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T-4 Handbook of Material Properties Data Bases

Vol. Ic: Equations of State

Edited by
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Prepared by Vickie Montoya, Group T-4

PREFACE

Since its inception in 1971, the Equation of State and Opacity Group (T-4) of the Los Alamos National Laboratory, has developed theories and models and calculated, compiled, and analyzed equation of state, opacity, and other related data. The Equation of State Library, initiated by my predecessor, John F. Barnes, contains these data in computer-based data files available to users for direct application.

This booklet is the first in a series of planned T-4 Handbooks to give the user an overview and background information on our computer-based libraries. It contains computer generated equation of state data in a compressed format for quick look-up. An expanded version will contain more detailed information. Although first in a series of planned publications, this booklet is not volume Ia, because logically a description of theories for equation of state models and of methods for calculations should precede the results of the equations of state that are summarized here. It is planned that volume Ia will give descriptions of theories and models, while volume Ib will be an expanded version of the present booklet. Other volumes will summarize opacities and conductivities.

Walter F. Huebner
Group Leader, T-4
3 May, 1984

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ABSTRACT

This manual is a compilation of descriptions of the equations of state (EOS) in the T-4 computerized library of material properties tables. The introduction gives a brief description of the library and of the physics theories and models which were used to calculate the equations of state. Then each EOS is described in detail. First, various physical parameters of each theoretical EOS are tabulated and compared with experiments when available. Then the method of generating the EOS is briefly described. Finally, the tables are plotted in terms of pressure and energy vs density along lines of constant temperature.

I. INTRODUCTION

The SESAME Equation-of-State (EOS) Library is a standardized, computer-based library which contains tables of thermodynamic properties for a wide range of materials over a wide range of physical regions (from ambient to astrophysical conditions). The Library currently contains data for about 70 materials, including metals, minerals, polymers, mixtures, and simple atomic and molecular species. The purpose of this document is to sufficiently describe each of the EOS's so that the users of the Library may make educated decisions as to whether a particular EOS is appropriate for their needs.

In the Library, pressure and energy (and in some cases free energy) are tabulated as functions of density and temperature. For some materials, separate pressure and energy tables are available for the thermal electronic and thermal ionic contributions. These are called two-temperature tables.

The Library has been developed and is maintained by the Equation of State and Opacity Group (T-4) of the Theoretical Division of Los Alamos National Laboratory. It is available to all interested parties both inside and outside the Laboratory.

This document will describe the Library as it is in June 1984. However, the Library is actually in a constant state of flux. EOS's for existing materials are upgraded when appropriate, and new ones are being constantly added. Most of the EOS's are generated by the members of Group T-4; however, we are constantly on the lookout for quality EOS's generated by others (e.g., the National Bureau of Standards and Lawrence Livermore National Laboratory) to add to the Library.

The aim of the custodians of the SESAME Library is to include thermodynamically self-consistent EOS's that are computed with the best available physics models and that agree with available experimental data--given realistic time constraints.

II. HISTORICAL DEVELOPMENT

The SESAME Equation-of-State Library came into existence in 1971 under the direction of J. Barnes. Initially, all the EOS's were calculated using a procedure developed by J. Barnes and J. Rood. They generated about 30 EOS's from 1972 to 1975, and since many of these remain in the Library, their method will be described in some detail. Even though the method is semi-empirical and is based on fairly simple physical models, the EOS's produced are generally adequate, especially for high-temperature applications. In fact, we have no more sophisticated models today for generating the EOS's of complicated compounds.

Above 1 eV (1 eV = 11604.5 K), Barnes and Rood used old MAPLE EOS tables. The MAPLE tables were for the most part calculated by R. D. Cowan using a Thomas-Fermi-Dirac model[1] for the electronic part of the EOS. Two corrections were added to this basis: a nuclear contribution and an empirical correction,[*] the purpose of which was to force the experimental zero-pressure density and bulk modulus to be reproduced. The MAPLE EOS's were adequate at high temperatures, but unreliable at low temperatures. Most notably, they did not always accurately reproduce experimental Hugoniot data. When Barnes and Rood began the SESAME library, they developed a method which would improve the low-temperature region.

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[*] Information provided by J. Barnes at Los Alamos National Laboratory.

They generated the pressures on the cold curve with a "modified-Morse" model at low density:

$$P_c = a\eta^{2/3} (\eta e^{b_r v} - e^{b_a v}),$$

where

$$v \equiv 1 - \eta^{-1/3} ,$$

$$\eta \equiv \rho/\rho_o ,$$

$$b_a \equiv 3 + b_r - 3B_o , \text{ and}$$

B_o = experimental adiabatic bulk modulus at T=0.

The constants b_r and a were determined by matching the mod-Morse cold curve onto a Thomas-Fermi-Dirac cold curve used at higher densities. (Sometimes, a straight Thomas-Fermi model was used in order to obtain a better match.)

For the finite temperature isotherms (below 1 eV), Barnes and Rood ignored thermal excitation of the electrons and assumed that the total pressure is given by the cold curve contribution plus a lattice contribution:

$$P(\rho,T) = P_c(\rho) + P_n(\rho,T) \quad .$$

The thermal nuclear contribution was calculated with a Debye model. This requires knowledge of the Grüneisen parameter as a function of density which can be obtained either from the cold curve or, in some cases, from experimental data. No melting was included.

After the pressure table was calculated, the energies were computed by integration. The EOS was then compared with experimental Hugoniot data. If necessary, the coefficients in the Debye model were adjusted in order to produce a good match between the theoretical EOS and Hugoniot experiments.

After the SESAME low-temperature table was completed, the MAPLE table was shifted so that the 1-eV isotherms of the two tables would match. There was always a slight discontinuity since the mod-Morse EOS did not include electron thermal contributions.

In expansion below 1 eV, Barnes and Rood used a virial series EOS. The coefficients of the virial expansion were determined by matching the thermal pressure and the slope of the thermal pressure with respect to density at ρ_0 (reference density). The van der Waals loops were generally replaced by vapor pressures calculated from a Maxwell construction, unless a tension region was specifically requested. This technique seemed to reproduce other theoretical estimates of critical points well.

This procedure for calculating EOS's has been called the Barnes-Cowan-Rood technique. It is referred to often in the detailed descriptions of the Library equations of state which follow.

III. CURRENT PHYSICAL MODELS

Barnes and Rood did an excellent job at providing a large number of EOS's for a wide variety of materials. However, in the years since that time, other researchers have been improving on the EOS's added to the SESAME Library by using more sophisticated physical theories and models.

If computing time permits, the researchers in T-4 use the following method for generating an equation of state. They first assume that the pressures and energies are a sum of three separate contributions: cold curve (i.e., zero-kelvin), nuclear thermal, and electron thermal ($P_{total} = P_c + P_n + P_e$).

The cold curve contributions are calculated with electron band theory using a formulation such as APW (augmented plane wave), LMTO (linearized muffin-tin orbital), or KKR (Korringa, Kohn, and Rostoker).

The electron thermal contributions are calculated from the INFERNO model[2] (due to D. A. Liberman), which is described next in some detail.

In the INFERNO model, an atomic nucleus is placed at the center of a spherical cavity. Exterior to the cavity is an electrically neutral jellium sea. Interior to the cavity, sufficient electrons are included to neutralize the nuclear charge. To implement a solution to this system, the approximations made are similar to those in typical band structure calculations:

1) The electrons are treated as independent particles in a self-consistent field.

2) Exchange and correlation are treated with a local density approximation.

3) Statistical averages are treated in the mean-field approximation.

4) The charge density is equivalent to the "muffin-tin" approximation used in solid-state calculations.

The model has several features which combine to yield superior results to previous models for electronic thermal excitation:

1) All electrons are treated with an internally consistent formulation so that "continuum lowering" is automatically included. The transition from bound state to narrow resonance and then to broad resonance states is smooth as the density or temperature is changed.

2) The model accommodates wide ranges in density and temperature. For example, calculations have covered compression ranges of 10^{-4} to 10^{3} and temperature ranges of 10^{-2} to 10^{4} eV.

3) Since the Dirac equation is used, shell structure effects are automatically included, making INFERNO superior to Thomas-Fermi-Dirac theory in this regard.

4) The high-density limit is essentially the Thomas-Fermi-Dirac model.

5) The low density is an ionization model for ions in equilibrium with free electrons.

The zero-temperature isotherms obtained from the INFERNO model agree better with those from band structure calculations than do the cold curves obtained from Thomas-Fermi-Dirac theory. On the other hand, band theory has not been adequately developed to handle finite temperatures. Therefore, the atom-in-jellium model is presently the method of choice for computing the contribution to the EOS from the thermal excitation of electrons.

Both the Thomas-Fermi-Dirac and the atom-in-jellium models are most appropriate for metallic elements. However, they can be used for nonmetallic elements and adapted to compounds and mixtures with some loss in accuracy in the low-pressure region.

For mixtures and certain elements inappropriate for INFERNO, an adequate model for the electronic EOS is still Thomas-Fermi-Dirac theory.

After the zero-degree and electron thermal contributions are calculated, the PANDA[3,4] code is used to calculate the nuclear thermal components and to assemble the final EOS. The nuclear thermal EOS takes account of solid lattice vibrations, translational nuclear motion (for the fluid), intramolecular vibration, and rotation.

The solid lattice vibrational terms can be calculated using either a Debye or Einstein model. A number of different options to calculate the Einstein or Debye temperature and the Grüneisen parameter are provided in PANDA. The Einstein or Debye temperature and the Grüneisen parameter at ambient density can be calculated in PANDA or can be determined for experimental data and input to PANDA. PANDA also offers interpolation models (including a virial expansion) which go to an ideal gas at high temperatures and low densities. These will crudely describe melting and vaporization in place of a more rigorous liquid model.

For fluids, PANDA has the option to calculate contributions to the center-of-mass motion of the molecules using the CRIS model. This model is based on a thermodynamic perturbation expansion about a hard-sphere fluid in which the zero-temperature isotherm of the solid is used to obtain the effective pair potential.

Vibrational and rotational contributions for molecules are calculated using the harmonic oscillator-rigid rotator approximation. Vibrational frequencies and rotational constants obtained from spectroscopic data must be supplied to PANDA.

IV. OTHER PHYSICAL MODELS

Many other physical theories and models besides the ones described in the previous section have been used to calculate the equation-of-state tables in the SESAME library. Most notably, many good ones have come from the equation-of-state group at

Lawrence Livermore National Laboratory. Since these were used for some of the EOS's in SESAME, they will be described in more detail below. Also described are theories developed at places other than Los Alamos National Laboratory and Lawrence Livermore National Laboratory but which are used frequently in the calculation of EOS's included in the SESAME library.

ACTEX Model (developed by Forrest Rogers at Lawrence Livermore National Laboratory)

The ACTEX (Activity Expansion) model[5-7] treats ionization equilibrium in the presence of plasma coupling and allows for the fact that the heavy ions may be strongly coupled (liquid-like), whereas the electrons are only moderately coupled (gas-like). The theory begins with a many-body perturbation expansion of the grand canonical ensemble partition function. Three distinct renormalizations are required to handle the general problem, accounting for (1) formation of electron-nucleus composites, (2) coupling of the composite particles to the plasma, and (3) strong coupling of heavy ions having charge $Z > 1$.

To carry out numerical calculations, it is necessary to obtain multielectron bound and scattering states. This is accomplished through the introduction of effective pair potentials. These potentials are composed of a long-range term plus exponentially screened Coulomb terms for each shell of core electrons. The parameters in the potential are determined from experimental spectroscopic data, and plasma-screening effects are then added to the long-range tail. The perturbation expansion breaks down at low temperature and at high densities.

SAHA Model (OCCIPITAL) (as implemented by C. Rouse at Lawrence Livermore National Laboratory)

The OCCIPITAL code calculates the complete solution to Saha's equation for partially ionized dense plasmas and liquid metals, which is then modified with the Debye-Hückel corrections for ionization potentials and Planck's theoretical partition function.[8,9] The EOS generated by OCCIPITAL is exact in the ideal gas limit, accurate in the weakly coupled Coulomb region, but becomes increasingly inaccurate with the onset of strong Coulomb interactions and electron degeneracy.

APW

The most sophisticated method to calculate the zero-kelvin pressure-volume isotherm is with rigorous electron band theory based on the self-consistent augmented plane wave (APW) method.[10] Contributions from lattice vibrations of the nuclei are not calculated by this model; but when they are added (as determined from Grüneisen-Debye models), the resultant zero-pressure volume is normally within 3% of experiment.

LMTO

An alternative way to calculate a zero-kelvin isotherm with electron band theory is to use the linear-muffin-tin-orbital (LMTO) method.[11,12] The augmented plane wave method is time consuming for computer calculations.

By making certain approximations which lead to the LMTO method, the calculation time for an EOS point can be reduced by one or two orders of magnitude with very little loss of accuracy.

Band-theory calculations yield a $T = 0$ isotherm for a lattice of immobile atoms, the static lattice. These results must be corrected for zero-point lattice vibrations to obtain the actual $T = 0$ isotherm. The appropriate pressure correction within the Grüneisen model is $\gamma \Delta E/V$, where ΔE may be taken as the zero-point phonon energy:

$$\Delta E = \frac{9}{8} k_B \Theta_D \quad .$$

KKR

Another method for solving the Schrödinger equation in a crystal lattice was devised by Korringa, Kohn, and Rostoker. It involves the same assumptions made in the APW method and is equally accurate. Two programs devised by Williams at IBM are in use in T-4. The LMTO programs used at Lawrence Livermore National Laboratory are a very good approximation to KKR in most circumstances and are computationally faster.

Pseudopotential Perturbation Theory for Simple Metals

The physical basis for the interatomic potential for simple metals is the adiabatic approximation in which the electron energy is calculated as a function of the ionic positions. The pseudopotential model for simple metals provides the means of applying the adiabatic approximation to determine an effective interatomic potential between ions.[13] From the pseudopotential expansion for the electron energies, one can write the total system energy (ion cores plus conduction electrons) as the sum of a two-body central force interaction between ions plus contributions that depend only on the total volume of the system. The total volume of the system does appear as an explicit parameter in the two-body interaction, and hence, a change in volume alters the pair-wise interaction between ions. (Three-body and higher interactions result from third and higher order terms in the perturbation expansion of the electron-ion pseudopotential interaction.[14]) The utility of pseudopotential theory for statistical mechanics arises from the property that at fixed volume the ions may take any arrangement without changing the effective ion-ion interaction.

GRAY Model (developed by R. Grover, D. Young, and E. Royce at Lawrence Livermore National Laboratory)

GRAY[15,16] uses a combination of physics models, experimental data, and analytic fits to experimental data to calculate the EOS of monatomic materials in the solid, melt, and liquid regions.

The EOS of the solid is based on the Dugdale-MacDonald form of the Grüneisen-Debye model. The total pressure (or energy) at a given temperature and density is the sum of the zero-degree pressure (or energy) and the thermal pressure (or energy) which is in turn a sum of independent contributions from electron excitations and atomic motions. The nuclear part of the thermal EOS is based on the nuclear Grüneisen gamma coefficient γ_G. An analytic fit for γ_G as a function of volume is put into GRAY. The electronic thermal EOS is based on the free electron model: $g_e \propto V^{2/3}$, where g_e is the electronic specific heat coefficient. GRAY uses the analytic fits for γ_G and experimental Hugoniot data to determine the zero-degree pressure and energy, $P_o(V)$ and $E_o(V)$, by the following formulas:

$$\gamma_G(V) = V \frac{P_H(V) - P_o(V)}{E_H(V) - E_o(V)} \quad ,$$

where $P_H(V)$ and $E_H(V)$ are the Hugoniot pressure and energy, and

$$P_o = - \frac{\partial E_o}{\partial V} \quad .$$

No internal rotational or vibrational contributions to the EOS are taken into account.

The melting transition is calculated according to the Lindemann law. The equation of state of the liquid is given by a scaling law; that is, the solid Grüneisen EOS at a given temperature and density is corrected with various terms which depend on the ratio of the temperature to the melting temperature at that density. The basis of the scaling law is contained in the equation for the specific heat of the liquid:

$$C_v = C_{vs} - \frac{3R}{2} \frac{\alpha T/T_m}{1 + T/T_m} ,$$

where C_{vs} is the lattice heat capacity of the solid, T_m is the melting temperature, and α is a constant determined by fitting soft-sphere data on heat capacity as a function of temperature.

The experimental data used directly in the GRAY model are normal state data at 1 atm and room temperature (reference density, sound velocity, Grüneisen gamma, and the electronic specific heat coefficient); the melting temperature at 1 atm; and the cohesive energy.

TFNUC (implemented by F. Ree at Lawrence Livermore National Laboratory)

TFNUC calculates an electronic equation of state using the Thomas-Fermi statistical atom model with the Kirzhnits form of quantum and exchange corrections.[17] Ionic motion contributions[18] are then added to the electronic EOS. These are based on Grüneisen-like theory at low temperature and one component plasma theory at high temperature with an interpolation scheme in between. In the low-temperature region, the Grüneisen gamma, γ_G, is expressed in three different analytic forms. Below a density ρ_G, TFNUC uses the same γ_G as used in GRAY. This forces the TFNUC EOS to join smoothly with the GRAY EOS. Above a density ρ_K, γ_G is a polynomial function of volume determined by a least squares fit to Kopyshev's numerical data. In between ρ_G and ρ_K, the analytic form of γ_G is designed to smoothly join the GRAY and the Kopyshev Grüneisen gamma coefficients. The best values for ρ_G and ρ_K are determined empirically by the user in such a way as to minimize the difference between ρ_G and ρ_K, yet also preserve a smooth transition between the upper and lower analytic forms of γ_G. TFNUC also includes a Lindemann law melt consistent with the GRAY melting line.

Soft-sphere Model (developed by David Young at Lawrence Livermore National Laboratory)

The soft-sphere model is based on Monte Carlo computer calculations[19] of fluids with interparticle potentials of the form $\phi(r) = \epsilon(\sigma/r)^n$, where $4 \leq n \leq 12$, ϵ and σ are constants, and r is the interparticle distance. The computer calculations of pressure and energy were fit with simple functions that consisted of ideal gas, static lattice, and configurational heat-capacity terms. Two further modifications[20,21] are needed to make the model usable for liquid metals. First, a negative cohesive term must be added to the pressure and energy. Since the attractive part of the interparticle interaction is poorly understood, a mean-field term is used. Second, some liquid metals have substantial electron heat-capacity contributions that cannot be accounted for with the soft-sphere heat-capacity term alone. Hence, this soft-sphere term is multiplied by a factor which can be greater than unity.

Since the parameters in the soft-sphere model cannot easily be predicted from liquid metal data, the model is used to fit experimental data. Specifically, the model parameters are determined by a best fit to enthalpy, volume, and sound speed isobars.

TIGER

TIGER[22,23] calculates the EOS of a heterogeneous mixture containing gaseous, liquid, and solid components. Since ionization is ignored, the range of validity is low temperature (kT < 1 eV) and low density. Generally, TIGER is used in the region in which the equation of state is sensitive to the chemical equilibrium between molecules and the dissociated species of the molecules.

The chemical potential of gaseous species i is calculated with the following formula:[24]

$$\mu_i = \mu_i^o(T) + RT\, \ln(n_i\, RT/V_g) + \int_{V_g}^{\infty} \left[\frac{\partial P}{\partial n_i} - \frac{RT}{V_g}\right] d\, V_g \quad ,$$

where n_i is the number of moles of species i, V_g is the gaseous molar volume, and $\mu_i^o(T)$ is the chemical potential at 1 atmosphere. The pressure, P, for the gaseous mixtures is calculated with the empirical Becker-Kistiakowsky-Wilson equation:[25]

$$PV_g/RT = 1 + xe^{\beta x} \quad ,$$

where

$$x = \kappa \sum_i n_i k_i / [n_g V_g (T + \Theta)^{\alpha}] \quad .$$

The constants α, β, Θ, and κ are usually given the values of $\alpha = 0.5$, $\beta = 0.1$, $\Theta = 400$ K, and $\kappa = 11.85$. The quantity n_g is the total number of moles of the gaseous species, and k_i is the "covolume" of species i. The numerical values of k_i are computed as follows. For each atom, the distance from the molecular center of mass is computed. Then the van der Waals radius is added to this distance. The volume is assumed to be 42.8 r^3, where r is the largest of all distances computed in this manner.

The chemical potentials of the condensed species are evaluated by

$$\mu_i^* = \mu_i^{o*}(T) + \int_{1\ \mathrm{atm}}^{P} V_i^*\, dP \quad \text{, where}$$

$$V_i^*(P,T) = A_1 + A_2P + A_3P^2 + A_4T \quad .$$

The values of the constants A_i are determined from experimental data on sound speed, thermal expansion, and Hugoniot measurements.

The concentration of each of the gaseous and solid species in equilibrium is determined according to the Gibbs and stoichiometry conditions: the first states that the chemical potentials of the reactants and products are equal, and the second condition is that the total number of atoms in one mole of a certain molecule is constant (e.g., the total number of silicon and oxygen atoms in one mole of SiO_2 is constant). These two conditions result in a number of relations with the same number of unknown concentrations (n_i and n_i^*) of the species. TIGER solves these iteratively. The EOS can then be calculated from knowing what the values of n_i and n_i^* are.

V. TABLES IN THE SESAME LIBRARY

The SESAME Library contains tables of pressure; internal energy; and, in some cases, free energy as functions of temperature and density. In addition, for some materials, the total pressure and energy are separated into electronic and nuclear components. The following types of tables can be found in the Library:

301: total pressure and energy tables

303: ionic EOS (including cold curve and zero-point contributions)

304: thermal electronic tables

305: thermal nuclear tables (including zero-point contribution)

306: cold curve

The 301 tables are the sum of the 304, 305, and 306 tables.

The data for all these tables are automatically produced every time an EOS is generated using either of the two methods described in Sections II and III. However, until very recently there was little interest in the two-temperature tables, and these data were not saved. The only way, then, to generate accurate two-temperature tables is to recalculate the EOS's for most existing materials. As an alternative, R. Albers has developed an approximate scheme to separate the total pressure and energy surfaces into the two components. A Cowan ion model is used to calculate the thermal nuclear EOS (the 305 table) which may then be subtracted from the total thermal EOS to find the thermal electronic component (the 304 table). There are a number of fixes in the procedure which smooth the data and prevent crossing isotherms.

This procedure was used to generate two-temperature tables for many of the older materials in the SESAME Library. Starting in 1982, all new material EOS's from T-4 have directly ~~calculated two-~~temperature tables. The individual EOS descriptions indicate whether the approximate scheme (via the code TWOTEMP) was used.

Equations of state developed in places other than Los Alamos National Laboratory only have the 301 tables (total pressure and energy).

VI. SESAME SOFTWARE

SESAME Subroutine Library

The SESAME Subroutine Library was developed to simplify use of tabular EOS data. SESAME tables are transmitted to users on magnetic tapes in a card image format that can be read and interpreted by the user's computing system. The user is also supplied with FORTRAN subroutines that preprocess the data into a compact binary file and update this file as needed. The user is supplied with subroutines that search this file for a given material, load data into a local array, and compute thermodynamic functions by search and interpolation. Linear and rational function interpolation schemes are available for one and two dimensions.

Routines are available to compute P and E (and their first derivatives) as functions of ρ and T and also to compute P and T (and their first derivatives) as functions of ρ and E. Physical process paths can be computed from the EOS's such as isochores, isentropes, and

Hugoniots. Vapor-liquid coexistence curves, thermodynamic behavior of foams, and phase transitions can also be determined.

Display Codes

Group T-4 has a number of in-house display codes that combine various subroutines mentioned in the preceding section to provide tabular and graphical representation of the EOS data.

Both two- and three-dimensional graphics codes exist. Black-and-white capability exists for use with Tektronix, microfilm, and microfiche output; color graphics capability also exists. The codes use DISSPLA graphics software hat can be made available to external users to adapt to their own systems.

VII. OBTAINING THE SESAME LIBRARY

To obtain SESAME EOS data and the subroutine library, a user should send a list of the materials required to the following address:

SESAME Library, T-4, MS-B925
Los Alamos National Laboratory
Los Alamos, NM 87545.

The subroutine library will be copied onto one tape, and tabular data will be written on another. Instructions, included with the tapes, explain how to preprocess the data tapes and how to use the library routines. Users will be charged a nominal fee to cover costs to T-4.

The tapes will be written in an 80-character card image format that is compatible with the user's computing facilities. Standard options include the BCD character set for 7-track tapes and the EBCDIC character set for 9-track tapes. The tapes may be either blocked or unblocked, with either 800, 1600, or 6250 BPI. The user should specify either 7-track or 9-track tapes, the character set, density, and any other appropriate parameters.

The number of data tapes needed depends upon the tape format, the number of materials requested, and the size of the tables. As a rough guide, allow

one 7-track tape, 800 BPI, for each 20-25 materials,

one 9-track tape, 800 BPI, for each 25-30 materials,

one 7-track tape, 1600 BPI, for each 40-50 materials,

one 9-track tape, 1600 BPI, for each 50-60 materials.

The general Group T-4 telephone number is (505) 667-7024 or (505) 667-5751.

VIII. DETAILED DESCRIPTION OF EQUATIONS OF STATE

Following are detailed descriptions and plots of each equation of state in the SESAME Library. Each description is divided into three parts. The first section contains some general information which is self-explanatory. The second section is a compilation of physical data. For convenience, experimental values of the physical parameters are listed along with the values which are actually reflected by the theoretical EOS. (The theoretical values have an asterisk in front of them.) In some cases, these physical parameters were input for the models that were used to calculate the EOS, and in other cases, these quantities were calculated from the output. It is usually noted in the descriptions whether the theoretical values are input or output.

The physical parameters which are included are

A -- atomic weight
Z -- atomic number
ρ_o -- normal density (density of material at room temperature and 1 atmosphere)

$P(T = 298.15\ K, \rho_o)$ -- pressure (in the SESAME table) at room temperature and normal density
$E(T = 298.15\ K, \rho_o)$ -- energy (in the SESAME table) at room temperature and normal density
$T(P = 10^{-6}\ GPa, \rho_o)$ -- temperature (in the SESAME table) at a very low pressure (near zero) and normal density
T_m -- melting temperature of material at 1 atmosphere
T_c -- temperature at critical point (point at maximum of the gas-liquid coexistence curve in a P vs ρ diagram; at all

temperatures below T_c, the gas and liquid will physically separate).

P_c -- pressure at critical point
ρ_c -- density at critical point

γ_o -- Grüneisen gamma $[\gamma = V \frac{\partial P}{\partial E}|_v]$ at normal density and room temperature
B_o -- bulk modulus at normal density and room temperature
Θ_D -- Debye temperature at normal density
E_{coh} -- cohesive energy
U_S -- shock velocity (as measured in a Hugoniot experiment)
U_p -- particle velocity (as measured in a Hugoniot experiment)

(Note: The Hugoniot of a material can be expressed as a functional relationship between U_S and U_p.)

Users of the SESAME Library should beware that, although the values of the above parameters are for the most part given at room temperature and normal density, often the models which were used to generate the equations of state expect the values to be at zero-kelvin. Many of the tables are normalized incorrectly because of the fact that room-temperature values of bulk modulus and Grüneisen gamma, for example, were used in models which expected zero-kelvin values. The differences in the equations of state, however, would be very slight if they were renormalized correctly.

The third section of the detailed description gives a brief outline of the physics models and theories which were used to calculate the EOS tables. Usually only a sentence or two is included to describe the models here; more detail is given about the physics in Sections II, III, and IV. The third section also has information about whether the EOS has a melting transition, whether it has van der Waals loops or a Maxwell construction in the vapor-liquid coexistence region, and how the EOS compares with experimental data (most often Hugoniot data). Comments on the thermodynamic consistency of the table are also included.

Also associated with each equation of state in the following section are plots. The first is a plot of pressure vs density along isotherms. Actually the logs of these values are plotted since the ranges covered by the EOS's are very large. The values of the isotherms in kelvin are printed to the right of the plot. The second plot is of the log of energy vs the log of density along isotherms.

The units used in this manual are

temperature	kelvin or eV (1 eV ≡ 11604.5 K)
density	Mg/m^3 or g/cm^3 (1 Mg/m^3 ≡ 1 g/cm^3)
pressure	GPa (1 GPa ≡ 0.01 MBar)
energy	MJ/kg (1 MJ/kg ≡ 0.01 $Mbar{-}cm^3/g$)
shock velocity U_S	km/s
particle velocity U_p	km/s

REFERENCES

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IX. INDEX OF MATERIALS AND SESAME NUMBERS

Material	SESAME Number
Air (dry)	5030
Alumina	7410
Aluminum	3712, 3713
Ammonia	5520
Argon	5171, 5172
Beryllium	2020
Brass	4100
Calcium Carbonate	7330
Carbon Liquid	7831
Carbon Phenolic	7541
Copper	3330, 3331, 3332
Deuterium	5263
Deuterium-Tritium	5271
Gold	2700
Helium	5760, 5761, 5762
Hydrogen	5250, 5251
Iron	2140, 2145
Krypton	5180
Lead	3200
Lithia-Boria	7252
Lithium	2290, 2291
Lithium Deuteride	7242, 7243
Lithium Hydride	7371
Methane	5500, 5501, 5502
Mica	7520
Molybdenum	2980, 2981, 2982, 2983
Neon	5410, 5411
Nevada Alluvium	7111
Nickel	3100
Nitrogen	5000, 5001
Oxygen	5010, 5011
PBX-9502	8180
PBX-9502 (high explosive)	8200
Platinum	3730

Polyethylene (branched, completely deuterated)	7160
Polyethylene (branched, low density)	7171
Polyethylene (Marlex)	7180
Polystyrene	7590
Polyurethane	7560
Quartz	7380, 7381, 7382
Sodium	2448
Solar Mix (Ross-Aller)	5280
Stainless Steel (304)	4270
Teflon (Polytetrafluoroethylene)	7190
Tungsten	3541
Tungsten Carbide	3560
Uranium	1540
Water	7150, 7152
Westerly Granite	7390

SESAME #1540

Material: Uranium
Originator: J. Barnes and J. Rood
Date of Origin: March 1973
Type of Tables Included: 301, 303, 304, 305
Limits: $0 < \rho < 3.8 \times 10^5$ g/cm^3
$0 < T < 3.7 \times 10^8$ K

BASIC PHYSICAL DATA

$A = 238.03$
$Z = 92$
$\rho_o = 18.983$ g/cm^3

$P(T = 298.15 \text{ K}, \rho_o) = 1.0207$ GPa
$E(T = 298.15 \text{ K}, \rho_o) = 2.3946 \times 10^{-2}$ MJ/kg
$T(P = 10^{-6} \text{ GPa}, \rho_o) = 2.939 \times 10^{-4}$ K

$T_m = 1405.5$ K [Ref. 1]

$T_c = *\ 9837$ K (calculated)

$\gamma_o = *\ 2.257$ (calculated)
2.07 [Ref. 2]

$B_o = *\ 112.2$ GPa (used in calculation of EOS)
100.7 GPa [Ref. 2]

$\theta_D = *\ 207.0$ K (used in calculation of EOS)

$E_{coh} = *\ 2.20$ MJ/kg (used in calculation of EOS)

Hugoniot fit: $U_S = 2.51 + 1.51\, U_p$ km/s
[Ref. 3]

DESCRIPTION OF PHYSICS

This equation of state was generated using the standard Barnes-Cowan-Rood method. The electronic part of the EOS is from Thomas-Fermi-Dirac theory; the cold curve is based on a modified-Morse model; and the thermal nuclear contributions are based on a Debye model below 1 eV. (See Part II for a more detailed description of this method.)

The zero-pressure experimental bulk modulus and density are reproduced by this EOS, and the fit to experimental Hugoniot data is good. However, the equation of state is not accurate at low temperatures in expansion.

The melting transition is not included in this EOS.

The thermodynamic consistency of this EOS is good.

The two-temperature tables for this EOS were derived from the TWOTEMP code and are very noisy.

REFERENCES

1. Handbook of Chemistry and Physics, R. C. Weast, Ed. (CRC Press, Cleveland, Ohio, 1976).

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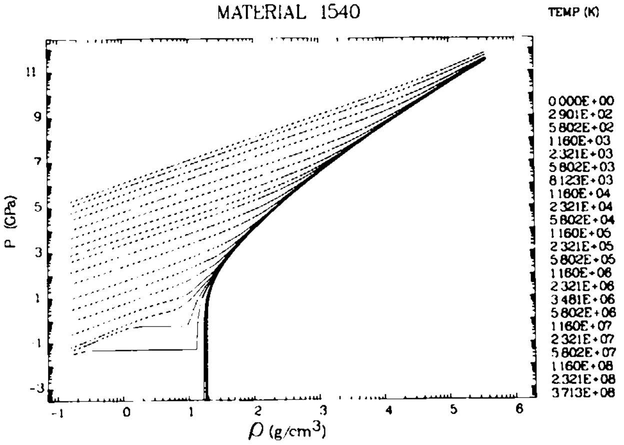
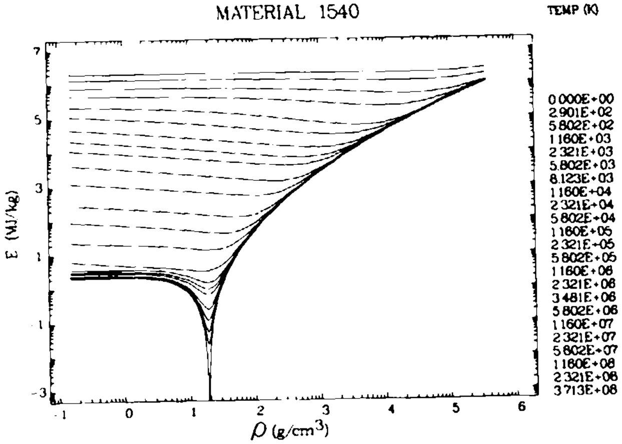
3. S. P. Marsh, LASL Shock Hugoniot Data (University of California Press, Berkeley, 1980).


MATERIAL 1540
TEMP (K)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08
P (GPa)
11
9
7
5
3
1
1
-3
-1
0
1
2
3
4
5
6
ρ (g/cm3)


MATERIAL 1540
TEMP (K)
E (MJ/kg)
7
5
3
1
-1
-3
-1
0
1
2
3
4
5
6
ρ (g/cm3)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08

SESAME #2020

Material: Beryllium
Originator: J. Barnes and J. Rood
Date of Origin: July 1973
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho < 3.7 \times 10^4$ g/cm^3
$0 < T < 3.7 \times 10^8$ K

BASIC PHYSICAL DATA

$A = 9.0122$
$Z = 4$
$\rho_o = 1.845$ g/cm^3

$P(T = 298.15$ K, $\rho_o) = 0.3704$ GPa
$E(T = 298.15$ K, $\rho_o) = 0.1980$ MJ/kg
$T(P = 10^{-6}$ GPa, $\rho_o) = 8.3065 \times 10^{-4}$ K

$T_m = 1551$ K [Ref. 1]

$T_c = 10665$ K [Ref. 2]
9109 K [Ref. 3]
* 9823 K (calculated)

$\gamma_o =$ * 1.014 (calculated)
1.16 [Ref. 4]
$B_o =$ * 120.8 GPa (used in calculation of EOS)
102.3 GPa [Ref. 4]

$E_{coh} =$ * 35.6 MJ/kg (used in calculation of EOS) [Ref. 5]

$\theta_D =$ * 1000 K
1160 K [Ref. 4]

Hugoniot Fit: $U_s = 7.99 + 1.13\ U_p$ km/s
[Ref. 6]

DESCRIPTION OF PHYSICS

This equation of state was generated using the standard Barnes-Cowan-Rood method. The electronic part of the EOS was calculated with Thomas-Fermi-Dirac theory; the cold curve is based on a modified-Morse model; the ionic contributions are calculated with a model by R. D. Cowan above 1 eV and a Debye model below 1 eV. (See Part II for a detailed discussion of this procedure of EOS generation.)

The zero-pressure experimental density and bulk modulus are reproduced by this EOS, and the fit to experimental Hugoniot data is good. Also, the critical point is fairly close to estimates made by Merts and Magee,[2] as well as Thompson.[3] However, this EOS was not generally designed for the hot, expanded liquid metal region and it is not to be trusted there.

The thermodynamic consistency is good everywhere.

No melting transition is included in this EOS.

The two-temperature tables were derived from the code TWOTEMP and are noisy.

A tension region for spall has been added.

REFERENCES

1. Handbook of Chemistry and Physics, R. C. Weast, Ed. (CRC Press, Cleveland, Ohio, 1976).

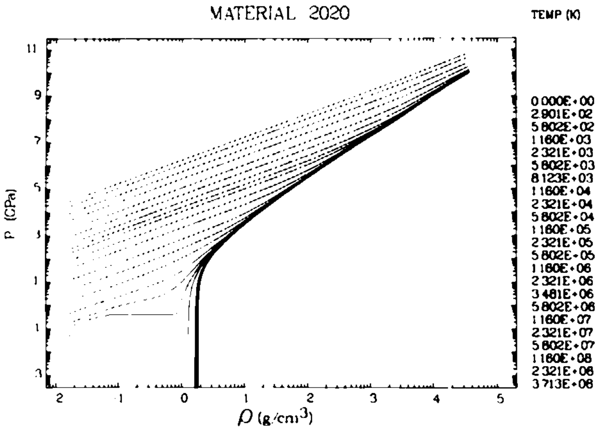
2. A. L. Merts, N. H. Magee, Jr., "Low Temperature Equation of State for Metals," Los Alamos Scientific Laboratory report LA-5068 (Jan. 1973).

3. S. L. Thompson, "Improvements in CHART D Radiation Hydrodynamics Code: Analytic Equations of State," Sandia Laboratories, Albuquerque, report SC-RR-70-28 (1970).

4. K. A. Gschneidner, Jr., Solid State Physics 16, 275 (1964).

5. L. Brewer, "Cohesive Energies of the Elements," Lawrence Berkeley Laboratory report LBL-3720 (1975).

6. S. P. Marsh, LASL Shock Hugoniot Data (University of California Press, Berkeley, 1980).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TEMP (K)
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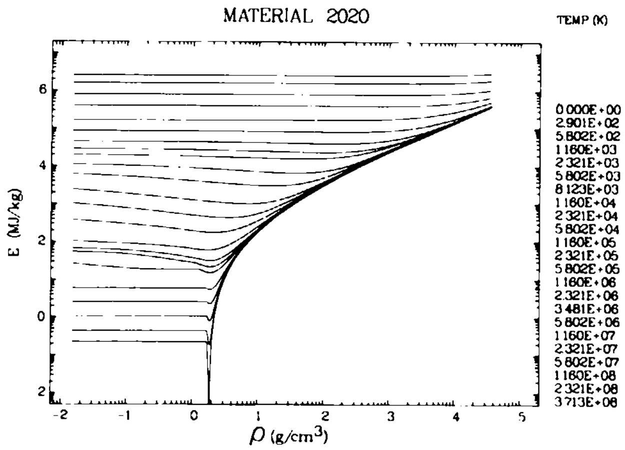
2 901E+02
5 802E+02
1 160E+03
2 321E+03
5 802E+03
8 123E+03
1 160E+04
2 321E+04
5 802E+04
1 160E+05
2 321E+05
5 802E+05
1 160E+06
2 321E+06
3 481E+06
5 802E+06
1 160E+07
2 321E+07
5 802E+07
1 160E+08
2 321E+08
3 713E+08
P (GPa)
11
9
7
5
3
1
1
3
2
1
0
1
2
3
4
5
ρ (g/cm3)


MATERIAL 2020
TEMP (K)
E (MJ/kg)
6
4
2
0
2
-2
-1
0
1
2
3
4
5
ρ (g/cm³)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08

SESAME #2140

Material: Iron
Originator: J. Barnes and J. Rood
Date of Origin: August 1973
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho < 1.57 \times 10^5$ g/cm^3
$0 < T < 3.7 \times 10^8$ K

BASIC PHYSICAL DATA

$A = 55.850$
$Z = 26$
$\rho_o = 7.85$ g/cm^3

$P(T = 298.15\ \mathrm{K}, \rho_o) = 1.1233$ GPa
$E(T = 298.15\ \mathrm{K}, \rho_o) = 7.0505 \times 10^{-2}$ MJ/kg
$T(P = 10^{-6}\ \mathrm{GPa}, \rho_o) = 4.4979 \times 10^{-4}$ K

$T_m = 1535$ K [Ref. 1]

$T_c = 9340$ K [Ref. 2]
6750 K [Ref.3]
* 8830 K (calculated)

$\gamma_o = 1.81$ [Ref. 4]
* 2.035 (calculated)
$B_o = 171.6$ [Ref. 4]
* 165.7 GPa (calculated)

$E_{coh} =$ * 7.243 MJ/kg (used in calculation of EOS)

$\theta_D = 464$ K [Ref. 1]
* 470 K (used in calculation of EOS)

Hugoniot Fit: $U_s = 4.955 + 0.454\ U_p$ km/s for $0.1 < U_p < 0.33$

$$U_s = 2.049 + 3.79\ U_p \text{ km/s for } 0.34 < U_p < 0.79$$

$$U_s = 3.635 + 1.802\ U_p - 0.0333\ U_p^2 \text{ for } 1. < U_p < 7.7 \text{ [Ref. 5]}$$

DESCRIPTION OF PHYSICS

The iron equation of state was calculated with the Barnes-Cowan-Rood method. The electronic part of the EOS was treated with Thomas-Fermi-Dirac theory, and the thermal nuclear part was determined by a Cowan model at temperatures above 1 eV and a Debye model for lower temperatures. The cold curve was based on the modified-Morse model with one exception. Since iron has a solid-solid phase transition (bcc → hcp), a composite cold curve was constructed. The lower portion (bcc) was based on ρ_o = 7.85 g/cm^3 and B_o = 165.7 GPa, and the hcp part of the cold curve was computed with values of ρ_o = 8.08 g/cm^3 and B_o = 149.5 GPa. The transition from the bcc to the hcp phase occurs at 8.4 g/cm^3 on the zero-kelvin isotherm. Since this cold curve was used in calculating all the finite-temperature isotherms, the phase transition persists at high temperatures. (See Part II for a detailed description of this procedure of EOS generation.)

The theoretical Hugoniot compares well with experiments until it reaches pressures of approximately 300 GPa, at which point it is slightly soft. The EOS also reproduces porous Hugoniot experiments well. The theoretical cold curve agrees well with three APW calculations by E. Kmetko; the largest discrepancy is 11% at four-fold compression. The mod-Morse cold curve does not approach the Thomas-Fermi-Dirac limit fast enough.

The thermodynamic consistency is good.

The two-temperature tables were derived later by the cold TWOTEMP and are noisy.

REFERENCES

1. Handbook of Chemistry and Physics, R. C. Weast, Ed. (CRC Press, Cleveland, Ohio, 1976).

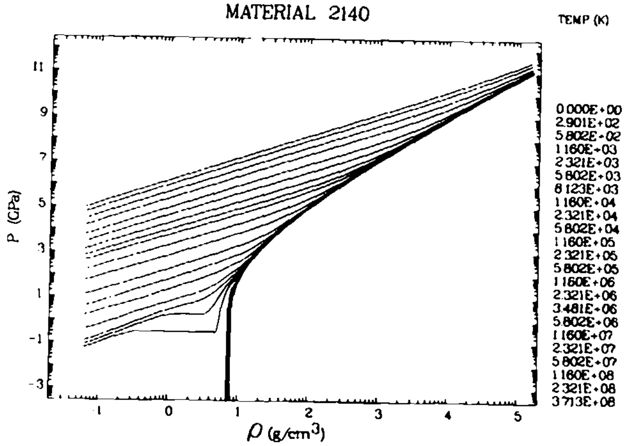
2. D. A. Young and B. J. Alder, "Critical Points of Metals from van der Waals Model," Phys. Rev. A 3 (1) (1971).

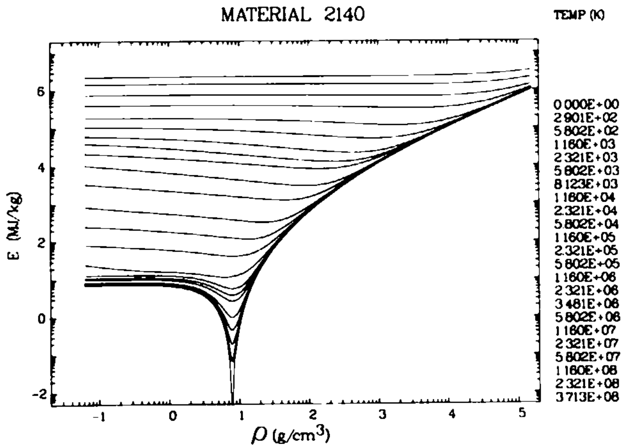
3. A. V. Grosse and A. D. Kirshenbaum, J. Inorg. Nucl. Chem. 25, 331 (1963).

4. K. A. Gschneidner, Jr., Solid State Physics 16, 275 (1964).

5. M. van Thiel, "Compendium of Shock Wave Data," Lawrence Livermore Laboratory report UCRL-50108, Rev. 1 (1977).

2140-5


MATERIAL 2140
TEMP (K)
P (GPa)
11
9
7
5
3
1
-1
-3
-1
0
1
2
3
4
5
ρ (g/cm^3)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08


MATERIAL 2140
TEMP (K)
E (MJ/kg)
6
4
2
0
-2
-1
0
1
2
3
4
5
ρ (g/cm^3)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08

SESAME #2145

Material: Iron
Originator: G. Kerley, J. Barnes, and J. Rood
Date of Origin: June 1977
Type of Tables Included: 301
Limits: $0 < \rho < 12.537$ g/cm^3
$0 < T < 11604.5$ K

BASIC PHYSICAL DATA

$A = 55.847$
$Z = 26$
$\rho_o = 7.91$ g/cm^3

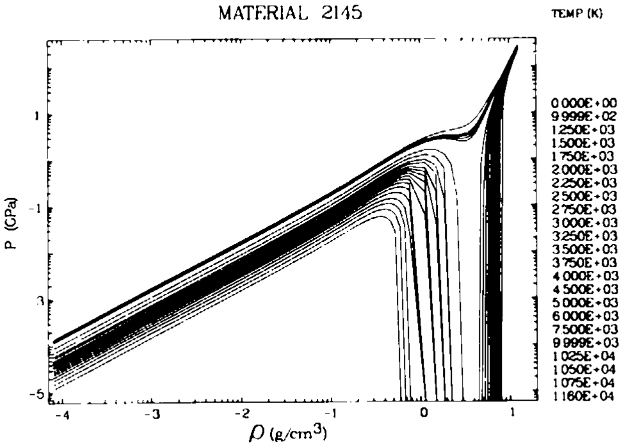
$P(T = 298.15\ \mathrm{K}, \rho_o) = 1.42235$ GPa
$E(T = 298.15\ \mathrm{K}, \rho_o) = 9.93465 \times 10^{-2}$ MJ/kg
$T(P = 10^{-6}\ \mathrm{GPa}, \rho_o) = 1.875 \times 10^{-4}$ K

$T_m = 1535$ K

Hugoniot Fit: See SESAME #2140

DESCRIPTION OF PHYSICS

This equation of state was generated for the reactor safety program and covers only a limited range of temperatures and densities. Information about the models used to generate this EOS is unknown.


MATERIAL 2145
TEMP (K)
P (GPa)
ρ (g/cm3)
1
-1
-3
-5
-4
-3
-2
-1
0
1
0.000E+00
9.999E+02
1.250E+03
1.500E+03
1.750E+03
2.000E+03
2.250E+03
2.500E+03
2.750E+03
3.000E+03
3.250E+03
3.500E+03
3.750E+03
4.000E+03
4.500E+03
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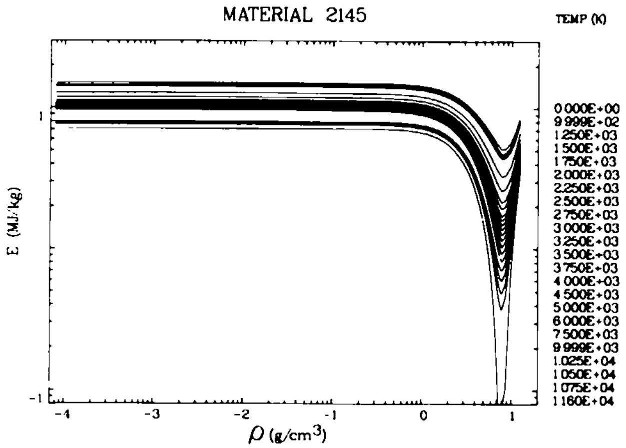
1.075E+04
1.160E+04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TEMP (K)
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1.500E+03
1.750E+03
2.000E+03
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2.750E+03
3.000E+03
3.250E+03
3.500E+03
3.750E+03
4.000E+03
4.500E+03
5.000E+03
6.000E+03
7.500E+03
9.999E+03
1.025E+04
1.050E+04
1.075E+04
1.160E+04
E (MJ/kg)
1
-1
-4
-3
-2
-1
0
1
ρ (g/cm³)

SESAME #2290

Material: Lithium [Ref. 1]
Originator: D. Steinberg (Lawrence Livermore
National Laboratory, B-Division)
Date of Origin: unknown
Type of Tables Included: 301
Limits: $0 < \rho < 53.26$ g/cm^3
$0 < T < 1.16 \times 10^7$ K

BASIC PHYSICAL DATA

$A = 6.939$
$Z = 3$
$\rho_o = 0.534$ g/cm^3

$P(T = 298.15\ K, \rho_o) = 0.71988$ GPa
$E(T = 298.15\ K, \rho_o) = 0.77464$ MJ/kg
No zero pressure point exists in this table.

$T_m = 453.7$ K [Ref. 2]

$\gamma_o = *\ 0.92$ (used in generating EOS)
$B_o = *\ 13.6$ GPa (used in generating EOS)

Hugoniot Fit: * $U_S = 0.477 + 1.066\ U_P$ km/s
(used in generating EOS)

DESCRIPTION OF PHYSICS

This lithium EOS was generated from an analytic Grüneisen EOS determined by D. Steinberg at Lawrence Livermore National Laboratory. The original analytic function gives pressure as a function of energy and density. However, the SESAME Library expects a table in which pressure and energy are given at each point of a rectangular grid of density and temperature. The method which was used to turn the analytic function into a

SESAME-formatted table is documented in Ref. 3.

Even though this EOS has been tabulated over a fairly wide range of temperatures and densities, its range of validity covers only the area between the principal adiabat and the Hugoniot. And it should only be used up to a density corresponding to a pressure of 5 B_0 on the Hugoniot.

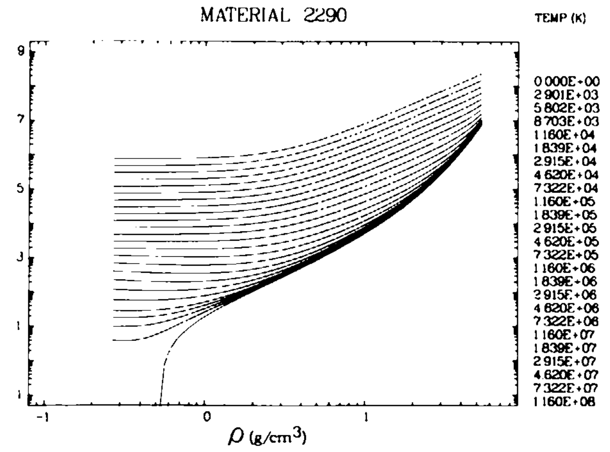
This equation of state is not thermodynamically consistent because of the method used to incorporate temperature.

REFERENCES

1. D. Steinberg, "A High Pressure Equation of State for Lithium," Lawrence Livermore Laboratory, B-Division Progress Report (July, 1973).

2. Sargent-Welch Periodic Table of the Elements (1968).

3. B. I. Bennett, "EOSSCAN: A Program to Display Equation-of-State Data," Los Alamos National Laboratory report LA-8737-MS (March 1981).



MATERIAL 2290
TEMP (K)
P (GPa)
9
7
5
3
1
1
-1
0
1
ρ (g/cm^3)
0.000E+00
2.901E+03
5.802E+03
8.703E+03
1.160E+04
1.839E+04
2.915E+04
4.620E+04
7.322E+04
1.160E+05
1.839E+05
2.915E+05
4.620E+05
7.322E+05
1.160E+06
1.839E+06
2.915E+06
4.620E+06
7.322E+06
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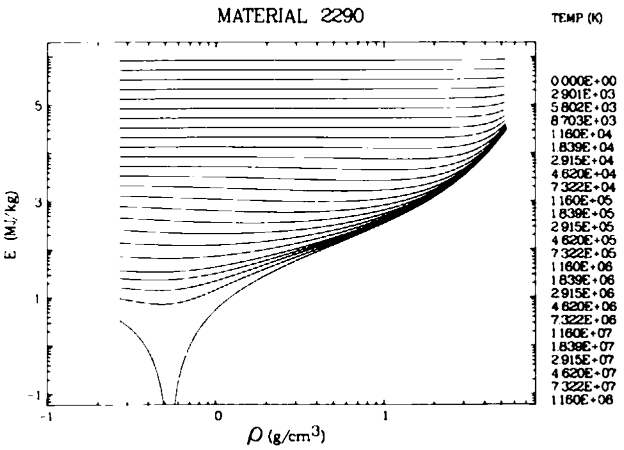
4.620E+07
7.322E+07
1.160E+08


MATERIAL 2290
TEMP (K)
E (MJ/kg)
5
3
1
-1
-1
0
1
ρ (g/cm^3)
0 000E+00
2 901E+03
5 802E+03
8 703E+03
1 160E+04
1 839E+04
2 915E+04
4 620E+04
7 322E+04
1 160E+05
1 839E+05
2 915E+05
4 620E+05
7 322E+05
1 160E+06
1 839E+06
2 915E+06
4 620E+06
7 322E+06
1 160E+07
1 839E+07
2 915E+07
4 620E+07
7 322E+07
1 160E+08

SESAME #2291

Material: Lithium [Ref. 1]
Originator: D. A. Young (Lawrence Livermore
National Laboratory, H-Division)
Date of Origination: 1978
Type of Tables Included: 301
Limits: $10^{-4} < \rho < 2$ g/cm^3
$453 < T < 3.67 \times 10^8$ K

BASIC PHYSICAL DATA

$A = 6.939$
$Z = 3$
$\rho_o = 0.518$ g/cm^3

$P(T = 298.15\text{ K}, \rho_o) = -0.33247$ GPa (outside range of table)
$E(T = 298.15\text{ K}, \rho_o) = 0.401455$ MJ/kg (cohesive energy)
(No zero pressure point exists in this table.)

$T_m = 453.7$ K [Ref. 2]
$= {}^*\,453.7$ K (used in calculation of EOS)

$T_c = {}^*\,3741$ K (calculated)

Hugoniot Fit: $U_s = 4.51 + 1.09\ U_p$ km/s [Ref. 3]

DESCRIPTION OF PHYSICS

This lithium EOS was generated for use in design studies of laser-fusion reactors employing a lithium "waterfall". That is why the upper limit of density is only four-fold compressed.

Three physics models were used: ACTEX for the ionized fluid, soft sphere for the liquid and vapor, and a liquid metal perturbation theory based on pseudopotentials for the hot, dense liquid. Three separate EOS's were computed in overlapping regions of the temperature-density plane, and then these were joined along optimal boundaries. A small amount of bilinear numerical interpolation was required for smooth joining. Fig. 1 shows the regions over which each theory was used.

Agreement of the EOS with experimental isobaric data [Ref. 4] (measuring volume, sound speed, and enthalpy) and experimental Hugoniot data [Refs. 3 and 5] is good.

The thermodynamic consistency of this EOS is good due to the fact that the energy was forced into consistency with the pressure in the interpolation regions. (Joining EOS subsurfaces invariably leads to inconsistency along boundaries.) However, this caused a kink in the ultrahigh pressure shock Hugoniot (in an area not accessed by a fusion reactor).

The quality of this EOS is high; it is a composite of three of the more advanced EOS models available.

The lithium EOS has a Maxwell construction in the two-phase, liquid-vapor region.

REFERENCES

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2. Sargent-Welch Periodic Table of the Elements (1968).

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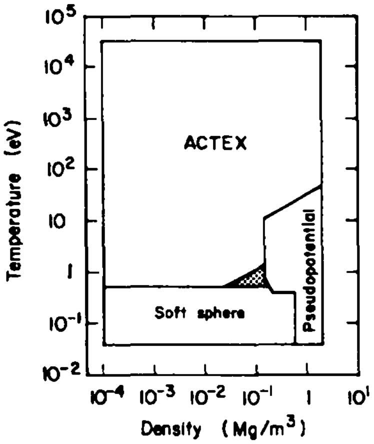
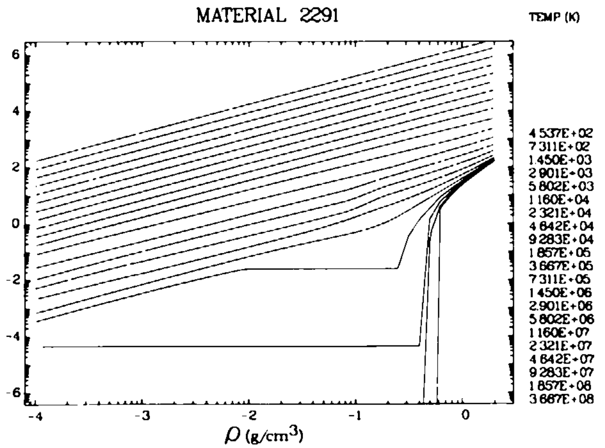


Fig. 1. Temperature-density plot showing the subregions covered by each of the theory codes used to calculate the EOS for lithium. The shaded area is where numerical interpolation was required to smoothly join two EOS subsurfaces.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TEMP (K)
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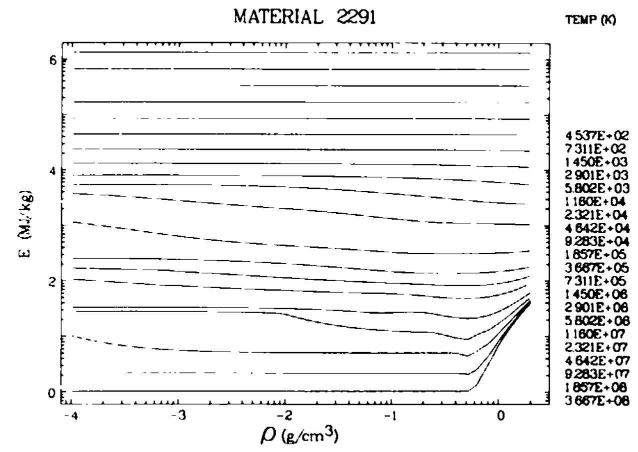
7.311E+02
1.450E+03
2.901E+03
5.802E+03
1.160E+04
2.321E+04
4.642E+04
9.283E+04
1.857E+05
3.667E+05
7.311E+05
1.450E+06
2.901E+06
5.802E+06
1.160E+07
2.321E+07
4.642E+07
9.283E+07
1.857E+08
3.667E+08
P (GPa)
6
4
2
0
-2
-4
-6
-4
-3
-2
-1
0
ρ (g/cm³)


MATERIAL 2291
TEMP (K)
E (MJ/kg)
6
4
2
0
-4
-3
-2
-1
0
ρ (g/cm³)
4.537E+02
7.311E+02
1.450E+03
2.901E+03
5.802E+03
1.160E+04
2.321E+04
4.642E+04
9.283E+04
1.857E+05
3.667E+05
7.311E+05
1.450E+06
2.901E+06
5.802E+06
1.160E+07
2.321E+07
4.642E+07
9.283E+07
1.857E+08
3.667E+08

SESAME #2448

Material: Sodium
Originator: B. Bennett
Date of Origin: June 1977
Types of Tables Included: 301
Limits: $0 < \rho < 1.3143\ \mathrm{g/cm^3}$
$0 < T < 1.015 \times 10^4$ K

BASIC PHYSICAL DATA

$A = 23.0$
$Z = 11$
$\rho_o = 1.011\ \mathrm{g/cm^3}$

$\rho_{ref} = {*}\ 0.96587\ \mathrm{g/cm^3}$ (computed from table at 298 K)
$0.971\ \mathrm{g/cm^3}$ (experiment)
$E(T = 298.15\ \mathrm{K}, \rho_{ref}) = 0.26914$ MJ/kg
$T(P = 0, \rho_{ref}) = 298.12$ K

$T_m = 370.96$ K (experiment)

$T_c = {*}\ 2538.58$ K (computed)
2503.25 K [Ref. 1]

$\gamma_o = 1.2$ [Ref. 2]
$B_o = 7.7$ GPa [Ref. 2]

$E_{coh} = 4.668$ MJ/kg [Ref. 3]

$\theta_D = 158$ K [Ref. 4]

Poisson's ratio: 1/3 (arbitrarily chosen)

DESCRIPTION OF PHYSICS

Cold Curve (T = 0 K isotherm)

An empirical model generated from a modified-Morse form [Ref. 5] above a density of $0.9453\rho_0$ and a Lennard-Jones (m,n) form with m = 1.85 and n = 8.08953 below this density was used. The latter guarantees agreement with the assumed cohesive energy.

Nuclear Vibration Contribution

A model which causes a transition from a Debye solid to an ideal gas was used [Ref. 6]. This model requires knowledge of the density dependence of the Debye temperature and the Grüneisen parameter. This was obtained from the so-called Chart-D model [Ref. 7].

Electronic Excitation Contribution

A modified Saha-type theory was used. This model requires a single ionization potential. A value of 5.12 eV was chosen. It is expected that, because of the magnitude of the critical temperature ~ 2500 K, the contribution to the equation of state due to electronic excitations should be small.

REFERENCES

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2. J. F. Barnes, "An Equation of State for Sodium over an Extended Temperature and Density Range," *Thermodynamics of Nuclear Materials 1974, Vol. I,* (International Atomic Energy Agency, Vienna, 1975), p. 327.

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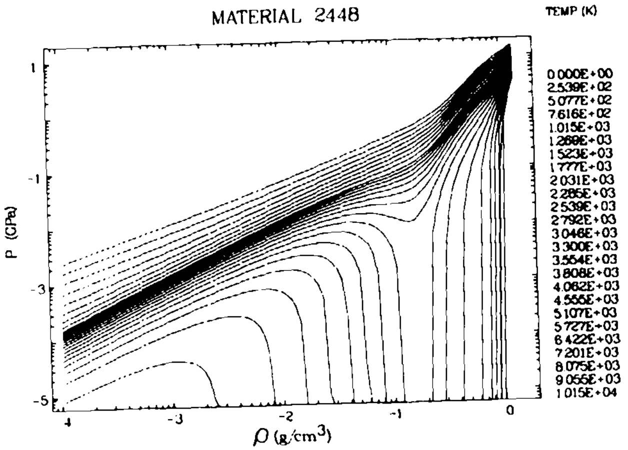
6. Kormer, Funtikov, Urlin, and Kolesnikova, JETP **15**, 447 (1962); Kormer, Sinitsyn, Funtikov, Urlin, and Blinov, JETP **20**, 811 (1965).

7. Thompson and Lauson, "Improvements in the Chart-Radiation-Hydrodynamic Code III," Sandia Laboratories report SC-RR-71 0714 (March, 1972).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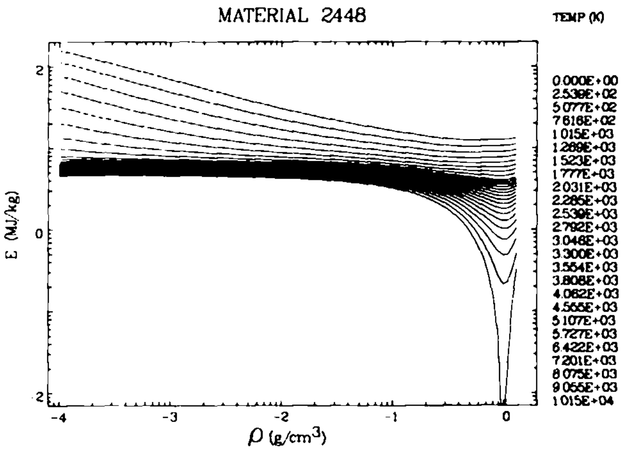
TEMP (K)
P (GPa)
1
-1
-3
-5
-4
-3
-2
-1
0
ρ (g/cm³)
0.000E+00
2.539E+02
5.077E+02
7.616E+02
1.015E+03
1.269E+03
1.523E+03
1.777E+03
2.031E+03
2.285E+03
2.539E+03
2.792E+03
3.046E+03
3.300E+03
3.554E+03
3.808E+03
4.062E+03
4.555E+03
5.107E+03
5.727E+03
6.422E+03
7.201E+03
8.075E+03
9.055E+03
1.015E+04


MATERIAL 2448
TEMP (K)
E (MJ/kg)
2
0
-2
-4
-3
-2
-1
0
ρ (g/cm³)
0.000E+00
2.539E+02
5.077E+02
7.616E+02
1.015E+03
1.269E+03
1.523E+03
1.777E+03
2.031E+03
2.285E+03
2.539E+03
2.792E+03
3.046E+03
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4.565E+03
5.107E+03
5.727E+03
6.422E+03
7.201E+03
8.075E+03
9.055E+03
1.015E+04

SESAME #2700

Material: Gold
Originator: A. Lindstrom and J. Rood
Date of Origin: January 1976
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 \leq \rho \leq 3.86 \times 10^5$ g/cm^3
$0 \leq T \leq 3.7 \times 10^8$ K

BASIC PHYSICAL DATA

$A = 196.97$
$Z = 79$
$\rho_o = 19.3$ g/cm^3

$P(T = 298.15\ \mathrm{K}, \rho_o) = 1.3101$ GPa
$E(T = 298.15\ \mathrm{K}, \rho_o) = 3.0641 \times 10^{-2}$ MJ/kg
$T(P = 10^{-6}\ \mathrm{GPa}, \rho_o) = 2.285 \times 10^{-4}$ K

$T_m = 1337.61$ K [Ref. 1]

$T_c =$ * 8460 K (calculated)

$\gamma_o =$ * 2.225 (used in calculation of EOS)
3.09 [Ref. 2]
$B_o =$ * 167.6 GPa (used in calculation of EOS)
176.6 GPa [Ref. 2]

$E_{coh} =$ * 1.748 MJ/kg (used in calculation)
1.868 MJ/kg [Ref. 3]

$\theta_D =$ * 165 K (used in calculation) [Ref. 1]

Hugoniot Fit: $U_s = 3.120 + 1.521\ U_p$ km/s
[Ref. 4]

DESCRIPTION OF PHYSICS

The gold equation of state was generated with the Barnes-Cowan-Rood method. The electronic contribution was calculated with Thomas-Fermi-Dirac theory. The cold curve is based on a modified-Morse model. The thermal nuclear EOS was calculated with a model from R. D. Cowan above 1 eV and a Debye model below 1 eV. (See Part II for a detailed discussion of this method of EOS generation.)

The theoretical EOS reproduces Hugoniot experiments well, although it is soft near the highest pressure experimental Hugoniot point. This EOS was not designed for the hot, expanded liquid metal region, so it should not be trusted there.

No melting transition has been included in this EOS.

The thermodynamic consistency is good everywhere.

The two-temperature tables were derived by the code TWOTEMP and are noisy.

A tension region for spall has been added.

REFERENCES

1. Handbook of Chemistry and Physics, R. C. Weast, Ed. (CRC Press, Cleveland, Ohio, 1976).

2. K. A. Gschneidner, Jr., Solid State Physics 16, 275 (1964).

3. L. Brewer, "Cohesive Energies of the Elements," Lawrence Berkeley Laboratory report LBL-3720 (1975).

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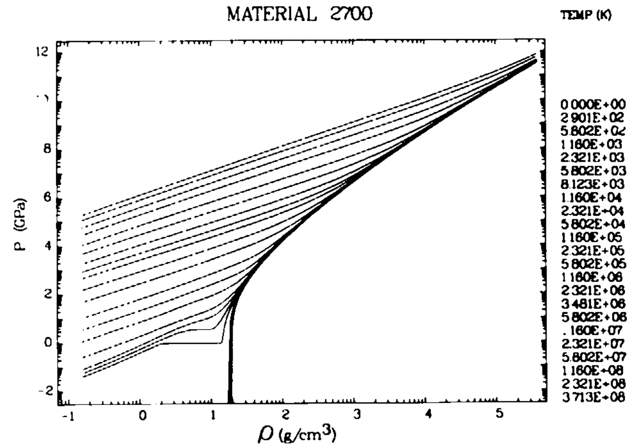
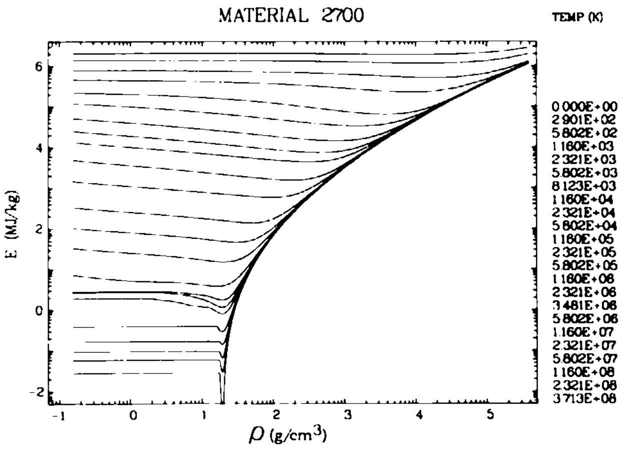

MATERIAL 2700
TEMP (K)
P (GPa)
12
10
8
6
4
2
0
-2
-1
0
1
2
3
4
5
ρ (g/cm^3)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08


MATERIAL 2700
TEMP (K)
E (MJ/kg)
6
4
2
0
-2
-1
0
1
2
3
4
5
ρ (g/cm3)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08

SESAME #2980

Material: Molybdenum
Originator: J. Barnes and J. Rood
Date of Origin: March 1973
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 \le \rho \le 2.04 \times 10^5$ g/cm^3
$0 \le T \le 3.7 \times 10^8$ K

BASIC PHYSICAL DATA

$A = 95.94$
$Z = 42$
$\rho_o = 10.2$ g/cm^3

$P(T = 298.15\ \text{K}, \rho_o) = 0.63866$ GPa
$E(T = 298.15\ \text{K}, \rho_o) = 4.2209 \times 10^{-2}$ MJ/kg
$T(P = 10^{-6}\ \text{GPa}, \rho_o) = 4.729 \times 10^{-4}$ K

$T_m = 2888$ K [Ref. 1]
2890 K [Ref. 2]
(There are a large number of measurements of the melting temperature in the literature; the two values cited here are averages of several measurements.)

$T_c = 14300$ K [Ref. 3]
14590 K [Ref. 4]
9470 K [Ref. 5]

$\gamma_o = 1.60$ [Ref. 1]
$B_o = 277.9$ GPa [Ref. 1]
267 Gpa [Ref. 6]
261.0 GPa [Ref. 7]

$E_{coh} = 6.85$ MJ/kg [Ref. 1]

$\theta_D = 459 \pm 11$ K [Ref. 1]

Hugoniot Fit: $U_s = 5.14 + 1.22\ U_p$ [Ref. 8]
$U_s = 5.1 + 1.266\ U_p$ [Ref. 9]

(Note: The values for the above parameters which were used in generating the EOS are unknown).

DESCRIPTION OF PHYSICS

This molybdenum equation of state was generated with the Barnes-Cowan-Rood method. The electronic part of the EOS is from Thomas-Fermi-Dirac theory; the cold curve is based on a modified-Morse model; and the thermal nuclear EOS is calculated with a model from R. D. Cowan above 1 eV and a Debye model below 1 eV. (See Part II for a detailed discussion of this method of EOS generation.)

The melting transition is not included in this EOS.

The two-temperature tables for this material were derived from the code TWOTEMP and are noisy.

A tension region for spall has been added.

REFERENCES

1. K. A. Gschneidner, Jr., Solid State Physics 16, 275 (1964).

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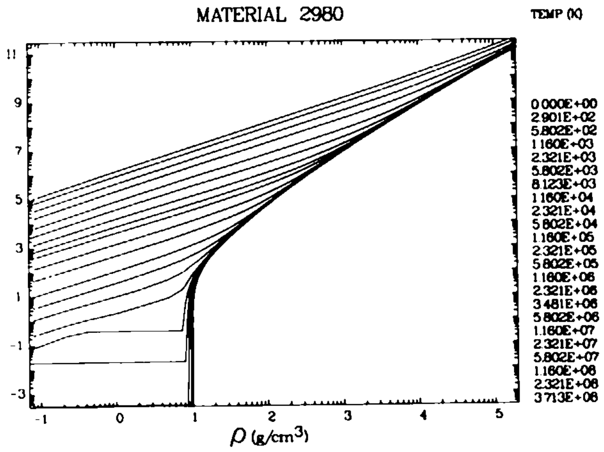
9. L. V. Al′tshuler, A. A. Bakanova, I. P. Dudoladov, E. A. Dynin, R. F. Trunin, and B. S. Chekin, Zhurnal Prikladnoi Mekhaniki i Tekhnicheskoi Fiziki 2, 3 (1981) [Sov. Phys. JAMTP 22 (2), 145 (19810].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TEMP (K)
P (GPa)
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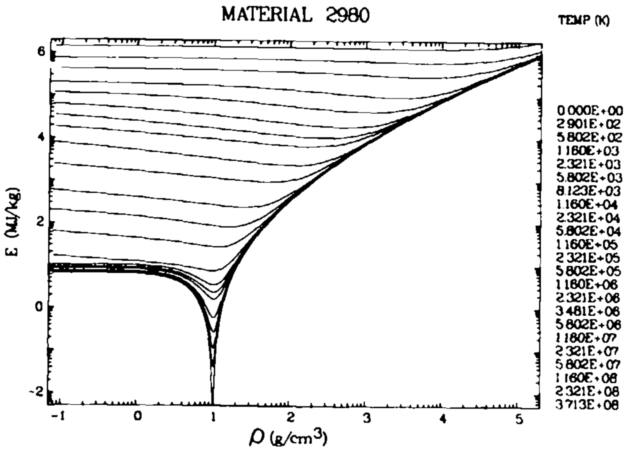
9
7
5
3
1
-1
-3
-1
0
1
2
3
4
5
ρ (g/cm³)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08

2980-6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TEMP (K)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08
E (MJ/kg)
6
4
2
0
-2
-1
0
1
2
3
4
5
ρ (g/cm3)

SESAME #2981

Material: Molybdenum
Originators: G. Kerley and J. Abdallah
Date of Origin: October 1980
Type of Tables Included: 301
Limits: $8.5 < \rho < 1000$ g/cm^3
$50 \le T \le 1.16 \times 10^6$ K

BASIC PHYSICAL DATA

$A = 95.94$
$Z = 42$
$\rho_o = 10.221$

$P(T = 298.15 \text{ K}, \rho_o) = 5.3983 \times 10^{-3}$ GPa
$E(T = 298.15 \text{ K}, \rho_o) = 2.8944 \times 10^{-5}$ MJ/kg
$T(P = 10^{-6} \text{ GPa}, \rho_o) = 296.75$ K

$T_m = 2888$ K [Ref. 1]
2890 K [Ref. 2]
* 2890 K (result of melting transition calculation)

(There are a large number of measurements of melting temperature in the literature; the two values cited here are averages of several measurements.)

No value for T_c is listed since this EOS only covers compression.

$\gamma_o = 1.60$ [Ref. 1]
* 1.70 (used in calculation of EOS)

$B_o = 277.9$ GPa [Ref. 1]
267 GPa [Ref. 3]
261.0 GPa [Ref. 4]
* 270.3 GPa (used in calculation of EOS)

E_{coh} = 6.85 MJ/kg [Ref. 1]
* 6.858 MJ/kg (used in calculation of EOS)

θ_D = 459 ± 11 K [Ref. 1]
* 450 K (used in calculation of EOS)

Hugoniot Fit: $U_S = 5.14 + 1.22\ U_p$ [Ref. 5]
$U_S = 5.1 + 1.266\ U_p$ [Ref. 6]
* $U_S = 5.1 + 1.24\ U_p$ (used in calculation of EOS)

DESCRIPTION OF PHYSICS

This molybdenum equation of state only covers the compression half-plane (densities greater than reference density). It was basically intended to be as accurate as possible for the purpose of analyzing Hugoniot impedance-matching experiments.

The cold curve is a composite of INFERNO and PANDA calculations. The PANDA part of the cold curve is constructed from experimental Hugoniot data and so covers densities accessed by experiment. The INFERNO calculations are used at higher densities and are smoothly joined onto the PANDA cold curve.

The electronic contribution to the EOS was calculated with the INFERNO model which solves the Dirac equation for an atom embedded in an electron gas. Shell structure effects are predicted by INFERNO, unlike Thomas-Fermi-Dirac theory which is based on a continuous electron distribution.

PANDA was also used to calculate the nuclear contribution to the EOS. In this portion of the EOS, solid lattice vibrations and fluid nuclear motion are taken into account.

The molybdenum EOS includes a melting transition. Separate equations of state were generated for the solid and liquid states, and then a composite surface was constructed by locating the phase boundary on each isotherm at the point where the Gibbs free energies are equal.

REFERENCES

1. K. A. Gschneidner, Jr., Solid State Physics 16, 275 (1964).
2. R. Hultgren, P. D. Desai, D. T. Hawkins, M. Gleiser, K. K. Kelley, and D. D. Wagman, Selected Values of the Thermodynamic Properties of the Elements (American Society for Metals, Metals Park, Ohio, 1973).
3. Li-chung Ming and M. H. Manghnani, J. Appl. Phys. 49 (1), 208 (1978).
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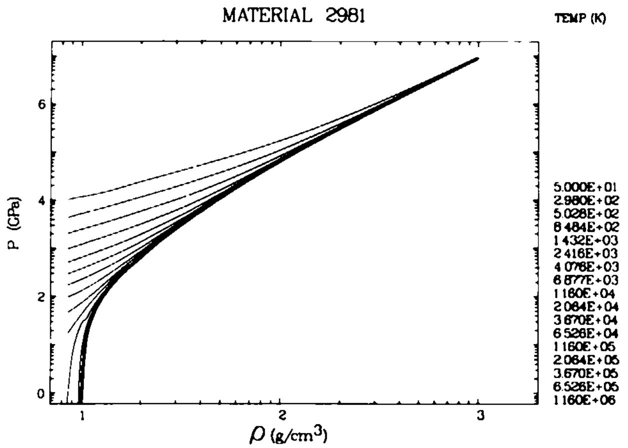
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5.028E+02
8.484E+02
1.432E+03
2.416E+03
4.076E+03
6.877E+03
1.160E+04
2.064E+04
3.670E+04
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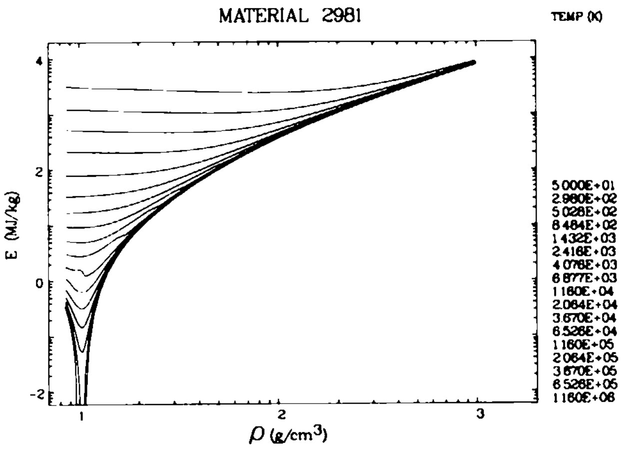
6.526E+05
1.160E+06

2981-6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TEMP (K)
E (MJ/kg)
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2
0
-2
1
2
3
ρ (g/cm³)
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2.980E+02
5.028E+02
8.484E+02
1.432E+03
2.416E+03
4.076E+03
6.877E+03
1.160E+04
2.064E+04
3.670E+04
6.526E+04
1.160E+05
2.064E+05
3.670E+05
6.526E+05
1.160E+06

SESAME #2982

Material: Molybdenum
Originator: R. C. Albers
Date of Origin: September 1982
Type of Tables Included: 306
Limits: $9.506 < \rho < 256.66$ g/cm^3
$T = 0$ K

BASIC PHYSICAL DATA

$A = 95.94$
$Z = 42$
$\rho_o = 10.256$ g/cm^3

$B_o =$ * 261 GPa (calculated)

DESCRIPTION OF PHYSICS

The zero-temperature cold curve was calculated with a self-consistent, semirelativistic, LMTO electronic band structure code for fcc molybdenum. Muffin-tin and ASA corrections are included. Angular momentum values up to g ($\ell = 4$) were kept.

SESAME #2983

Material: Molybdenum
Originator: K. Trainor
Date of Origin: March 1983
Type of Tables: 301, 303, 304, 305, 306
Limits: $10.2 < \rho < 250$ g/cm^3
$0 < T < 2.32 \times 10^6$ K

BASIC PHYSICAL DATA

$A = 95.94$
$Z = 42$
$\rho_o = 10.2$ g/cm^2

$P(T = 298.15\ \mathrm{K}, \rho_o) = 0.16024$ GPa
$E(T = 298.15\ \mathrm{K}, \rho_o) = 1.1587 \times 10^{-2}$ MJ/kg
$T(P = 10^{-4}\ \mathrm{GPa}, \rho_o) = 1.3509 \times 10^{-5}$ K

$T_m = 2888$ K [Ref. 1]
2890 K [Ref. 2]
* 2883 K (used in calculation)
(There are a large number of measurements of melting temperature in the literature; the two values cited here are averages of several measurements.)

No value for T_c is listed since this EOS only covers compression.

$\gamma_o = 1.60$ [Ref. 1]
* 1.36 (result of calculation)
$B_o = 277.9$ GPa [Ref. 1]
267 GPa [Ref. 3]
261.0 GPa [Ref. 4]
* 259 GPa (result of calculation)

$E_{coh} = 6.85$ MJ/kg [Ref. 1]

$\theta_D = 459 \pm 11$ K [Ref. 1]

Hugoniot Fit: $U_S = 5.14 + 1.22\ U_p$ km/s
[Ref. 5]
$U_S = 5.1 + 1.266\ U_p$ km/s
[Ref. 6]

DESCRIPTION OF PHYSICS

This equation of state for molybdenum was generated along with equations of state for copper (3332) and aluminum (3713) for the purpose of evaluating Hugoniot impedance-matching experiments. The goal was to calculate a set of EOS tables based on the same physics models.

The zero-kelvin isotherm was calculated with a semirelativistic band structure model (LMTO) based on the linear-muffin-tin-orbital method. (This is the same cold curve as SESAME #2982.)

The thermal electronic part of the EOS was generated with D. Liberman's self-consistent field model for condensed matter (INFERNO). INFERNO solves the Dirac equation for an atom embedded in an electron gas. Unlike EOS's based on Thomas-Fermi-Dirac theory, INFERNO thermodynamic surfaces exhibit shell structure effects. The nuclear thermal EOS was based on the Dugdale-MacDonald form of Grüneisen-Debye theory. Grüneisen gamma was calculated from the cold curve according to the following formula:

$$\gamma(V) = -\frac{1}{6} - \frac{1}{2}\left[\left(\frac{d\ \ell n\ B}{d\ \ell n\ V} + \frac{2}{3}\right)/\left(1 - \frac{2P}{3B}\right)\right]$$

where B is bulk modulus, V is volume, and P is pressure. Note that gamma is a function of density only, not temperature.

A melting transition is included in this EOS based on the Lindemann law. The equation of state of the liquid is given by a scaling law; that is, the solid Grüneisen EOS at a given temperature and density is corrected with various terms which depend on the ratio of the temperature to the melting temperature at that density.

At pressures between 50 and 200 GPa, the Hugoniot that this EOS predicts is a little soft compared with existing Hugoniot experiments; but above and below those pressures, it matches the data well.

Note that only compression is covered by this EOS since it was intended for analysis of Hugoniot experiments.

The EOS is thermodynamically consistent everywhere.

REFERENCES

1. K. A. Gschneidner, Jr., Solid State Physics 16, 275 (1964).

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3. Li-chung Ming and M. H. Manghnani, J. Appl. Phys. **49** (1), 208 (1978).

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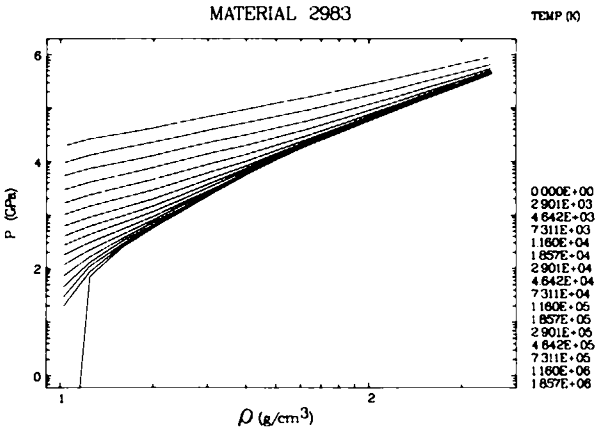
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TEMP (K)
P (GPa)
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2
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1
2
ρ (g/cm3)
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4.642E+03
7.311E+03
1.160E+04
1.857E+04
2.901E+04
4.642E+04
7.311E+04
1.160E+05
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7.311E+05
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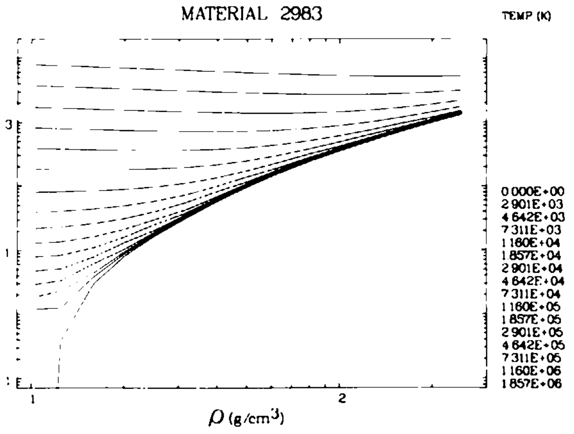
1.857E+06


MATERIAL 2983
TEMP (K)
E (MJ/kg)
3
1
ρ (g/cm³)
1
2
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2.901E+03
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7.311E+03
1.160E+04
1.857E+04
2.901E+04
4.642E+04
7.311E+04
1.160E+05
1.857E+05
2.901E+05
4.642E+05
7.311E+05
1.160E+06
1.857E+06

SESAME #3100

Material: Nickel
Originators: J. Barnes and J. Rood
Date of Origin: March 1973
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho < 1.7764 \times 10^5$ g/cm^3
$0 < T < 3.7 \times 10^8$ K

BASIC PHYSICAL DATA

$A = 58.710$
$Z = 28$
$\rho_o = 8.882$ g/cm^3

$P(T = 298.15\ \text{K}, \rho_o) = 1.2806$ GPa
$E(T = 298.15\ \text{K}, \rho_o) = 6.8903 \times 10^{-2}$ MJ/kg
$T(P = 10^{-6}\ \text{GPa}, \rho_o) = 2.359 \times 10^{-4}$ K

$T_m = 1726$ K [Ref. 1]
1728 K [Ref. 2]

$T_c = 9576$ K [Ref. 3]
6520 K [Ref. 4]
6000 K [Ref. 5]
* 9133 K (result of EOS calculation)

$\gamma_o = 1.88$ (an average of values found in the literature) [Ref. 1]
2.00 (calculated from shock wave data) [Ref. 1]
* 2.098 (result of EOS calculation)
$B_o = 190$ GPa [Ref. 1]
* 190 GPa (used in EOS calculation)

$E_{coh} = 7.29$ MJ/kg [Ref. 1]
* 7.27 MJ/kg (used in EOS calculation)

Θ_D = 427 ± 14 K [Ref. 1]
450 K (used in EOS calculation)

Hugoniot Fit: $U_S = 4.646 + 1.445\ U_p$ km/s [Ref. 6]
$U_S = 4.501 + 1.627\ U_p - 0.0264\ U_p^2$ km/s [Ref. 7]

DESCRIPTION OF PHYSICS

At higher temperatures (probably above 1 eV), this EOS was generated by mixing MAPLE equations of state for iron (using a number fraction of 0.802937) and molybdenum (using a number fraction of 0.197063). The average atomic weight of the resulting material was 60.8625. The mixed EOS was scaled so that the atomic weight would be 58.71 and the reference density, ρ_0, would be 8.882 g/cm^3.

At temperatures below 1 eV, the code MAXWELL computed the EOS. MAXWELL assumes that the pressures and energies are the sum of two contributions: a zero-degree contribution and a thermal nuclear contribution. The cold curve (zero-kelvin isotherm) is based on a modified-Morse model, and the thermal nuclear part is calculated by a Debye model. (See Part II for a detailed discussion of this procedure of EOS generation.)

The experimental zero-pressure density and bulk modulus are reproduced by this EOS, and the fit to experimental Hugoniot data is good. Also, the critical point is fairly close to an estimate made by Young and Alder. However, this EOS was not generally designed for the hot, expanded, liquid metal region and it is not to be trusted there.

No melting transition is included in this EOS.

The thermodynamic consistency is good everywhere.

The two-temperature tables for this material were derived by the code TWOTEMP and are noisy.

REFERENCES

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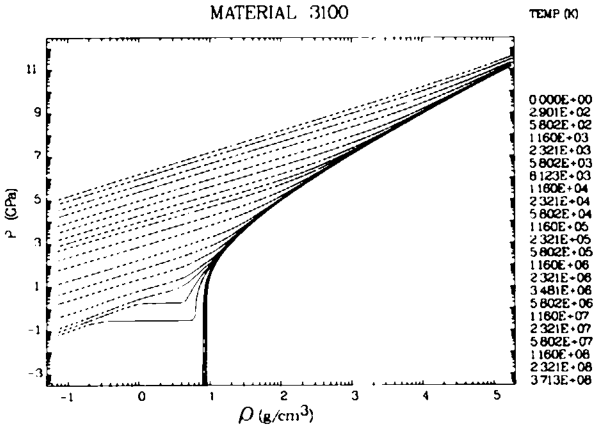
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TEMP (K)
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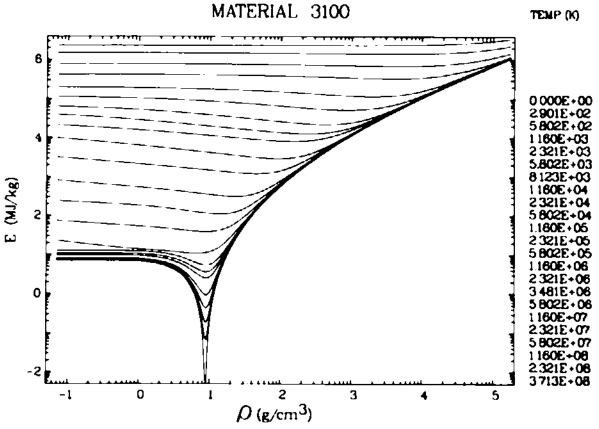
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08
P (GPa)
11
9
7
5
3
1
-1
-3
-1
0
1
2
3
4
5
ρ (g/cm3)


MATERIAL 3100

SESAME #3200

Material: Lead
Originators: J. Barnes and J. Rood
Date of Origin: April 1975 and August 1978
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho \; 2.268 \times 10^5$ g/cm^3
$0 < T < 3.7 \times 10^8$ K

BASIC PHYSICAL DATA

$A = 207.19$
$Z = 82$
$\rho_o = 11.34$ g/cm^3

$P(T = 298.15 \text{ K}, \rho_o) = 0.75759$ GPa
$E(T = 298.15 \text{ K}, \rho_o) = 3.1576 \times 10^{-2}$ MJ/kg
$T(P = 10^{-6} \text{ GPa}, \rho_o) = 3.948 \times 10^{-4}$ K

$T_m = 600.576$ K [Ref. 1]

$T_c = 5158$ K [Ref. 2]
5300 K [experiment reported in Ref. 2]
3530 K [Ref. 3]
* 5223 K (from calculation of EOS)

$\gamma_o = 2.84$ [Ref. 1]
2.62 ± 0.27 (average of values given in literature) [Ref. 1]
2.38 ± 0.35 (calculated from shock wave data) [Ref. 1]
2.629 [Ref. 4]
* 1.945 (used in calculation of EOS)
$B_o = 43.82$ GPa [Ref. 1]
45.4 GPa [Ref. 5]
* 45.63 GPa (used in calculation of EOS)

E_{coh} = 0.949 MJ/kg [Ref. 1]
* 0.939 MJ/kg (used in calculation of EOS)

θ_D = 102 ± 5 K [Ref. 1]
* 105 K (used in calculation of EOS)

Hugoniot Fit: $U_S = 2.006 + 1.538\ U_p$ km/s (P < 1.2 Mb) [Ref. 5]
$U_S = 2.616 + 1.249\ U_p$ km/s (P > 1.2 Mb) [Ref. 5]
$U_S = 1.981 + 1.603\ U_p - 0.0378\ U_p^2$ km/s [Ref. 6]

DESCRIPTION OF PHYSICS

At higher temperatures (probably above 1 eV), this EOS was produced by scaling a MAPLE table for lead to an atomic weight of 207.19. Thomas-Fermi- Dirac physics describes the electronic contributions to pressure and energy in the MAPLE table, and the nuclear contributions are calculated with a model developed by R. D. Cowan.

Below 1 eV, the EOS was computed with the code MAXWELL, which assumes that the pressures and energies are the sum of a zero-degree contribution and a nuclear thermal contribution. The cold curve is calculated with a modified-Morse model, and the thermal nuclear EOS with a Debye model. (See Part II for a detailed discussion of this procedure of EOS generation.)

The experimental zero-pressure density and bulk modulus are reproduced by this EOS, and the fit to experimental Hugoniot data is good. Also the critical point is close to the estimate made by Young and Alder. However, this EOS was not generally designed for the hot, expanded, liquid metal region, and is not to be trusted there.

No melting transition is included in this EOS.

The thermodynamic consistency is good everywhere.

The two-temperature tables for this EOS were derived by the code TWOTEMP and are noisy.

A tension region for spall was added to this EOS.

REFERENCES

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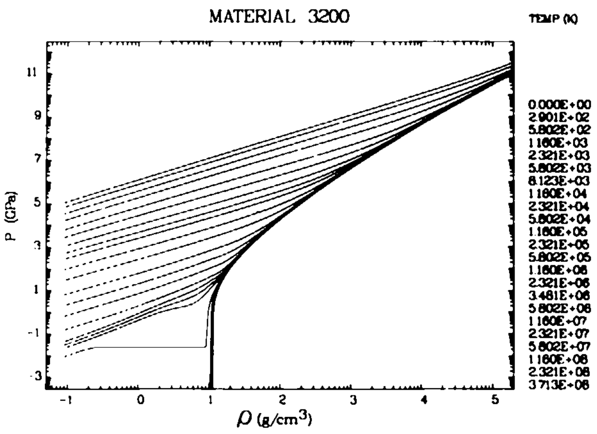
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P (GPa)
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3
4
5
ρ (g/cm^3)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
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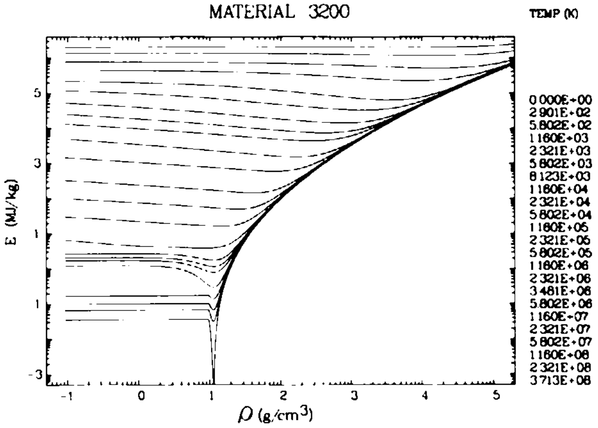
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TEMP (K)
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1.160E+03
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8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
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3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08
E (MJ/kg)
5
3
1
1
-3
-1
0
1
2
3
4
5
ρ (g/cm3)

SESAME #3330

Material: Copper
Originators: J. Barnes and J. Rood
Date of Origin: May 1974
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho < 1.786 \times 10^5$ g/cm^3
$0 < T < 3.7 \times 10^8$ K

BASIC PHYSICAL DATA

$A = 63.54$
$Z = 29$
$\rho_o = 8.93$ g/cm^3

$P(T = 298.15\text{ K}, \rho_o) = 1.3225$ GPa
$E(T = 298.15\text{ K}, \rho_o) = 7.4241 \times 10^{-2}$ MJ/kg
$T(P = 10^{-6}\text{ GPa}, \rho_o) = 2.277 \times 10^{-4}$ K

$T_m = 1356$ K [Ref. 1]
1355.95 K [Ref. 2]

$T_c = 6544$ K (Information provided by D. A. Young at Lawrence Livermore National Laboratory)
* 7580 K (from calculation of EOS)

$\gamma_o = 2.008$ [Ref. 3]
1.97 [Ref. 1]
2.00 ± 0.08 (average of values in literature) [Ref. 1]
* 2.00 (used in calculation of EOS)

$B_o = 133.5$ GPa [Ref. 1]
137 GPa (calculated from measurement of bulk sound velocity) [Ref. 4]
* 133.9 GPa (used in calculation of EOS)

$E_{coh} = 5.32$ MJ/kg [Ref. 1]
* 5.38 MJ/kg (used in calculation of EOS)

θ_D = 342 ± 2 K [Ref. 1]
* 343 (used in calculation of EOS)

Hugoniot Fit: $U_S = 4.007 + 1.466\ U_p$ km/s [Ref. 4]
$U_S = 3.889 + 1.520\ U_p - 0.00071\ U_p^2$ km/s [Ref. 5]
$U_S = 3.993 + 1.500\ U_p$ km/s [Ref. 6]

DESCRIPTION OF PHYSICS

An EOS for copper from Lawrence Livermore National Laboratory was joined onto an EOS generated by the code MAXWELL (which was probably run at temperatures lower than 1 eV). MAXWELL uses a modified-Morse model to calculate the zero-kelvin contributions to pressure and energy and a Debye model for the thermal nuclear part. (See Part II for a detailed description of this method of EOS generation.)

The experimental zero-pressure density and bulk modulus are reproduced by this EOS, and the comparison with experimental Hugoniot data is good. However, this EOS was not generally designed for the hot, expanded, liquid metal region and is not to be trusted there.

No melting transition was included in this EOS.

The thermodynamic consistency is good everywhere.

The two-temperature tables for this EOS were derived by the code TWOTEMP and are noisy.

REFERENCES

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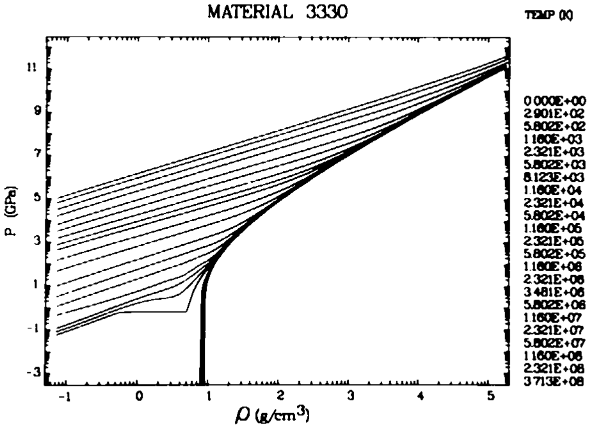
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4
5
ρ (g/cm³)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
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5.802E+05
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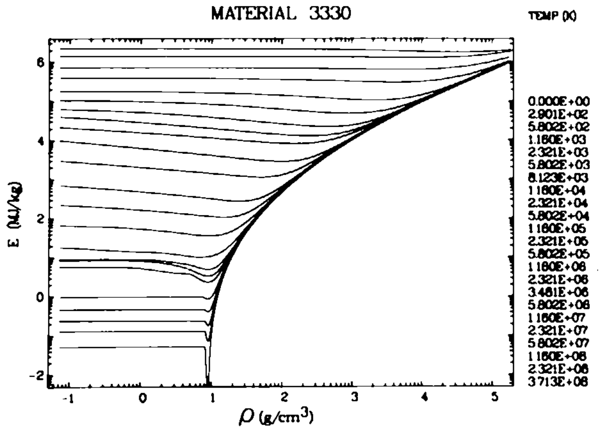
3.713E+08


MATERIAL 3330
TEMP (K)
E (MJ/kg)
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2
0
-2
-1
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1
2
3
4
5
ρ (g/cm³)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
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1.160E+06
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3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08

SESAME #3331

Material: Copper [Ref. 1]
Originator: K. Trainor
Date of Origin: 1980
Type of Tables Included: 301
Limits: $10^{-3} < \rho < 10^{3}$ g/cm^3
$300 < T < 5.8 \times 10^{8}$ K

BASIC PHYSICAL DATA

$A = 63.54$
$Z = 29$
$\rho_o = 8.93$ g/cm^3

$P(T = 298.15\ \mathrm{K}, \rho_o) = 2.1018 \times 10^{-4}$ GPa
$E(T = 298.15\ \mathrm{K}, \rho_o) = 0.11825$ MJ/kg
$T(P = 10^{-4}\ \mathrm{GPa}, \rho_o) = 300$ K

T_m = 1356 K [Ref. 2]
1355.95 K [Ref. 3]
* 1356 K (used in calculation of EOS)

T_c = 6544 K (Information provided by D. A. Young at Lawrence Livermore National Laboratory)
* 6544 K (result of calculation of EOS)

γ_o = 2.008 [Ref. 4]
1.97 [Ref. 2]
2.00 ± 0.08 (average of values in literature) [Ref. 2]
* 1.97 (used in calculation of EOS)
B_o = 133.5 GPa [Ref. 2]
137 GPa (calculated from measurement of bulk sound velocity)[Ref. 5]

E_{coh} = 5.32 MJ/kg [Ref. 2]
* 5.34 MJ/kg (used in calculation of EOS)

Θ_D = 342 ± 2K [Ref. 2]

Hugoniot Fit: $U_S = 4.007 + 1.466\ U_p$ km/s [Ref. 5]
$U_S = 3.889 + 1.520\ U_p - 0.00071\ U_p^2$ km/s [Ref. 6]
$U_S = 3.933 + 1.500\ U_p$ km/s [Ref. 7]
* $U_S = 4.007 + 1.48\ U_p$ km/s (used in calculation of EOS)

DESCRIPTION OF PHYSICS

The purpose of generating this EOS was to construct a global equation of state using the best available physical theories.

Six different theoretical models were used in the generation:

1) rigorous electron band theory based on the self-consistent augmented plane wave (APW) method for the zero-kelvin isotherm in compression

2) semi-empirical Grüneisen-Debye model for the multiphase region at densities from normal density to two-fold compressed (GRAY)

3) Thomas-Fermi-Kirzhnits theory with nuclear corrections for the rest of the compression EOS (TFNUC)

4) semi-empirical soft-sphere model for liquid metals at low temperatures below liquid density

5) rigorous quantum-statistical-mechanical theory based on a many-body perturbation expansion (ACTEX) for the high-temperature ionization equilibrium region

6) Saha model based on the Planck-Larkin partition function (OCCIPITAL) for the moderate-temperature ionization equilibrium region.

The composite pressure and energy surfaces were constructed by joining the separate EOS subsurfaces along the boundaries shown in Fig. 2. At high temperature, the models merged smoothly into one another. At low temperature, however, the physics is more complex, and there were in some cases substantial mismatches between adjacent theories. In this case, portions of each EOS subsurface on either side of a boundary had to be replaced with numerical interpolation to ensure a smooth and continuous join.

The copper EOS has a melting transition based on the Lindemann law. The theoretical melting line matches experimental measurements of the melting temperature as a function of pressure up to 6 GPa. The two-phase region in expansion is a Maxwell construction (not van der Waals loops).

Experimental data are reproduced well. Experiments which have been compared to this EOS include Hugoniot experiments, porous Hugoniot experiments, isobaric data, compressibility data, and release isentrope measurements.

The thermodynamic consistency is good everywhere except on the boundaries between the various physical models.

REFERENCES

1. A complete description of this EOS is given in K. Trainor, J. Appl. Phys. 54 (5), 2372 (1983).
2. K. A. Gschneidner, Jr., Solid State Physics 16, 275 (1964).
3. J. Akella and G. C. Kennedy, J. Geophys. Res. 76 (20), 4969 (1971).
4. J. Ramakrishnan, R. Boehler, G. H. Higgins, and G. C. Kennedy, J. Geophys. Res. 83 (B7), 3535 (1978).
5. M. van Thiel, "Compendium of Shock Wave Data," Lawrence Livermore Laboratory report UCRL-50108, Rev. 1 (1977).
6. L. V. Al'tshuler, A. A. Bakanova, I. P. Dudoladov, E. A. Dynin, R. F. Trunin, and B. S. Chekin, Zhurnal Prikladnoi Mekhaniki i Tekhnicheskoi Fiziki 2, 3 (1981) [Sov. Phys. JAMTP 22 (2), 195 (1981)].
7. A. C. Mitchell and W. J. Nellis, J. Appl. Phys. 52 (5), 3363 (1980).

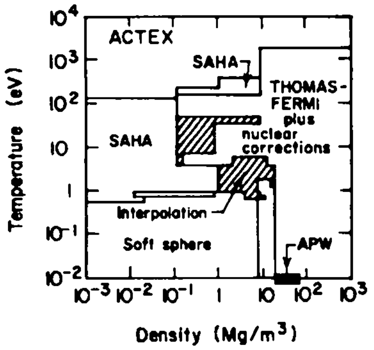
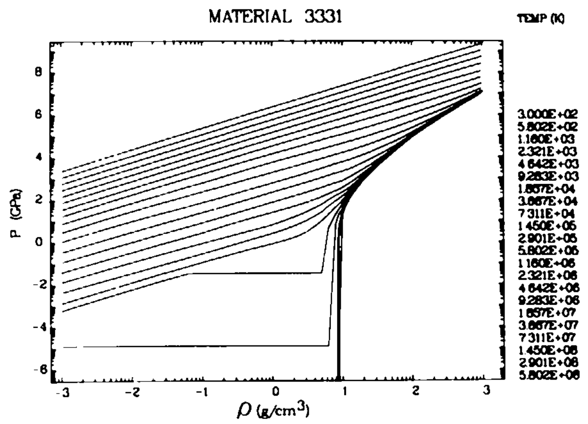
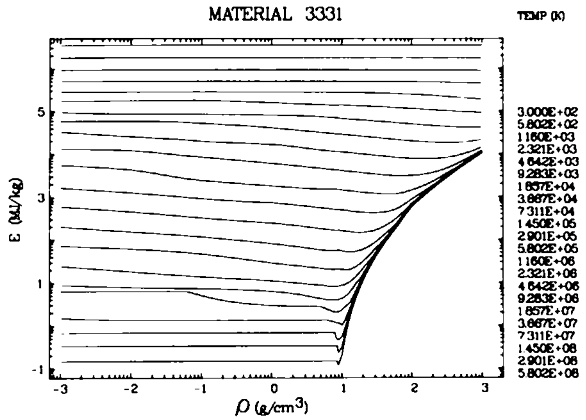


Fig. 2. Temperature-density plot showing the subregions covered by each of the theory codes used to calculate the EOS for copper. The shaded areas are regions in which numerical interpolation was required to smoothly join two EOS subsurfaces.


MATERIAL 3331
TEMP (K)
P (GPa)
8
6
4
2
0
-2
-4
-6
-3
-2
-1
0
1
2
3
ρ (g/cm3)
3.000E+02
5.802E+02
1.160E+03
2.321E+03
4.642E+03
9.283E+03
1.857E+04
3.687E+04
7.311E+04
1.450E+05
2.901E+05
5.802E+05
1.160E+06
2.321E+06
4.642E+06
9.283E+06
1.857E+07
3.687E+07
7.311E+07
1.450E+08
2.901E+08
5.802E+08


MATERIAL 3331
TEMP (K)
5
3
1
-1
ε (MJ/kg)
-3
-2
-1
0
1
2
3
ρ (g/cm3)
3.000E+02
5.802E+02
1.160E+03
2.321E+03
4.642E+03
9.283E+03
1.857E+04
3.667E+04
7.311E+04
1.450E+05
2.901E+05
5.802E+05
1.160E+06
2.321E+06
4.642E+06
9.283E+06
1.857E+07
3.667E+07
7.311E+07
1.450E+08
2.901E+08
5.802E+08

SESAME #3332

Material: Copper
Originator: K. Trainor
Date of Origin: March 1983
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $8.93 < \rho < 1000$ g/cm^3
$0 < T < 1.16 \times 10^6$ K

BASIC PHYSICAL DATA

$A = 63.54$
$Z = 29$
$\rho_o = 8.93$ g/cm^3

$P(T = 298.15\text{ K}, \rho_o) = 1.3603$ GPa
$E(T = 298.15\text{ K}, \rho_o) = 0.15831$ MJ/kg
$T(P = 10^{-4}\text{ GPa}, \rho_o) = 9.2797 \times 10^{-3}$ K

$T_m = 1356$ K [Ref. 1]
1355.95 K [Ref. 2]
* 1356.55 K (used in calculation of EOS)

No value for T_c is included since this EOS only covers compression.

$\gamma_o = 2.008$ [Ref. 3]
1.97 [Ref. 1]
2.00 ± 0.08 (average of values in literature) [Ref. 1]
* 0.90 (result of calculation)

$B_o = 133.5$ GPa [Ref. 1]
137 GPa (calculated from measurement of bulk sound velocity) [Ref. 4]
* 157 GPa (result of calculation)

$E_{coh} = 5.32$ MJ/kg [Ref. 1]

$\Theta_D = 342 \pm 2$ K [Ref. 1]

Hugoniot Fit: $U_S = 4.007 + 1.466\ U_p$ km/s [Ref. 4]

$U_S = 3.889 + 1.520\ U_p - 0.00071\ U_p^2$ km/s [Ref. 5]

$U_S = 3.933 + 1.500\ U_p$ km/s [Ref. 6]

(No Hugoniot fit was explicitly used in the calculation of this EOS.)

DESCRIPTION OF PHYSICS

This equation of state for copper was generated along with equations of state for aluminum (#3713) and molybdenum (#2983) for the purpose of evaluating high-pressure, impedance-matching Hugoniot experiments. The goal was to calculate a set of EOS tables based on a consistent set of physics models.

The zero-kelvin isotherm was calculated by A. McMahan (Lawrence Livermore National Laboratory) with rigorous band theory based on the self-consistent, augmented plane wave (APW) method.

The thermal electronic part of the EOS was generated with D. Liberman's self-consistent field model for condensed matter (INFERNO). This model solves the Dirac equation for an atom embedded in an electron gas. Unlike equations of state based on Thomas-Fermi-Dirac theory, INFERNO thermodynamic surfaces exhibit shell structure effects.

The thermal nuclear contribution to the EOS was calculated with the Dugdale-MacDonald form of Grüneisen-Debye theory. Grüneisen gamma is derived from the cold curve according to the following formula:

$$\gamma(V) = -\frac{1}{6} - \frac{1}{2}\,\frac{\dfrac{d\,\ell n\,B}{d\,\ell n\,V} + \dfrac{2}{3}}{1 - \dfrac{2P}{3B}} \quad ,$$

where B is bulk modulus, V is volume, and P is pressure. Note that gamma is a function of density only, not temperature.

A melting transition is included in this EOS based on the Lindemann law. The equation of state of the liquid is given by a scaling law; that is, the solid Grüneisen EOS at a given temperature and density is corrected with terms which depend on the ratio of the temperature to the melting temperature at that density.

At pressures above 100 GPa, the Hugoniot that this EOS predicts is slightly stiff compared with existing Hugoniot experiments. Below, it matches the data well.

Note that only compression is covered by this EOS since it was intended for analysis of Hugoniot experiments.

The EOS is thermodynamically consistent everywhere.

REFERENCES

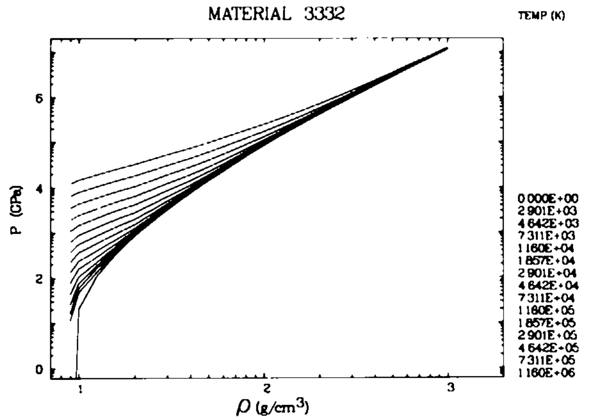
1. K. A. Gschneidner, Jr., Solid State Physics 16, 275 (1964).

2. J. Akella and G. C. Kennedy, J. Geophys. Res. 76 (20), 4969 (1971).

3. J. Ramakrishnan, R. Boehler, G. H. Higgins, and G. C. Kennedy, J. Geophys. Res. 83 (B7), 3535 (1978).

4. M. van Thiel, "Compendium of Shock Wave Data," Lawrence Livermore Laboratory report UCRL-50108, Rev. 1 (1977).

5. A. C. Mitchell and W. J. Nellis, J. Appl. Phys. 52 (5), 3363 (1981).


MATERIAL 3332
TEMP (K)
P (GPa)
0
2
4
6
1
2
3
ρ (g/cm³)
0 000E+00
2 901E+03
4 642E+03
7 311E+03
1 160E+04
1 857E+04
2 901E+04
4 642E+04
7 311E+04
1 160E+05
1 857E+05
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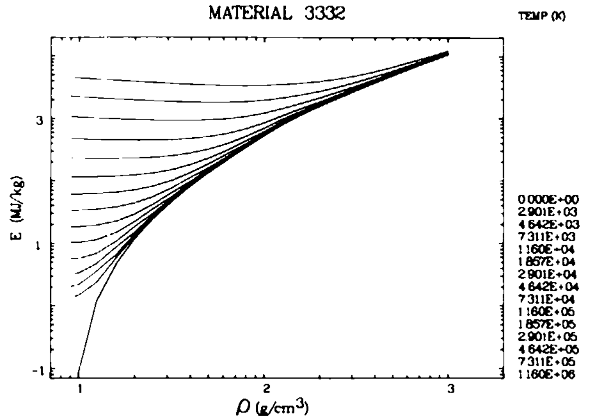
4 642E+05
7 311E+05
1 160E+06


MATERIAL 3332
TEMP (K)
E (MJ/kg)
3
1
-1
1
2
3
ρ (g/cm^3)
0.000E+00
2.901E+03
4.642E+03
7.311E+03
1.160E+04
1.857E+04
2.901E+04
4.642E+04
7.311E+04
1.160E+05
1.857E+05
2.901E+05
4.642E+05
7.311E+05
1.160E+06

SESAME #3541

Material: Tungsten
Originator: B. Bennett
Date of Origin: September 1979
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho < 1.9312 \times 10^{4}$ g/cm^3
$0 < T < 1.16 \times 10^{8}$ K

BASIC PHYSICAL DATA

$A = 183.85$
$Z = 74$
$\rho_0 = 19.237$ g/cm^3

$P(T = 300\text{ K}, \rho_0) = 4.3891 \times 10^{-3}$ GPa
$E(T = 300\text{ K}, \rho_0) = 1.9451 \times 10^{-4}$ MJ/kg
$T(P = 10^{-6}\text{ GPa}, \rho_0) = 298.5$ K

T_m = 3653 K [Ref. 1]
3690 K (Information provided by G. R. Gathers at Lawrence Livermore National Laboratory)
3695 K [Ref. 2]

T_c = 13400 ± 1400 K [Ref. 3]
11950 K [Ref. 4]
18538 K [Ref. 5]
* 17401 K (calculated)

γ_0 = 1.78 [Ref. 1]
1.68 (average of values found in literature) [Ref. 1]
* 1.47 (calculated)

B_o = 307 GPa [Ref. 6]
329.6 GPa [Ref. 1]
314 GPa (calculated from shock wave data) [Ref. 7]
* 313 GPa (used in calculation of EOS)

E_{coh} = 4.54 MJ/kg [Ref. 1]
* 4.67 MJ/kg (used in calculation of EOS)

Θ_D = 388 ± 17 K [Ref. 1]

Hugoniot Fit: $U_S = 4.04 + 1.23\ U_p$ km/s [Ref. 8]
$U_S = 4.015 + 1.252\ U_p$ km/s [Ref. 9]
* $U_S = 4.025 + 1.239\ U_p$ km/s (used in calculation of EOS)

DESCRIPTION OF PHYSICS

The tungsten EOS was calculated with the codes CANDIDE (Thomas-Fermi-Dirac theory for the electrons) and EOS_IS. The zero-kelvin isotherm was obtained from Hugoniot data assuming the Dugdale-MacDonald form for Grüneisen gamma. A Lennard-Jones tail was used for densities less than ρ_o. The nuclear vibration contributions were also based on the Dugdale-MacDonald form of Grüneisen-Debye theory, but with a transition to ideal gas high temperatures.

No melting transition per se is included in this table, and it has van der Waals loops in expansion instead of a Maxwell construction.

This tungsten EOS reproduces experimental principal Hugoniot data. Also, vapor pressures computed from the table should give reasonable agreement with experiment.

The two-temperature tables for this material were derived from the code TWOTEMP and are noisy.

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3. W. Fucke and U. Seydel, High Temp.-High Pressures 12, 419 (1980).
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5. D. A. Young and B. J. Alder, Phys. Rev. A 3, 364 (1971).
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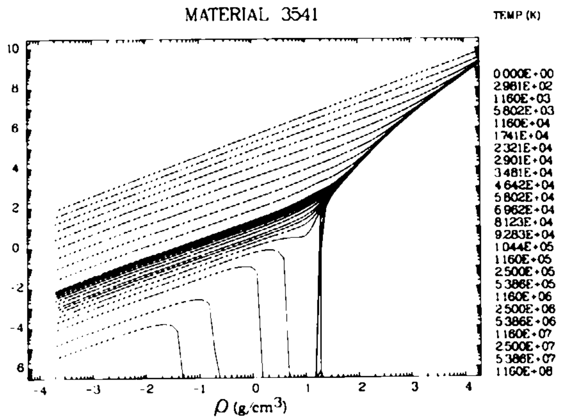
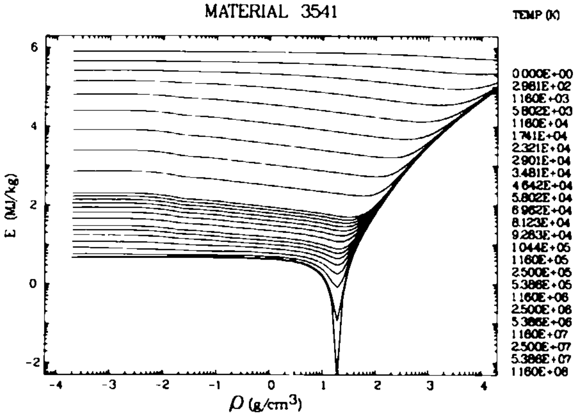
7. M. van Thiel, "Compendium of Shock Wave Data," Lawrence Livermore Laboratory report UCRL-50108, Rev. 1 (1977).
8. S. P. Marsh, LASL Shock Hugoniot Data (University of California Press, Berkeley, 1980).

9. L. V. Al'tshuler, A. A. Bakanova, I. P. Dudoladov, E. A. Dynin, R. F. Trunin, and B. S. Chekin, Zhurnal Prikladnoi Mekhaniki i Tekhnicheskoi Fiziki 2, 3 (1981) [Sov. Phys. JAMTP 22 (2), 195 (1981)].


MATERIAL 3541
TEMP (K)
P (GPa)
10
8
6
4
2
0
-2
-4
6
ρ (g/cm3)
-4
-3
-2
-1
0
1
2
3
4
0.000E+00
2.981E+02
1.160E+03
5.802E+03
1.160E+04
1.741E+04
2.321E+04
2.901E+04
3.481E+04
4.642E+04
5.802E+04
6.962E+04
8.123E+04
9.283E+04
1.044E+05
1.160E+05
2.500E+05
5.386E+05
1.160E+06
2.500E+06
5.386E+06
1.160E+07
2.500E+07
5.386E+07
1.160E+08


MATERIAL 3541
TEMP (K)
6
4
2
0
-2
E (MJ/kg)
-4
-3
-2
-1
0
1
2
3
4
ρ (g/cm3)
0.000E+00
2.981E+02
1.160E+03
5.802E+03
1.160E+04
1.741E+04
2.321E+04
2.901E+04
3.481E+04
4.642E+04
5.802E+04
6.962E+04
8.123E+04
9.283E+04
1.044E+05
1.160E+05
2.500E+05
5.386E+05
1.160E+06
2.500E+06
5.386E+06
1.160E+07
2.500E+07
5.386E+07
1.160E+08

SESAME #3560

Material: Tungsten Carbide
Composition: Tungsten Carbide (94 wt %)
Cobalt (6 wt %)
Originator: R. C. Albers
Date of Origin: November 1981
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho < 1.5048 \times 10^4$ g/cm^3
$0 < T < 3.48 \times 10^8$ K

BASIC PHYSICAL DATA

$\bar{A} = 94.1909$
$\bar{Z} = 38.75335$
$\rho_o = 14.97$ g/cm^3

$P(T = 298.15\text{ K}, \rho_o) = 2.9187 \times 10^{-3}$ GPa
$E(T = 298.15\text{ K}, \rho_o) = 3.1184 \times 10^{-6}$ MJ/kg
$T(P = 10^{-6}\text{ GPa}, \rho_o) = 297.4$ K

$T_m = 3143$ K [Ref. 1]

Boiling Temperature = 6273 K [Ref. 1]

$\gamma_o = 1.5$ [Ref. 2]

$B_o = 362.4$ GPa (from shock wave data on tungsten carbide)
$= 360$ GPa (at $P = 0$, $T = 298.15$ K in table)

$E_{coh} = 4.63$ MJ/kg [Ref. 3]

DESCRIPTION OF PHYSICS

The cold curve was generated by fitting shock wave data [Ref. 3]. An average atom Thomas-Fermi-Dirac model was used for the thermal electronic excitations. A Chart-D Grüneisen ion model was used for the ion (nuclear) contributions to the EOS. There is a nonequilibrium region in the vapor dome area (van der Waals loops) because no Maxwell construction was performed.

The theoretical Hugoniot reproduces experimental shock wave data [Ref. 4].

REFERENCES

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2. Grüneisen constant of 1.50 is taken from Meyers and Murr, "Shock Wave and High-Strain-Rate phenomena in Metals," in Proceedings of the International Conference on Metallurgical Effects of High-Strain Rate Deformation and Fabrication, Albuquerque, NM, 1980 M. A. Meyers and L. E. Murr, Eds. (Plenum Press, New York, 1981), P. 1077.

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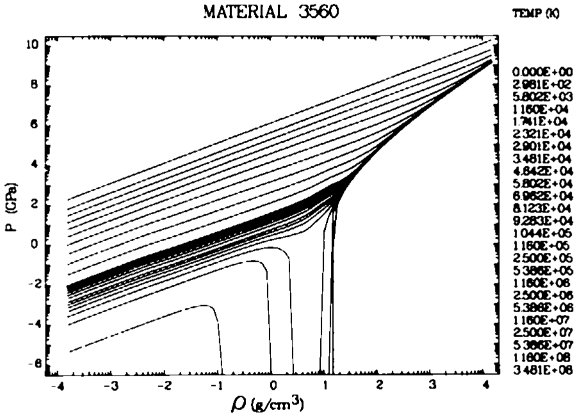
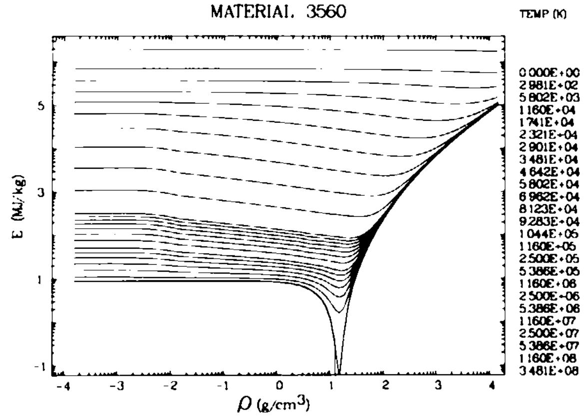
4. S. P. Marsh, LASL Shock Hugoniot Data (University of California Press, Berkeley, 1980).


MATERIAL 3560
TEMP (K)
0.000E+00
2.981E+02
5.802E+03
1.160E+04
1.741E+04
2.321E+04
2.901E+04
3.481E+04
4.642E+04
5.802E+04
6.962E+04
8.123E+04
9.283E+04
1.044E+05
1.160E+05
2.500E+05
5.386E+05
1.160E+06
2.500E+06
5.386E+06
1.160E+07
2.500E+07
5.386E+07
1.160E+08
3.481E+08
P (GPa)
10
8
6
4
2
0
-2
-4
-6
-4
-3
-2
-1
0
1
2
3
4
ρ (g/cm³)


MATERIAL 3560
TEMP (K)
E (MJ/kg)
5
3
1
-1
-4
-3
-2
-1
0
1
2
3
4
ρ (g/cm3)
0 000E+00
2 981E+02
5 802E+03
1 160E+04
1 741E+04
2 321E+04
2 901E+04
3 481E+04
4 642E+04
5 802E+04
6 962E+04
8 123E+04
9 283E+04
1 044E+05
1 160E+05
2 500E+05
5 386E+05
1 160E+06
2 500E+06
5 386E+06
1 160E+07
2 500E+07
5 386E+07
1 160E+08
3 481E+08

SESAME #3712

Material: Aluminum
Originator: K. Trainor
Date of Origin: 1982
Type of Tables Included: 301
Limits: $10^{-3} < \rho < 10^{3}$ g/cm^3
$300 < T < 2.3 \times 10^{8}$ K

BASIC PHYSICAL DATA

$A = 26.9815$
$Z = 13$
$\rho_o = 2.7$ g/cm^3

$P(T = 300\ \mathrm{K}, \rho_o) = 1.8525 \times 10^{-4}$ GPa
$E(T = 300\ \mathrm{K}, \rho_o) = 2.4950 \times 10^{-5}$ MJ/kg
$T(P = 10^{-4}\ \mathrm{GPa}, \rho_o) = 300$ K

$T_m = 933.25$ K [Ref. 1]
* 933.2 K (used in calculation of EOS)

$T_c = 5726$ K [Ref. 2]
5220 K [Ref. 3]
* 5726 K (calulated)

$\gamma_o = 2.136$ [Ref. 4]
2.19 [Ref. 5]
* 2.136 (used in calculation of EOS)
$B_o = 73.58$ GPa [Ref. 5]
77 GPa (calculated from shock wave data) [Ref. 6]

$E_{coh} = 11.9$ MJ/kg [Ref. 5]
* 11.9 MJ/kg (used in calculation of EOS)

$\Theta_D = 423 \pm 5$ K [Ref. 5]

Hugoniot Fit: $U_S = 5.386 + 1.339\ U_p$ km/s [Ref. 7]

* $U_S = 5.35 + 1.375\, U_p + 0.0118\, U_p^2 + 1.8 \times 10^{-4}\, U_p^3$ km/s [Ref. 8]
(used in calculation of EOS)

DESCRIPTION OF PHYSICS

The purpose of constructing this equation of state was to create a wide-range table incorporating the best possible physical theories that would match available experimental data. Seven different EOS models were used:

1) rigorous electron band theory based on the self-consistent, augmented plane wave (APW) method for the zero-kelvin isotherm in compression,

2) semi-empirical Grüneisen-Debye model for the multiphase (solid-melt-liquid) region at densities from normal density to two-fold compressed,

3) Thomas-Fermi-Kirzhnits theory with nuclear corrections for the rest of the compression EOS (TFNUC),

4) semi-empirical soft-sphere model for liquid metals at low temperatures below liquid density,

5) rigorous quantum-statistical-mechanical theory based on a many-body perturbation expansion (ACTEX) for the high-temperature ionization equilibrium region,

6) Saha model based on the Planck-Larkin partition function (OCCIPITAL) for the

moderate-temperature ionization equilibrium region, and

7) liquid metal perturbation theory generalized to account for electronic excitation of conduction and core electrons.

The composite pressure and energy surfaces were constructed by joining the separate EOS subsurfaces along the boundaries shown in Fig. 3. In some cases, there were mismatches between adjacent theories, and numerical interpolation was necessary to smoothly join two subsurfaces.

This aluminum EOS has a theoretical melting transition based on the Lindemann law, which matches experiments measuring melting temperature as a function of pressure (up to 6 GPa). The two-phase region in expansion has a Maxwell construction (not van der Waals loops).

Experimental data are reproduced well. Experiments which have been compared with this EOS include principal and porous Hugoniot experiments, isobaric data, and compressibility data. Also R. G. McQueen (Group M-6, Los Alamos National Laboratory) has measured the point on the Hugoniot at which melt occurs is between 110 and 120 GPa. This EOS predicts that melting occurs at 130 GPa on the Hugoniot.

The thermodynamic consistency of this EOS is good everywhere except in the interpolation areas.

REFERENCES

1. R. Hultgren, P. D. Desai, D. T. Hawkins, M. Gleiser, K. K. Kelley, and D. D. Wagman, Selected Values of the Thermodynamic Properties of the Elements (American Society for Metals, Metals Park, Ohio, 1973).
2. D. A. Young, "A Soft-Sphere Model for Liquid Metals," Lawrence Livermore National Laboratory report UCRL-52352 (1977).
3. M. M. Martynyuk, Russ. J. of Phys. Chem. 51 (5), 705 (1977).
4. J. Ramakrishnan, R. Boehler, G. H. Higgins, and G. C. Kennedy, J. Geophys. Res. 83 (B7), 3535 (1978).
5. K. A. Gschneidner, Jr., Solid State Physics 16, 275 (1964).
6. M. van Thiel, "Compendium of Shock Wave Data," Lawrence Livermore Laboratory report UCRL-50108, Rev. 1 (1977).
7. A. C. Mitchell and W. J. Nellis, J. Appl. Phys. 52 (5), 3363 (1981).
8. S. P. Marsh, LASL Shock Hugoniot Data (University of California Press, Berkeley, 1980).
9. A complete description of this EOS is given in K. Trainor, "A New Full-Range Equation of State for Aluminum," in H-Division Quarterly Report (April through June 1982), Lawrence Livermore National Laboratory report UCID-18574-82-2 (1982), p. 20.

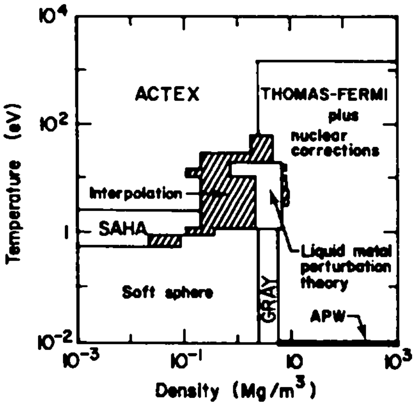
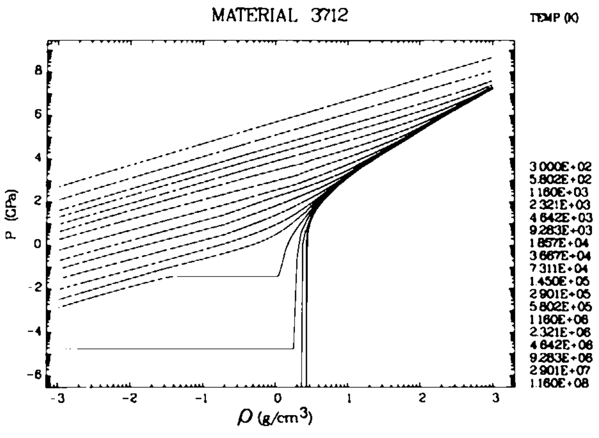
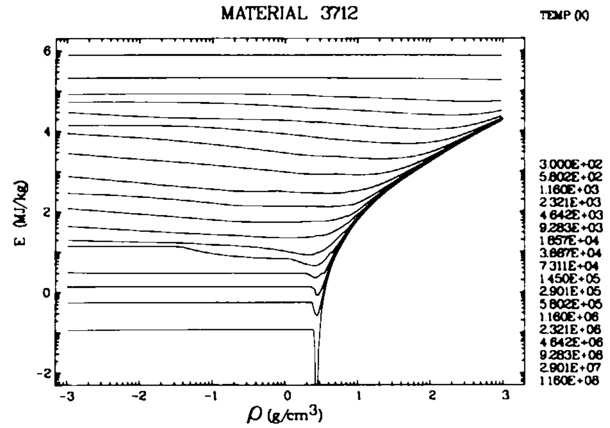


Fig. 3. Temperature-density plot showing the subregions covered by each of the theory codes used to calculate the EOS for aluminum. The shaded area is the region in which numerical intepolation was required to smoothly join two EOS subsurfaces.


MATERIAL 3712
TEMP (K)
3.000E+02
5.802E+02
1.160E+03
2.321E+03
4.642E+03
9.283E+03
1.857E+04
3.667E+04
7.311E+04
1.450E+05
2.901E+05
5.802E+05
1.160E+06
2.321E+06
4.642E+06
9.283E+06
2.901E+07
1.160E+08
P (GPa)
8
6
4
2
0
-2
-4
-6
-3
-2
-1
0
1
2
3
ρ (g/cm3)



MATERIAL 3712

SESAME #3713

Material: Aluminum
Originator: K. Trainor
Date of Origin: March 1983
Type of Tables Included: 301, 303, 304, 305,
306
Limits: $2.7 < \rho < 100\ \mathrm{g/cm^3}$
$0 < T < 1.16 \times 10^6\ \mathrm{K}$

BASIC PHYSICAL DATA

$A = 26.9815$
$Z = 13$
$\rho_o = 2.7\ \mathrm{g/cm^3}$

$P(T = 298.15\ \mathrm{K},\ \rho_o) = -1.9\ \mathrm{GPa}$
$E(T = 298.15\ \mathrm{K},\ \rho_o) = 0.3567\ \mathrm{MJ/kg}$
$T(P = 10^{-6}\ \mathrm{GPa},\ \rho_o) = 1145.8\ \mathrm{K}$

$T_m = 933.25$ K [Ref. 1]
* 933.5 K (used in calculation of EOS)

No value for T_c is included since this EOS only covers compression.

$\gamma_o = 2.136$ [Ref. 2]
2.19 [Ref. 3]
* 0.76 (result of EOS calculation)

$B_o = 73.58$ GPa [Ref. 3]
77 GPa (calculated from shock wave data) [Ref. 4]
* 82.02 GPa (result of EOS calculation)

$E_{coh} = 11.9$ MJ/kg [Ref. 3]

$\theta_D = 423 \pm 5$ K [Ref. 3]

Hugoniot Fit: $U_S = 5.386 + 1.339\ U_p$ km/s
[Ref. 5]
$U_S = 5.35 + 1.34\ U_p$ km/s
[Ref. 6]
(No Hugoniot fit was explicitly used in the calculation of this EOS.)

DESCRIPTION OF PHYSICS

This equation of state for aluminum was generated along with equations of state for copper (#3332) and molybdenum (#2983) for the purpose of evaluating high-pressure, impedance-matching Hugoniot experiments. The goal was to calculate a set of EOS tables based on a consistent set of physical models.

The zero-kelvin isotherm was calculated by A. McMahan (Lawrence Livermore National Laboratory) with rigorous band theory based on the self-consistent, augmented plane wave (APW) method.

The thermal electronic part of the EOS was generated with D. Liberman's self-consistent field model for condensed matter (INFERNO). This model solves the Dirac equation for an atom embedded in an electron gas. Unlike equations of state based on Thomas-Fermi-Dirac theory, INFERNO thermodynamic surfaces exhibit shell structure effects.

The thermal nuclear contribution to the EOS was calculated with the Dugdale-MacDonald form of Grüneisen-Debye theory. Grüneisen gamma is derived from the cold curve according to the following formula:

$$\gamma(V) = -\frac{1}{6} - \frac{1}{2}\left[\left(\frac{d\ \ell n\ B}{d\ \ell n\ V} + \frac{2}{3}\right)/\left(1 - \frac{2P}{3B}\right)\right] \quad .$$

where B is bulk modulus, V is volume, and P is pressure. Note that gamma is a function of density only, not temperature.

At pressures below 200 GPa, the Hugoniot that this EOS predicts is a little soft compared with Hugoniot experiments. Above that pressure, it matches the data well.

Note that only compression is covered by this EOS since it was intended for analysis of Hugoniot experiments.

The EOS is thermodynamically consistent everywhere.

REFERENCES

1. R. Hultgren, P. D. Desai, D. T. Hawkins, M. Gleiser, K. K. Kelley, and D. D. Wagman, Selected Values of the Thermodynamic Properties of the Elements (American Society for Metals, Metals Park, Ohio, 1973).

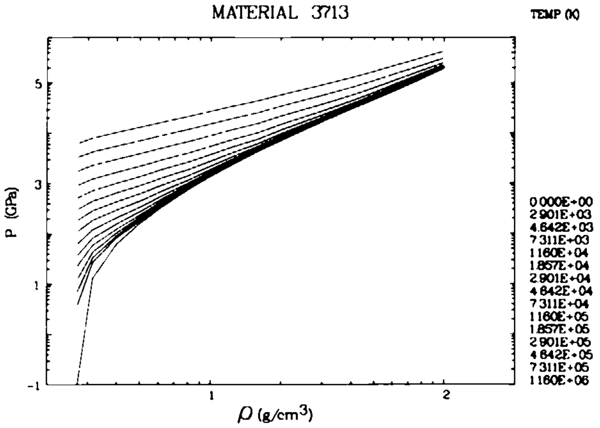
2. J. Ramakrishnan, R. Boehler, G. H. Higgins, and G. C. Kennedy, J. Geophys. Res. 83 (B7), 3535 (1978).

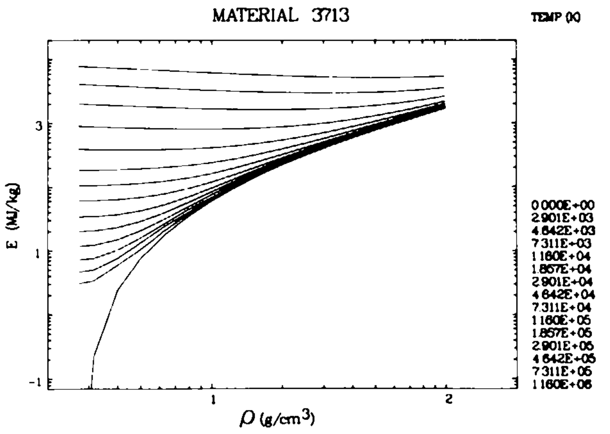
3. K. A. Gschneidner, Jr., Solid State Physics 16, 275 (1964).

4. M. van Thiel, "Compendium of Shock Wave Data," Lawrence Livermore Laboratory report UCRL-50108, Rev. 1 (1977).

5. A. C. Mitchell and W. J. Nellis, J. Appl. Phys. 32 (5), 3363 (1981).

6. S. P. Marsh, LASL Shock Hugoniot Data (University of California Press, Berkeley, 1980).


MATERIAL 3713
TEMP (K)
P (GPa)
5
3
1
-1
1
2
ρ (g/cm^3)
0.000E+00
2.901E+03
4.642E+03
7.311E+03
1.160E+04
1.857E+04
2.901E+04
4.642E+04
7.311E+04
1.160E+05
1.857E+05
2.901E+05
4.642E+05
7.311E+05
1.160E+06


MATERIAL 3713
TEMP (K)
E (MJ/kg)
3
1
-1
1
2
ρ (g/cm³)
0 000E+00
2 901E+03
4 642E+03
7 311E+03
1 160E+04
1 857E+04
2 901E+04
4 642E+04
7 311E+04
1 160E+05
1 857E+05
2 901E+05
4 642E+05
7 311E+05
1 160E+06

SESAME #3730

Material: Platinum
Originator: J. Barnes and J. Rood
Date of Origin: October 1972
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho < 2.1419 \times 10^4$ g/cm^3
$0 < T < 3.7 \times 10^8$ K

BASIC PHYSICAL DATA

$A = 195.09$
$Z = 78$
$\rho_o = 21.419$ g/cm^3

$P(T = 298.15\ \text{K}, \rho_o) = 1.2114$ GPa
$E(T = 298.15\ \text{K}, \rho_o) = 2.7909 \times 10^{-2}$ MJ/kg
$T(P = 10^{-6}\ \text{GPa}, \rho_o) = 2.48 \times 10^{-4}$ K

$T_m = 2042$ K [Ref. 1]

$T_c = 14650$ K [Ref. 2]
* 13704 K (calculated)

$\gamma_o = 2.92$ [Ref. 1]
2.56 (average of values in literature) [Ref. 1]
* 2.035 (calculated)

$B_o = 283.8$ GPa [Ref. 1]
249.2 GPa (calculated from shock wave data) [Ref. 3]
* 282.2 GPa (used in calculation of EOS)

$E_{coh} = 2.891$ MJ/kg [Ref. 1]
* 2.616 MJ/kg (used in calculation of EOS)

Θ_D = 234 K [Ref. 1]
* 240 K (used in calculation of EOS)

Hugoniot Fit: $U_S = 3.68 + 1.46\ U_p$ km/s [Ref. 4]
$U_S = 3.605 + 1.56\ U_p - 2.63 \times 10^{-3}\ U_p^2$ km/s [Ref. 5]

DESCRIPTION OF PHYSICS

Above 1 eV, a MAPLE table for platinum was scaled to match the reference density and atomic weight used. Below 1 eV, the code MAXWELL computed the EOS using a modified-Morse model for the zero-kelvin contributions to pressure and energy and a Debye model for the nuclear thermal contributions. (See Part II for a detailed description of this method of EOS generation.)

The experimental zero-pressure density and bulk modulus are reproduced by this EOS, and the comparison with experimental Hugoniot data is good. However, this EOS was not generally intended for the hot, expanded liquid metal region and is not to be trusted there.

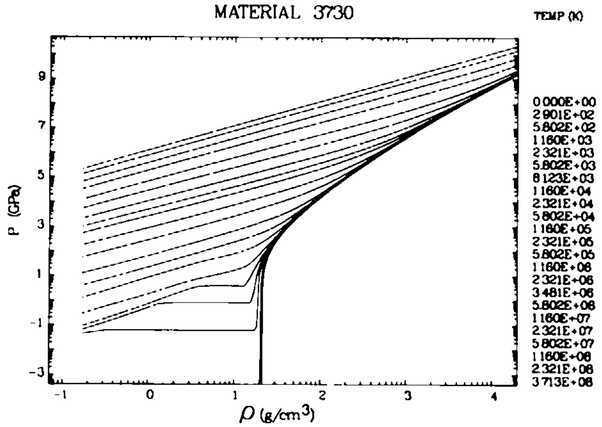
No melting transition is included in this table.

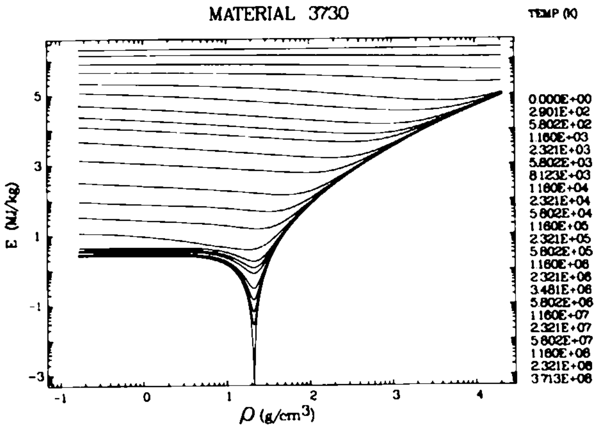
Thermodynamic consistency is good everywhere.

The two-temperature tables for this EOS were derived by the code TWOTEMP and are noisy.

REFERENCES

1. K. A. Gschneidner, Jr., Solid State Physics 16, 275 (1964).
2. D. A. Young and B. J. Alder, Phys. Rev. A 3 (1), 364 (1971).
3. M. van Thiel, "Compendium of Shock Wave Data," Lawrence Livermore Laboratory report UCRL-50108, Rev. 1 (1977).
4. S. P. Marsh, LASL Shock Hugoniot Data (University of California Press, Berkeley, 1980).
5. L. V. Al'tshuler, A. A. Bakanova, I. P. Dudoladov, E. A. Dynin, R. F. Trunin, and B. S. Chekin, Zhurnal Prikladnoi Mekhaniki i Teknicheskoi Fiziki 2, 3 (1981) [Sov. Phys. JAMTP 22 (2), 195 (1981)].


MATERIAL 3730
TEMP (K)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08
P (GPa)
9
7
5
3
1
-1
-3
ρ (g/cm3)
-1
0
1
2
3
4


MATERIAL 3730
TEMP (K)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08
E (MJ/kg)
5
3
1
-1
-3
-1
0
1
2
3
4
ρ (g/cm3)

SESAME #4100

Material: Brass
Composition: Cu 61.5 wt% or 63.237 at%
Zn 36.0 wt% or 35.975 at%
Pb 2.5 wt% or 0.788 at%
Originators: J. Barnes and A. Lindstrom
Date of Origin: May 1976
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $6.6016 \times 10^{-2} < \rho < 1.69 \times 10^{5}$ g/cm^3
$0 < T < 3.7 \times 10^{8}$ K

BASIC PHYSICAL DATA

$\bar{A} = 65.334$
$\bar{Z} = 29.777$
$\rho_o = 8.45$ g/cm^3

$P(T = 298.15\text{ K}, \rho_o) = 1.4327$ GPa
$E(T = 298.15\text{ K}, \rho_o) = 7.3038 \times 10^{-2}$ MJ/kg
$T(P = 10^{-6}\text{ GPa}, \rho_o) = 2.1 \times 10^{-4}$ K

$T_m = 1205$ K [Ref. 1]

$T_c =$ * 4642 K (calculated)

$B_o = 138.9$ GPa [Ref. 1]
* 100 GPa (used in calculation)

$E_{coh} =$ * 4.04 MJ/kg (used in calculation)

$\theta_D =$ * 335 K (used in calculation)

Hugoniot Fit: $U_S = 3.74 + 1.43\, U_p$ km/s
[Ref. 2]

DESCRIPTION OF PHYSICS

Above 1 eV, the brass EOS was calculated by mixing copper (SESAME #3330), zinc (a scaled SESAME #3330), and lead equations of state according to the number fractions given under composition. Below 1 eV, the code MAXWELL computed the EOS using a modified-Morse model for the zero-kelvin contributions to pressure and energy and a Debye model for the nuclear thermal contributions. (See Part II for a detailed description of this method of EOS generation.)

This EOS matches the experimental Hugoniot data well, but a low value of the bulk modulus was necessary to force a good match between theory and experiment.

This EOS was not generally intended for the hot, expanded liquid metal region and is not to be trusted there.

No melting transition was included in this EOS.

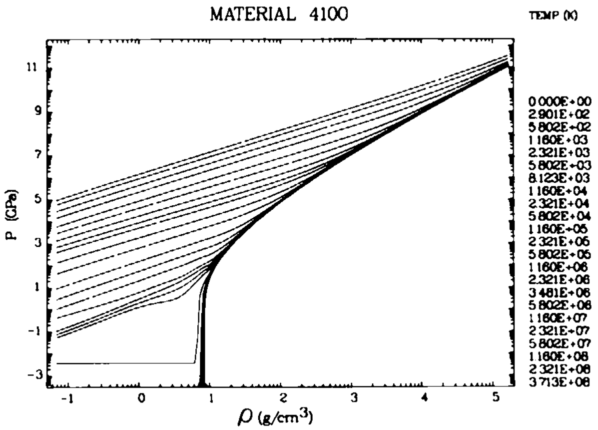
Thermodynamic consistency is good everywhere.

Two temperature tables for this EOS were derived from the code TWOTEMP and are noisy.

REFERENCES

1. Handbook of Chemistry and Physics, R. C. Weast, Ed. (CRC Press, Cleveland, Ohio, 1976).

2. S. P. Marsh, LASL Shock Hugoniot Data (University of California Press, Berkeley, 1980).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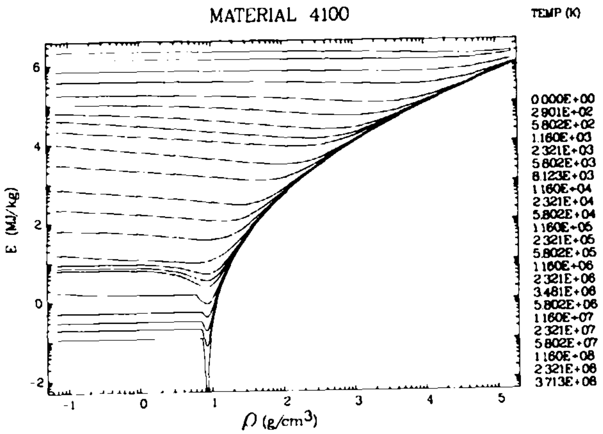
TEMP (K)
P (GPa)
11
9
7
5
3
1
-1
-3
-1
0
1
2
3
4
5
ρ (g/cm³)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08


MATERIAL 4100
TEMP (K)
E (MJ/kg)
6
4
2
0
-2
-1
0
1
2
3
4
5
ρ (g/cm^3)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08

SESAME #4270

Material: Stainless Steel (304)
Composition: Fe 70 wt%
Cr 19 wt%
Ni 11 wt%
Originator: A. Lindstrom
Date of Origin: 1976
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $6.1688 \times 10^{-2} < \rho < 1.5792 \times 10^{5}$ g/cm^3
$0 < T < 3.7 \times 10^{8}$ K

BASIC PHYSICAL DATA

$\bar{A} = 55.365$
$\bar{Z} = 25.802$
$\rho_o = 7.896$ g/cm^3

$P(T = 298.15\ K, \rho_o) = 1.1500$ GPa
$E(T = 298.15\ K, \rho_o) = 7.1136 \times 10^{-2}$ MJ/kg
$T(P = 10^{-6}\ GPa, \rho_o) = 2.62 \times 10^{-4}$ K

$T_c = *$ 8733 K (calculated)

$B_o = *$ 164.8 GPa (used in calculation of EOS)

$E_{coh} = *$ 7.3 MJ/kg (used in calculation of EOS)

$\Theta_D = *$ 470 K (used in calculation of EOS)

Hugoniot Fit: $U_S = 4.58 + 1.49\ U_p$ km/s [Ref. 1]

DESCRIPTION OF PHYSICS

Above 1 eV, three MAPLE tables were mixed to create the EOS for stainless steel: an iron table, a lead table that was scaled to simulate nickel, and an iron table that was scaled to simulate chromium.

Below 1 eV, the code MAXWELL computed the EOS using a modified-Morse model for the zero-kelvin contributions to pressure and energy and a Debye model for the nuclear thermal contributions. (See Part II for a detailed discussion of this method of EOS generation.)

This EOS matches experimental Hugoniot data for 304 stainless steel very well. However in the hot, expanded liquid metal region, it is not to be trusted.

No melting transition was included in this EOS.

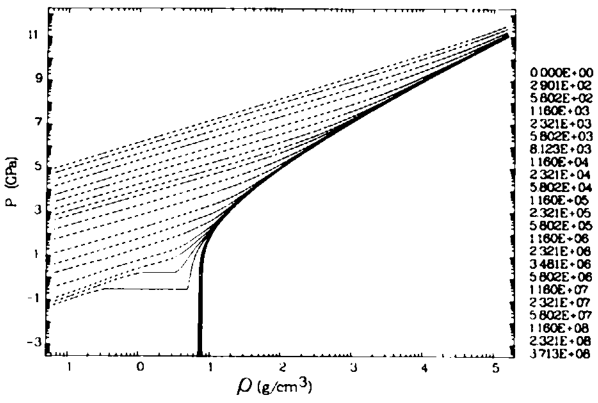
Thermodynamic consistency is good everywhere.

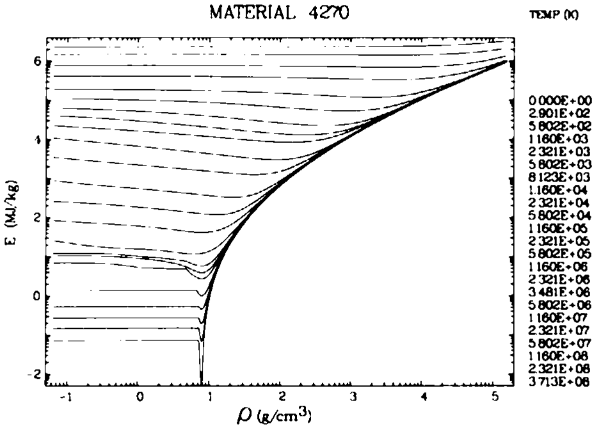
Two-temperature tables for this EOS were derived from the code TWOTEMP and are noisy.

REFERENCE

1. S. P. Marsh, LASL Shock Hugoniot Data (University of California Press, Berkeley, 1980).

MATERIAL 4270




MATERIAL 4270
TEMP (K)
E (MJ/kg)
6
4
2
0
-2
-1
0
1
2
3
4
5
ρ (g/cm3)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08

SESAME #5000

Material: Nitrogen
Composition: N_2
Originators: G. Kerley and J. Abdallah
Date of Origin: April 1981
Type of Tables Included: 301
Limits: $10^{-8} < \rho < 10^{4}$ g/cm^3
$0 < T < 10^{8}$ K

BASIC PHYSICAL DATA

$A = 14.0067$
$Z = 7$
$\rho_o = 0.85719$ g/cm^3

$P(T = 298.15\ \mathrm{K}, \rho_o) = 0.34730$ GPa
$E(T = 298.15\ \mathrm{K}, \rho_o) = 0.24689$ MJ/kg
$T(P = 10^{-6}\ \mathrm{GPa}, \rho_o) = 63.149$ K

$T_m = 63$ K [Ref. 1]

$T_c = 126$ K [Ref. 2]
$= 132$ K (calculated)

Binding Energy: 0.2472 MJ/kg [Ref. 3]
= 0.246 MJ/kg (calculated)

Hugoniot Fit: $U_S = 1.49 + 1.49\ U_p$ km/s
(for $2.3 < U_S < 7.4$ km/s)
$U_S = -1.0 + 2.0\ U_p$ km/s
(for $7.4 < U_S < 8.4$ km/s)
[Ref. 4]
$U_S = 4.06 + 0.92\ U_p$ km/s
(for $8.4 < U_S < 9.0$ km/s)

DESCRIPTION OF PHYSICS

The nitrogen EOS[5] was generated in response to a need for thermodynamic properties to be used in numerical modeling of detonations.

The fluid part of the nitrogen equation of state was calculated with the CRIS model, a thermodynamic perturbation theory in which the intermolecular forces are determined from the cold curve of the solid. The cold curve is described by a semi-empirical functional form in which certain parameters may be adjusted to fit experimental data for the liquid. The cold curve formulation includes effects of coupling among vibrational, rotational, and translational motions.

A crude model for the solid uses the same cold curve as that used in the CRIS model. However, it does not account for phase transitions associated with rotational ordering in the crystalline state. The melting transition was included in this EOS by calculating separate surfaces using the solid and liquid models and then finding the point at which the solid and liquid pressures and Gibbs free energies matched along each isotherm. Agreement of the melting curve with experimental data is fairly good.

This EOS does not include effects of molecular dissociation or electronic excitation, so it should not be completely believed at temperatures above where these effects start to become important (> 1 eV). Higher temperature isotherms were included mainly to prevent extrapolation problems. The theoretical EOS was compared with many different kinds of experiments: vaporization and critical point data, P-V-T data, and Hugoniot experiments. In general, agreement was very good. However, for particle velocities greater than 6.0 km/s, the theoretical Hugoniot was stiffer than experiments. This discrepancy is probably due to the increasing importance of dissociation at higher pressures.

REFERENCES

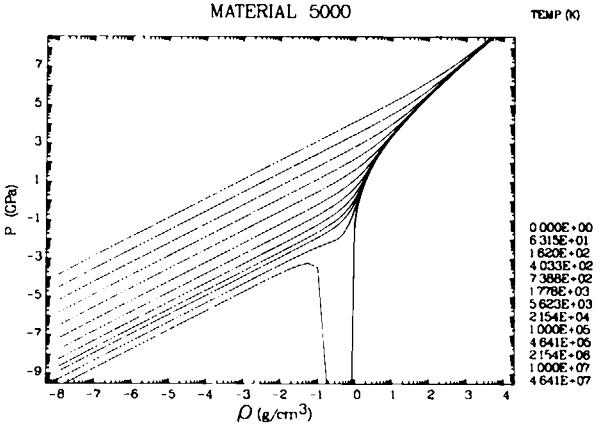
1. Sargent-Welch Periodic Table of the Elements (1968).

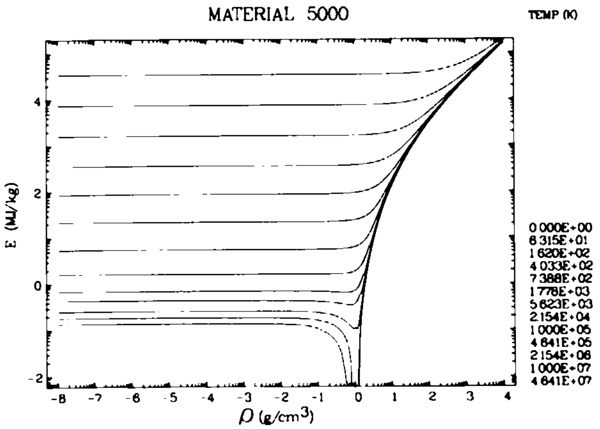
2. E. W. Washburn, International Critical Tables (McGraw-Hill, New York, 1926).

3. T. A. Scott, Phys. Lett. C 27, 90 (1976).

4. M. van Thiel, "Compendium of Shock Wave Data," Lawrence Livermore Laboratory report UCRL-50108, Rev. 1 (1977).

5. A complete description of the nitrogen EOS is contained in G. I. Kerley and J. Abdallah, Jr., J. Chem. Phys. 73 (10), 5337 (1980).


MATERIAL 5000
TEMP (K)
P (GPa)
7
5
3
1
-1
-3
-5
-7
-9
-8
-7
-6
-5
-4
-3
-2
-1
0
1
2
3
4
ρ (g/cm3)
0.000E+00
6.315E+01
1.620E+02
4.033E+02
7.388E+02
1.778E+03
5.623E+03
2.154E+04
1.000E+05
4.641E+05
2.154E+06
1.000E+07
4.641E+07


MATERIAL 5000
TEMP (K)
E (MJ/kg)
4
2
0
-2
-8
-7
-6
-5
-4
-3
-2
-1
0
1
2
3
4
ρ (g/cm3)
0 000E+00
6 315E+01
1 620E+02
4 033E+02
7 388E+02
1 778E+03
5 623E+03
2 154E+04
1 000E+05
4 641E+05
2 154E+06
1 000E+07
4 641E+07

SESAME #5001

Material: Nitrogen
Composition: N_2
Originator: National Bureau of Standards
Date of Origin: March 1982
Type of Tables Included: 301
Limits: $6.7125 \times 10^{-5} < \rho < 0.94015$ g/cm^3
$63.15 < T < 1.9 \times 10^3$ K

BASIC PHYSICAL DATA

$\bar{A} = 14.007$
$\bar{Z} = 7$
$\rho_o = 0.86778$ g/cm^3

$P(T = 298.15\ \mathrm{K}, \rho_o) = 0.38599$ GPa
$E(T = 298.15\ \mathrm{K}, \rho_o) = 9.9268 \times 10^{-2}$ MJ/kg
$T(P = 10^{-4}\ \mathrm{GPa}, \rho_o) = 63.18$ K

$T_m = 63$ K [Ref. 1]

$T_c = 126$ K [Ref. 2]
* 126.26 K (input)
$P_c = 3.39 \times 10^{-3}$ GPa [Ref. 2]
* 3.410034×10^{-3} GPa (calculated)
$\rho_c = 0.31096$ g/cm^3 [Ref. 2]
* 0.314 g/cm^3 (input)

Triple Point Temperature: 63.148 K [Ref. 3]
* 63.15 K (input)
Triple Point Pressure: * 1.246399×10^{-5} GPa (calculated)
Triple Point Density-Vapor: * 6.71247×10^{-3} g/cm^3 (calculated)
Triple Point Density-Liquid: * 8.67776×10^{-1} g/cm^3 (calculated)

DESCRIPTION OF PHYSICS

This nitrogen equation of state was calculated from a series of computer routines developed by the National Bureau of Standards which describe thermodynamic and transport properties of selected cryogens [Ref. 4]. The computer codes describe properties for gaseous and liquid states starting at the triple point. All of the properties are calculated from empirical equations which are derived from existing experimental data by a weighted least squares fit of mathematical models to those data. The uncertainty in the calculated pressure is 5% or less for the liquid at temperatures below the critical temperature and 0.3% everywhere else.

Beware that, although this EOS is very accurate, the temperature and density limits are restricted.

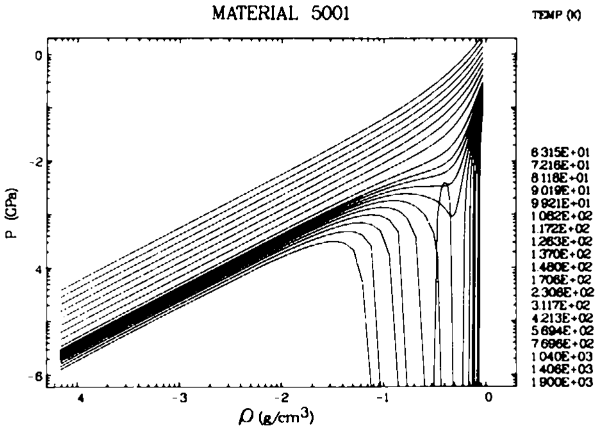
REFERENCES

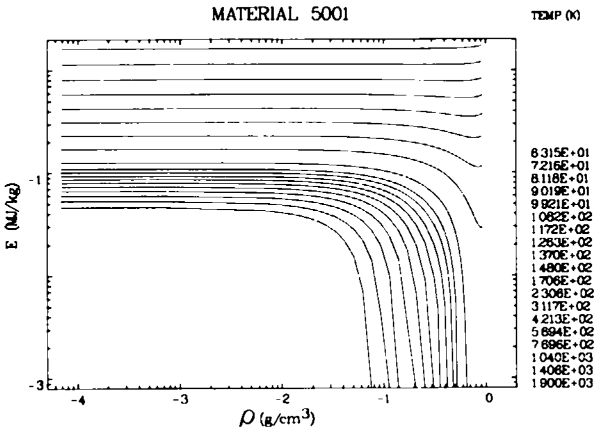
1. Sargent-Welch Periodic Table of the Elements (1968).

2. E. W. Washburn, International Critical Tables (McGraw-Hill, New York, 1926).

3. T. A. Scott, Phys. Lett. C 27, 90 (1976).

4. R. D. McCarty, "Interactive FORTRAN IV Programs for the Thermodynamic and Transport Properties of Selected Cryogens (Fluids Pack)," National Bureau of Standards Technical Note 1025 (October 1980).


MATERIAL 5001
TEMP (K)
P (GPa)
0
-2
4
-6
4
-3
-2
-1
0
ρ (g/cm^3)
6.315E+01
7.216E+01
8.118E+01
9.019E+01
9.921E+01
1.082E+02
1.172E+02
1.263E+02
1.370E+02
1.480E+02
1.706E+02
2.308E+02
3.117E+02
4.213E+02
5.694E+02
7.696E+02
1.040E+03
1.406E+03
1.900E+03


MATERIAL 5001
TEMP (K)
E (MJ/kg)
-1
-3
-4
-3
-2
-1
0
ρ (g/cm^3)
6.315E+01
7.216E+01
8.118E+01
9.019E+01
9.921E+01
1.082E+02
1.172E+02
1.263E+02
1.370E+02
1.480E+02
1.706E+02
2.306E+02
3.117E+02
4.213E+02
5.694E+02
7.696E+02
1.040E+03
1.406E+03
1.900E+03

SESAME #5010

Material: Oxygen [Ref. 1]
Composition: O_2
Originator: G. Kerley and J. Abdallah
Date of Origin: April 1981
Type of Tables Included: 301
Limits: $10^{-8} < \rho < 10^{4}$ g/cm^3
$0 < T < 10^{8}$ K

BASIC PHYSICAL DATA

$\bar{A} = 16.0$
$\bar{Z} = 8$
$\rho_o = 1.262$ g/cm^3

$P(T = 298.15\ K, \rho_o) = 0.54339$ GPa
$E(T = 298.15\ K, \rho_o) = 0.2390$ MJ/kg
$T(P = 10^{-6}\ GPa, \rho_o) = 54.39$ K

$T_m = 54.35$ K [Ref. 2]

$T_c = 154$ K [Ref. 3]
* 162.2 K (calculated)

Binding Energy: 0.2709 MJ/kg [Ref. 4]
* 0.266 MJ/kg (used in calculation of EOS)

Hugoniot Fit: $U_s = 1.171 + 1.788\ U_p - 0.6709\ U_p^2$ km/s [Ref. 5]
(for liquid oxygen at 76.9 K)

DESCRIPTION OF PHYSICS

The oxygen EOS was generated in response to a need for thermodynamic properties to be used in numerical modeling of detonations.

The fluid part of the oxygen equation of state was calculated with the CRIS model, a thermodynamic perturbation theory in which the intermolecular forces are determined from the cold curve of the solid. The cold curve is based on a semi-empirical functional form in which certain parameters may be adjusted in order to fit experimental data for the liquid. The cold curve formulation includes effects of coupling among vibrational, rotational, and translational motions.

A crude model for the solid uses the same cold curve as that for the CRIS model. However, it does not account for phase transitions associated with rotational ordering in the crystalline state. The melting curve for oxygen was determined by finding where the pressures and Gibbs free energies of the solid and liquid phases match at each temperature. Agreement of this melting curve with experimental data is fairly good.

This EOS does not include effects of molecular dissociation or electronic excitation, so it should not be entirely believed at temperatures above the point at which these effects start to become important (> 1 eV). Higher temperature isotherms were included to prevent extrapolation problems.

The theoretical EOS was compared with many different kinds of experimental measurements: vapor-liquid coexistence curve, critical point, static compression data, internal energies, and Hugoniots.

The general agreement with the data was very good. However, at particle velocities greater than 4.0 km/s, the theoretical Hugoniot is stiffer than the experiments. Ths discrepancy is probably due to the increasing importance of dissociation at higher pressures. Also, the experimentally measured isotherm at 51 K (solid phase) disagrees with calculations.

REFERENCES

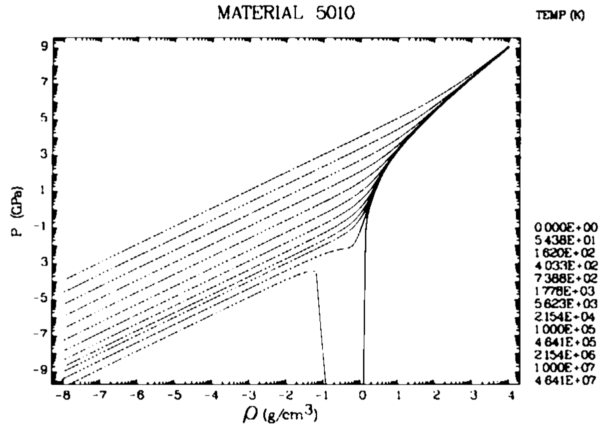
1. A complete description of the oxygen EOS is contained in G. I. Kerley and J. Abdallah, Jr., J. Chem. Phys. 73 (10), 5337 (1980).

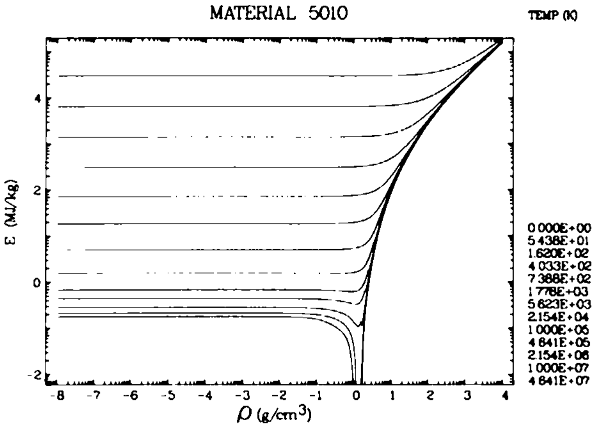
2. Sargent-Welch Periodic Table of the Elements (1968).

3. E. W. Washburn, International Critical Tables (McGraw-Hill, New York, 1926).

4. G. E. Jelinek, L. J. Slutsky and A. M. Karo, J. Phys. Chem. Solids 33, 1279 (1972).

5. M. van Thiel, "Compendium of Shock Wave Data," Lawrence Livermore Laboratory report UCRL-50108, Rev. 1 (1977).


MATERIAL 5010
TEMP (K)
P (GPa)
9
7
5
3
1
-1
-3
-5
-7
-9
-8
-7
-6
-5
-4
-3
-2
-1
0
1
2
3
4
ρ (g/cm³)
0 000E+00
5 438E+01
1 620E+02
4 033E+02
7 388E+02
1 778E+03
5 623E+03
2 154E+04
1 000E+05
4 641E+05
2 154E+06
1 000E+07
4 641E+07


MATERIAL 5010
TEMP (K)
ε (MJ/kg)
4
2
0
-2
-8
-7
-6
-5
-4
-3
-2
-1
0
1
2
3
4
ρ (g/cm3)
0 000E+00
5 438E+01
1.620E+02
4 033E+02
7 388E+02
1 778E+03
5 623E+03
2.154E+04
1 000E+05
4 641E+05
2.154E+06
1 000E+07
4 641E+07

SESAME #5011

Material: Oxygen
Composition: O_2
Originator: National Bureau of Standards
Date of Origin: March 1982
Type of Tables Included: 301
Limits: $1.0481 \times 10^{-7} < \rho < 1.4169$ g/cm^3
54.36 K $< T < 400$ K

BASIC PHYSICAL DATA

$\bar{A} = 15.9994$
$\bar{Z} = 8$
$\rho_o = 1.3062$ g/cm^3

$P(T = 298.15\text{ K}, \rho_o) = 0.58147$ GPa
$E(T = 298.15\text{ K}, \rho_o) = 5.8010 \times 10^{-2}$ MJ/kg
$T(P = 10^{-4}\text{ GPa}, \rho_o) = 54.38$ K

$T_m = 54.35$ K [Ref. 1]

$T_c = 154$ K [Ref. 2]
* 154.481 K (input)
$P_c = 5.04 \times 10^{-3}$ GPa [Ref. 2]
* 5.042218×10^{-3} GPa (calculated)
$\rho_c = 0.4299$ g/cm^3 [Ref. 2]
* 0.436144 g/cm^3 (input)

Triple Point Temperature: 54.38 K [Ref. 3]
* 54.359 K (input)
Triple Point Pressure: * 1.490085×10^{-7} GPa (calculated)
Triple Point Density-Vapor: * 1.04812×10^{-5} g/cm^3 (calculated)
Triple Point Density-Liquid: * 1.30619 g/cm^3 (calculated)

DESCRIPTION OF PHYSICS

This oxygen equation of state was calculated from a series of computer routines developed by the National Bureau of Standards which describe thermodynamic and transport properties of selected cryogens [Ref. 4]. The computer programs describe the properties of the gaseous and liquid states starting at the triple point. All of the properties are calculated from empirical equations which are derived from experimental data by a weighted least squares fit of mathematical models to those data. The uncertainty in the calculated pressures is 5% for the liquid at temperatures below the critical temperature, 0.25% for the gas at $T < T_c$, and 0.15% for the fluid at $T > T_c$.

Beware that, although the EOS is very accurate, the temperature and density limits are restricted.

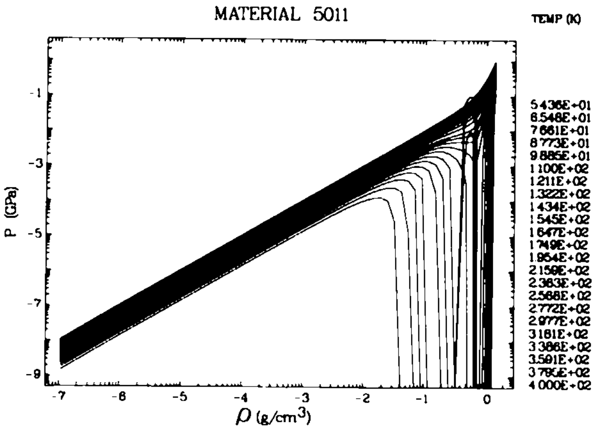
REFERENCES

1. Sargent-Welch Periodic Table of the Elements (1968).

2. E. W. Washburn, International Critical Tables (McGraw-Hill, New York, 1926).

3. R. L. Mills and E. R. Grilly, Phys. Rev. **99**, 480 (1955).

4. R. D. McCarty, "Interactive FORTRAN IV Computer Programs for the Thermodynamic and Transport Properties of Selected Cryogens (Fluids Pack)," National Bureau of Standards Technical Note 1025 (October 1980).


MATERIAL 5011
TEMP (K)
P (GPa)
-1
-3
-5
-7
-9
-7
-6
-5
-4
-3
-2
-1
0
ρ (g/cm^3)
5.436E+01
6.548E+01
7.661E+01
8.773E+01
9.885E+01
1.100E+02
1.211E+02
1.322E+02
1.434E+02
1.545E+02
1.647E+02
1.749E+02
1.954E+02
2.158E+02
2.363E+02
2.568E+02
2.772E+02
2.977E+02
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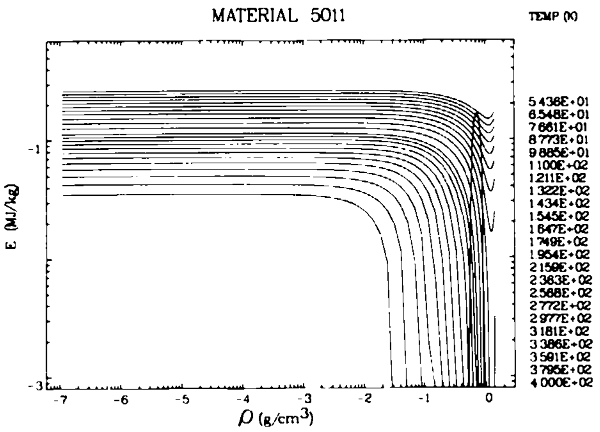
3.795E+02
4.000E+02


MATERIAL 5011
TEMP (K)
E (MJ/kg)
ρ (g/cm3)
-1
-3
-7
-6
-5
-4
-3
-2
-1
0
5 436E+01
6.548E+01
7 661E+01
8 773E+01
9 885E+01
1 100E+02
1.211E+02
1 322E+02
1 434E+02
1.545E+02
1 647E+02
1 749E+02
1.954E+02
2 159E+02
2 363E+02
2.568E+02
2 772E+02
2 977E+02
3 181E+02
3 386E+02
3 591E+02
3 795E+02
4 000E+02

SESAME #5030

Material: Dry Air [Ref. 1]
Composition: N_2 78.09 at%
O_2 20.95 at%
Ar 0.96 at%
Originator: H. Graboske (Lawrence Livermore National Laboratory)
Type of Tables Included: 301
Limits: $10^{-7} < \rho < 15$ g/cm^3
$0.015 < T < 3 \times 10^4$ eV

BASIC PHYSICAL DATA

$\bar{A} = 14.80304$
$\bar{Z} = 7.37296$
$\rho_o = 1.293 \times 10^{-3}$ g/cm^3

$P(T = 298.15\ \mathrm{K}, \rho_o) = 1.0757 \times 10^{-4}$ GPa
$E(T = 298.15\ \mathrm{K}, \rho_o) = 0.31313$ MJ/kg
$T(P = 10^{-4}\ \mathrm{GPa}, \rho_o) = 277.8$ K

DESCRIPTION OF PHYSICS

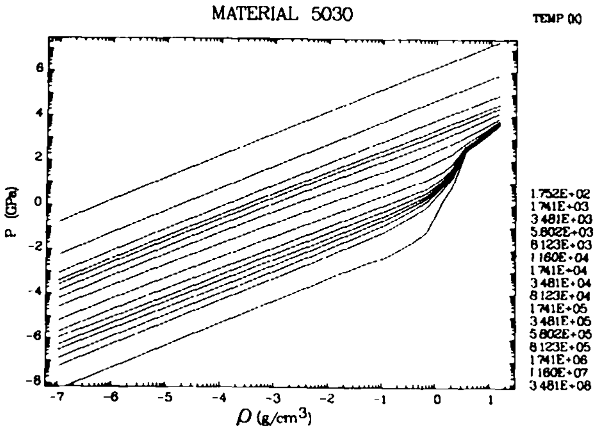
The low-density region of the EOS for air was calculated with a Lawrence Livermore National Laboratory code called FMIN which is based on a free energy Coulomb perturbation expansion. Full molecular physics is included in the form of vibrational-rotational coupling corrections. The equation of state in this region agrees excellently with the National Bureau of Standards theoretical molecular EOS. The high-density region is treated with a computer code which uses Thomas-Fermi physics to describe the electrons and includes temperature-dependent exchange and correlation effects. The nuclear contribution is a Monte Carlo-based ion fluid which goes to a Debye solid in the high-density limit. Numerical interpolation was used to smoothly join the two different physical models.

Thermodynamic consistency is good everywhere in this EOS.

Three Hugoniot experiments have been performed on air by W. J. Nellis, et al. at Lawrence Livermore National Laboratory. The theoretical EOS is in very poor agreement with the highest pressure experiment (70 GPa).

REFERENCE

1. A complete description of this EOS is given in H. C. Graboske, "A New EOS for Air," Lawrence Livermore Laboratory internal document UCID-16901 (1976).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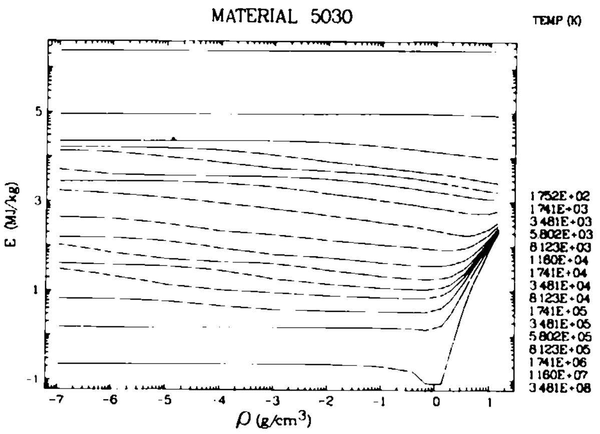
TEMP (K)
P (GPa)
6
4
2
0
-2
-4
-6
-8
-7
-6
-5
-4
-3
-2
-1
0
1
ρ (g/cm3)
1.752E+02
1.741E+03
3.481E+03
5.802E+03
8.123E+03
1.160E+04
1.741E+04
3.481E+04
8.123E+04
1.741E+05
3.481E+05
5.802E+05
8.123E+05
1.741E+06
1.160E+07
3.481E+08


MATERIAL 5030
TEMP (K)
E (MJ/kg)
5
3
1
-1
-7
-6
-5
-4
-3
-2
-1
0
1
ρ (g/cm³)
1.752E+02
1.741E+03
3.481E+03
5.802E+03
8.123E+03
1.160E+04
1.741E+04
3.481E+04
8.123E+04
1.741E+05
3.481E+05
5.802E+05
8.123E+05
1.741E+06
1.160E+07
3.481E+08

SESAME #5171

Material: Argon [Ref. 1]
Composition: Ar
Originator: National Bureau of Standards
Date of Origin: 1969
Type of Tables Included: 301
Limits: $4.0563 \times 10^{-3} < \rho < 1.5587$ g/cm^3
83.8 K $< T < 400$ K

BASIC PHYSICAL DATA

$A = 39.948$
$Z = 18$
$\rho_o = 1.4142$ g/cm^3

$P(T = 298.15 \text{ K}, \rho_o) = 0.26796$ GPa
$E(T = 298.15 \text{ K}, \rho_o) = 0.17902$ GPa
$T(P = 10^{-4} \text{ GPa}, \rho_o) = 83.81$ K

$T_m = 83.75$ K [Ref. 2]

$T_c = 151$ K [Ref. 3]
* 150.86 K (input)
$P_c = 5.0 \times 10^{-3}$ GPa [Ref. 3]
* 4.89805×10^{-3} GPa (calculated)
$\rho_c = 0.536$ g/cm^3 [Ref. 3]
* 0.5357 g/cm^3 (input)

Triple Point Temperature: * 83.80 K (input)
Triple Point Pressure: * 6.890708×10^{-5} GPa (calculated)
Triple Point Density-Vapor: * 4.0563×10^{-3} g/cm^3 (calculated)
Triple Point Density-Liquid: * 1.4142 g/cm^3 (calculated)

DESCRIPTION OF PHYSICS

This argon equation of state was calculated from a series of computer routines developed by the National Bureau of Standards which describe thermodynamic and transport properties of selected cryogens [Ref. 1]. The computer programs contain analytic equations which describe the EOS for both the liquid and vapor phases. The analytic equations are empirical; they are fits to experimental data. In general, the equation of state represents the different sources of experimental data to within the accuracy of the data except in the region of the critical point. The types of data which were taken into consideration for the analytic EOS were P-V-T data, vapor pressure data, and coexistence density data. The uncertainty in the calculated pressures is 10% for the liquid at temperatures below the critical temperature and 0.3% everywhere else.

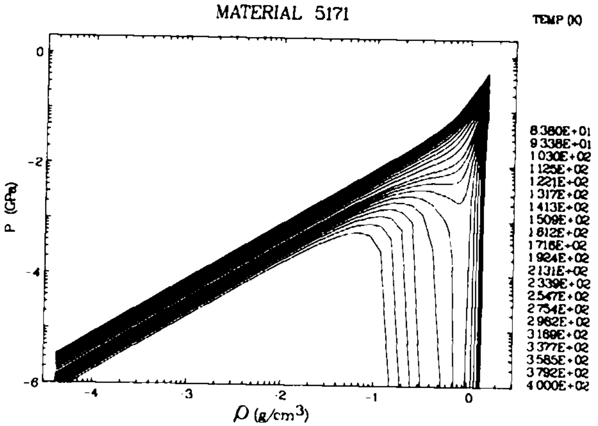
Beware that, although the EOS is very accurate, the temperature and density limits are restricted.

REFERENCES

1. A complete description of the argon EOS is given in A. L. Gosman, R. D. McCarty, and J. G. Hust, "Thermodynamic Properties of Argon from the Triple Point to 300K at Pressures to 1000 Atmospheres," National Standard Reference Data Series - National Bureau of Standards 27 (March, 1969).

2. Sargent-Welch Periodic Table of the Elements (1968).

3. N. B. Vargaftik, Tables on the Thermophysical Properties of Liquids and Gases 2nd Ed. (John Wiley and Sons, New York, 1975).


MATERIAL 5171
TEMP (K)
0
-2
-4
-6
P (GPa)
-4
-3
-2
-1
0
ρ (g/cm^3)
8.380E+01
9.338E+01
1.030E+02
1.125E+02
1.221E+02
1.317E+02
1.413E+02
1.509E+02
1.612E+02
1.716E+02
1.924E+02
2.131E+02
2.339E+02
2.547E+02
2.754E+02
2.962E+02
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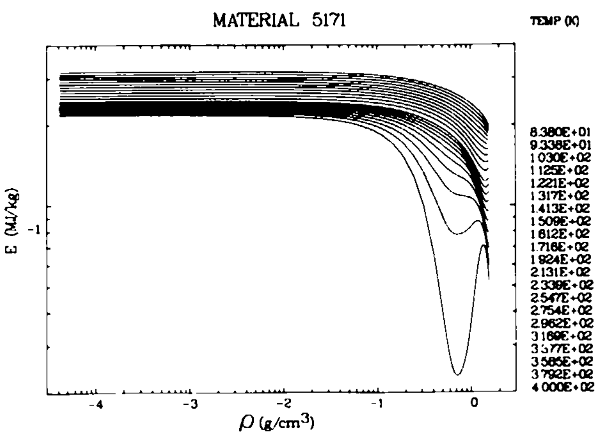
3.792E+02
4.000E+02


MATERIAL 5171
TEMP (K)
8.380E+01
9.338E+01
1.030E+02
1.125E+02
1.221E+02
1.317E+02
1.413E+02
1.509E+02
1.612E+02
1.716E+02
1.924E+02
2.131E+02
2.339E+02
2.547E+02
2.754E+02
2.962E+02
3.169E+02
3.377E+02
3.585E+02
3.792E+02
4.000E+02
E (MJ/kg)
-1
-4
-3
-2
-1
0
ρ (g/cm3)

SESAME #5172

Material: Argon [Ref. 1]
Originator: J. Wolford (Lawrence Livermore National Laboratory)
Date of Origin: October 1980
Type of Tables Included: 301
Limits: $10^{-5} \leq \rho \leq 10^{3}$ g/cm^3
$1.16 \times 10^{2} \leq T \leq 1.16 \times 10^{8}$ K

BASIC PHYSICAL DATA

$A = 39.948$
$Z = 18$
$\rho_o = 1.4$ g/cm^3

$P(T = 298.15$ K, $\rho_o) = 0.33043$ GPa
$E(T = 298.15$ K, $\rho_o) = 0.10131$ MJ/kg
(No zero pressure point in table)

$T_m = 83.75$ K [Ref. 2]

$T_c = 151$ K [Ref. 3]
$P_c = 5 \times 10^{-3}$ GPa [Ref. 3]
$\rho_c = 0.536$ g/cm^3 [Ref. 3]

DESCRIPTION OF PHYSICS

This argon equation of state is a wide-ranging global EOS which covers ideal gas, ionic equilibrium, ideal plasma, neutral fluid, multiphase, solid, and metallic solid conditions. Fig. 4 shows the regions in temperature-density space in which each condition occurs.

Below 1.0 eV in temperature and 0.1 g/cm^3 in density, argon is a neutral fluid, and the EOS can be described by a Lennard-Jones 6-12 fluid model. At densities between 0.1 g/cm^3

and 1.4 g/cm^3, and up to temperatures of 10 eV, the argon EOS was calculated with a high-density fluid perturbation theory (called r^{-6}). This theory uses a pair potential with an exponential repulsive term and an inverse sixth-power attractive term which is added as a perturbation to the free energy of the hard-sphere reference state.

In the ionization equilibrium region, two different theories were used. Over most of the region, the EOS was calculated with a rigorous quantum- statistical-mechanical theory based on a many-body perturbation expansion (ACTEX). At very low densities or very high temperatures (where argon is an ideal gas), a Saha model based on the Planck-Larkin partition function was considered suitable.

The zero-degree isotherm in compression was generated with electron band theory based on the self-consistent linear-muffin-tin-orbital(LMTO) method.

For the rest of the compression half-plane ($\rho > \rho_o$), the electronic part of the EOS was calculated with Thomas-Fermi theory modified with the Kirzhnits correction which accounts for the quantum-mechanical nature of the electron through exchange and correlation terms added to the electron distribution function. The contributions due to nuclear motion were described by semi-empirical Mie-Grüneisen theory at low temperatures and one-component-plasma theory at high temperatures.

Along boundaries where theories did not match, bicubic spline interpolation was used to smoothly merge adjoining models. See the shaded regions in Fig. 4.

Favorable comparisons exist with the following experimental data: critical point data, Soviet low-pressure P-V-T data, static high-pressure data, Soviet shock tube data, and Hugoniot data.

The argon EOS has a Maxwell construction instead of van der Waals loops in the two-phase region.

REFERENCES

1. A complete description of the argon EOS is given in J. K. Wolford and K. S. Long, "Extended Argon Equation of State," Lawrence Livermore Laboratory internal document UCID-18574-80-4 (1980).

2. Sargent-Welch Periodic Table of the Elements (1968).

3. N. B. Vargaftik, Tables on the Thermophysical Properties of Liquids and Gases 2nd Ed. (John Wiley and Sons, New York, 1975).

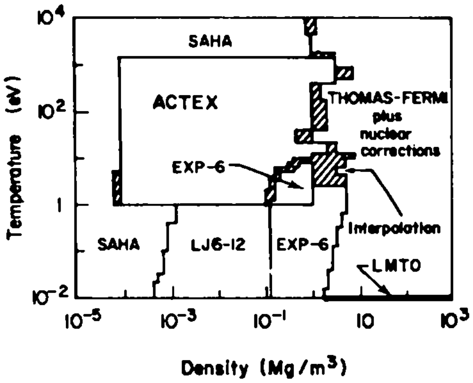
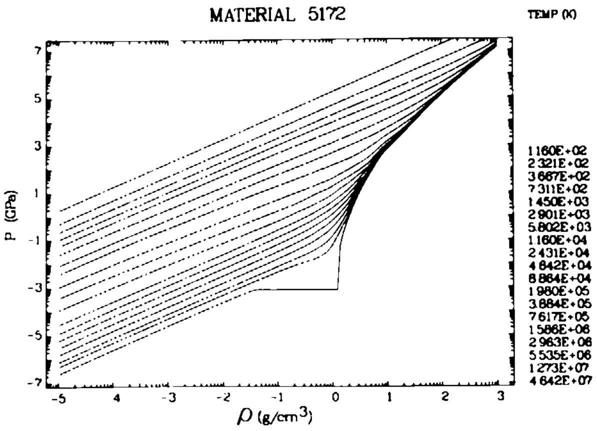
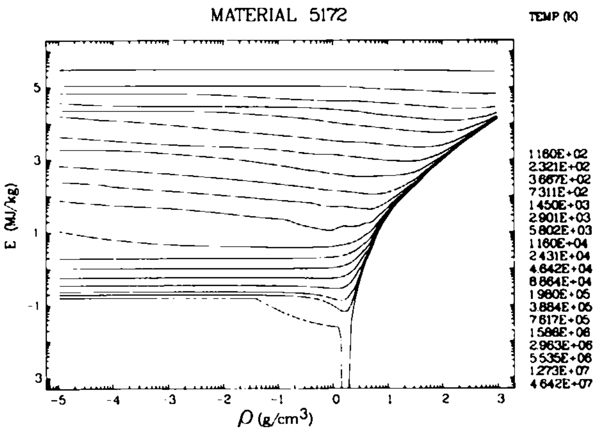


Fig. 4. Temperature-density plot showing the subregions covered by each of the theory codes used to calculate the EOS for argon. The shaded areas are regions in which numerical interpolation was required to smoothly join two EOS subsurfaces.


MATERIAL 5172
TEMP (K)
7
5
3
1
-1
-3
-5
-7
P (GPa)
-5
4
-3
-2
-1
0
1
2
3
ρ (g/cm3)
1 160E+02
2 321E+02
3 667E+02
7 311E+02
1 450E+03
2 901E+03
5.802E+03
1.160E+04
2 431E+04
4 642E+04
8 864E+04
1 980E+05
3.884E+05
7 617E+05
1 586E+06
2 963E+06
5 535E+06
1 273E+07
4 642E+07


MATERIAL 5172
TEMP (K)
E (MJ/kg)
5
3
1
-1
3
-5
-4
-3
-2
-1
0
1
2
3
ρ (g/cm³)
1.160E+02
2.321E+02
3.667E+02
7.311E+02
1.450E+03
2.901E+03
5.802E+03
1.160E+04
2.431E+04
4.642E+04
8.864E+04
1.960E+05
3.884E+05
7.617E+05
1.586E+06
2.963E+06
5.535E+06
1.273E+07
4.642E+07

SESAME #5180

Material: Krypton [Ref. 1]
Originator: G. I. Kerley
Date of Origin: December 1980
Type of Tables Included: 301
Limits: $10^{-6} < \rho < 10$ g/cm^3
$100 < T < 10^7$ K

BASIC PHYSICAL DATA

$A = 83.8$
$Z = 36$
$\rho_o = 2.5005$ g/cm^3

$P(T = 298.15\text{ K}, \rho_o) = 0.29370$ GPa
$E(T = 298.15\text{ K}, \rho_o) = 4.7337 \times 10^{-2}$ MJ/kg
$T(P = 10^{-6}\text{ GPa}, \rho_o) = 116.8$ K

$T_m = 115.85$ K [Ref. 2]

$T_c = 209$ K [Ref. 3]
$* \ 225$ K (calculated)
$P_c = 5.49 \times 10^{-3}$ GPa [Ref. 3]
$* \ 6.90 \times 10^{-3}$ GPa (calculated)
$\rho_c = 0.911$ g/cm^3
$* \ 0.795$ g/cm^3 (calculated)

$\gamma_o = * \ 2.05$ (used in calculation)

$\theta_D = * \ 64.5$ K (used in calculation) [Ref. 4]

Hugoniot Fit: No Hugoniot experiments have been performed on krypton.

DESCRIPTION OF PHYSICS

The liquid and vapor phases of krypton were computed with the CRIS model, which is based upon perturbation theory. The fluid EOS requires an expression for the potential energy of a molecule in the force field of its neighbors; this function was derived from the zero-kelvin isotherm of the solid. The cold curve was constructed by fitting a Grüneisen-Debye model to low-temperature compression data for solid krypton and then smoothly joining that onto Thomas-Fermi-Dirac statistical atom theory used at higher densities. Thomas-Fermi-Dirac theory was also used to calculate contributions from thermal electronic excitation at finite temperatures.

The solid EOS at finite temperatures is based on a Debye model which takes into account contributions from zero-point and thermal lattice vibrations. Agreement between theory and experimental data for Helmholtz free energy vs temperature is very good in the case of krypton, which shows that the Debye model is satisfactory in this case.

The fluid EOS also compares very well with measured isothermal compression data, sound speeds, and vaporization data. The Hugoniot has not been experimentally explored yet for krypton; however, a theoretical prediction for it has been included in this writeup.

Melting is included in this EOS, and the experimental melting curve agrees fairly well with theoretical predictions up to 240 K.

The krypton EOS has van der Waals loops instead of a Maxwell construction.

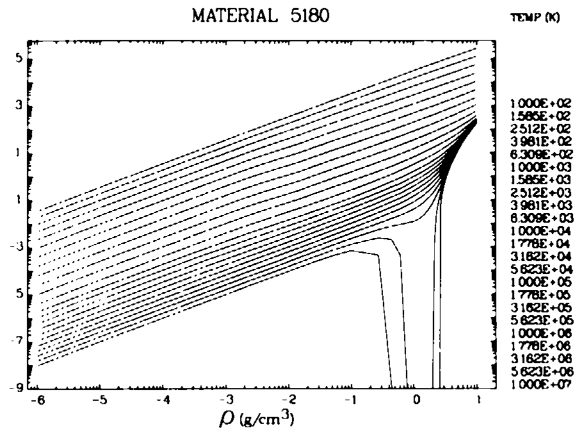
REFERENCES

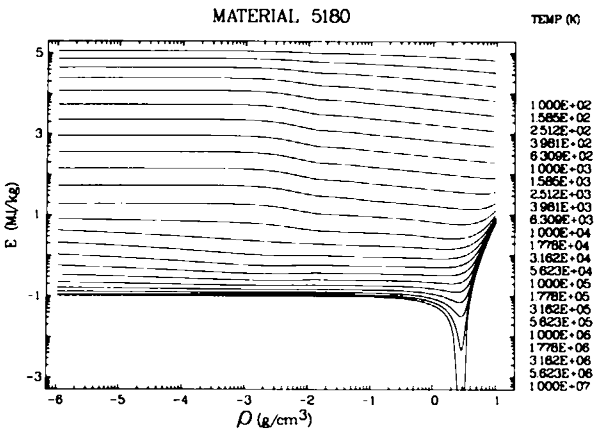
1. A complete description of how the krypton EOS was constructed is given in G. I. Kerley and P. M. Henry, "Theoretical Equations of State for the Rare Gases," Los Alamos Scientific Laboratory report LA-8062 (January 1980).

2. Sargent-Welch Periodic Table of the Elements (1968).

3. N. B. Vargaftik, Tables on the Thermophysical Properties of Liquids and Gases 2nd Ed. (John Wiley and Sons, Inc., New York, 1975).

4. G. L. Pollack, Rev. Mod. Phys. **36**, 748 (1964).


MATERIAL 5180
TEMP (K)
P (GPa)
5
3
1
1
-3
5
-7
-9
-6
-5
-4
-3
-2
-1
0
1
ρ (g/cm^3)
1.000E+02
1.585E+02
2.512E+02
3.981E+02
6.309E+02
1.000E+03
1.585E+03
2.512E+03
3.981E+03
6.309E+03
1.000E+04
1.778E+04
3.162E+04
5.623E+04
1.000E+05
1.778E+05
3.162E+05
5.623E+05
1.000E+06
1.778E+06
3.162E+06
5.623E+06
1.000E+07


MATERIAL 5180
TEMP (K)
E (MJ/kg)
5
3
1
-1
-3
-6
-5
-4
-3
-2
-1
0
1
ρ (g/cm3)
1.000E+02
1.585E+02
2.512E+02
3.981E+02
6.309E+02
1.000E+03
1.585E+03
2.512E+03
3.981E+03
6.309E+03
1.000E+04
1.778E+04
3.162E+04
5.623E+04
1.000E+05
1.778E+05
3.162E+05
5.623E+05
1.000E+06
1.778E+06
3.162E+06
5.623E+06
1.000E+07

SESAME #5250

Material: Hydrogen
Originator: National Bureau of Standards
Date of Origin: 1980
Type of Tables Included: 301
Limits: $1.2745 \times 10^{-6} < \rho < 0.10069$ g/cm^3
$13.8 < T < 400$ K

BASIC PHYSICAL DATA

$A = 1.00797$
$Z = 1$
$\rho_o = 7.7083 \times 10^{-2}$ g/cm^3

$P(T = 298.15 \text{ K}, \rho_o) = 0.22909$ GPa
$E(T = 298.15 \text{ K}, \rho_o) = 2.8835$ MJ/kg
$T(P = 10^{-4} \text{ GPa}, \rho_o) = 13.83$ K

$T_c =$ * 32.938 K (used in calculation)
$P_c =$ * 1.283768×10^{-3} GPa (calculated)
$\rho_c =$ * 1.568×10^{-2} g/cm^3 (used in calculation)

Triple Point Temperature: * 13.8 K (used in calculation)
Triple Point Pressure: * 7.043101×10^{-5} GPa (calculated)
Triple Point Density-Vapor: * 6.3727×10^{-5} g/cm^3 (calculated)
Triple Point Density-Liquid: * 3.8217×10^{-2} g/cm^3 (calculated)

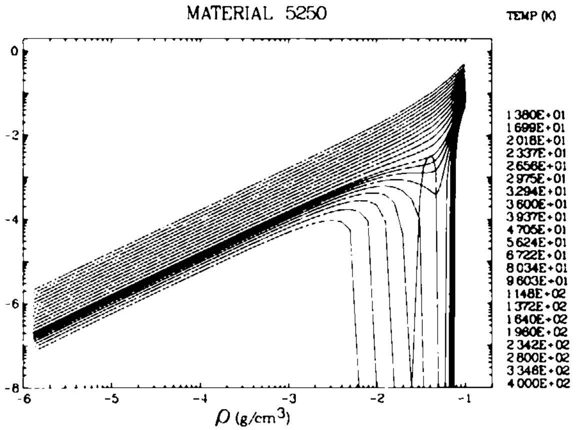
DESCRIPTION OF PHYSICS

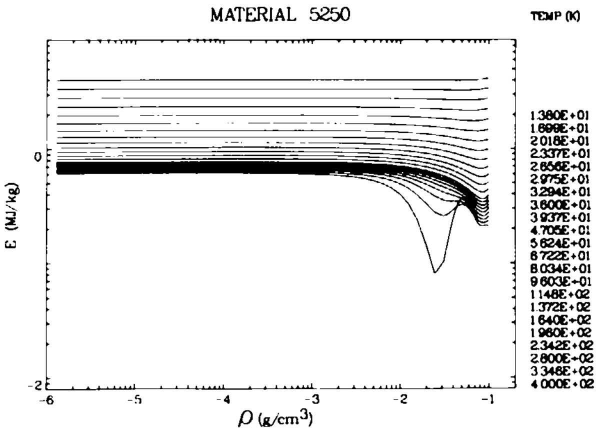
This hydrogen equation of state was calculated from a series of computer routines developed by the National Bureau of Standards which describe the thermodynamic and transport properties of selected cryogens [Ref. 1]. The computer programs describe properties for the gaseous and liquid states starting at the triple point. The EOS is calculated from a 32-term empirical equation which was derived from a weighted, least squares fit of experimental data. The uncertainty in the pressure is 5% for the liquid at temperatures below the critical temperature, 0.25% for the gas at $T < T_c$, and 0.2% everywhere else.

Beware that, although this EOS is very accurate, the temperature and density limits are restricted.

REFERENCE

1. R. D. McCarty, "Interactive FORTRAN IV Computer Programs for the Thermodynamic and Transport Properties of Selected Cryogens (Fluids Pack)," National Bureau of Standards Technical Note 1025 (October 1980).


MATERIAL 5250
TEMP (K)
P (GPa)
0
-2
-4
-6
-8
-6
-5
-4
-3
-2
-1
ρ (g/cm^3)
1.380E+01
1.699E+01
2.018E+01
2.337E+01
2.656E+01
2.975E+01
3.294E+01
3.600E+01
3.937E+01
4.705E+01
5.624E+01
6.722E+01
8.034E+01
9.603E+01
1.148E+02
1.372E+02
1.640E+02
1.960E+02
2.342E+02
2.800E+02
3.348E+02
4.000E+02


MATERIAL 5250
TEMP (K)
E (MJ/kg)
0
-2
-6
-5
-4
-3
-2
-1
ρ (g/cm3)
1.380E+01
1.699E+01
2.018E+01
2.337E+01
2.656E+01
2.975E+01
3.294E+01
3.600E+01
3.937E+01
4.705E+01
5.624E+01
6.722E+01
8.034E+01
9.603E+01
1.148E+02
1.372E+02
1.640E+02
1.960E+02
2.342E+02
2.800E+02
3.346E+02
4.000E+02

SESAME #5251

Material: Hydrogen
Composition: Natural Mix of Hydrogen Isotopes
Originators: R. C. Albers and J. D. Johnson
Date of Origin: September 1974
Type of Tables Included: 301, 303, 304
Limits: $0 \le \rho \le 1.7517 \times 10^{3}$ g/cm^{3}
$0 \le T \le 3.7 \times 10^{8}$ K

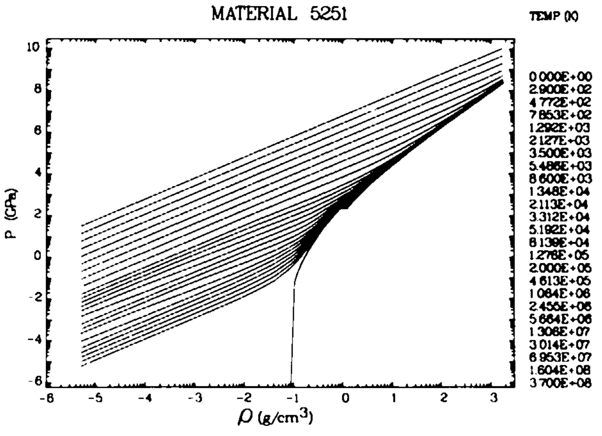
BASIC PHYSICAL DATA

$A = 1.00797$
$Z \quad 1$
$\rho_o = 8.8385 \times 10^{-2}$ g/cm^{3}

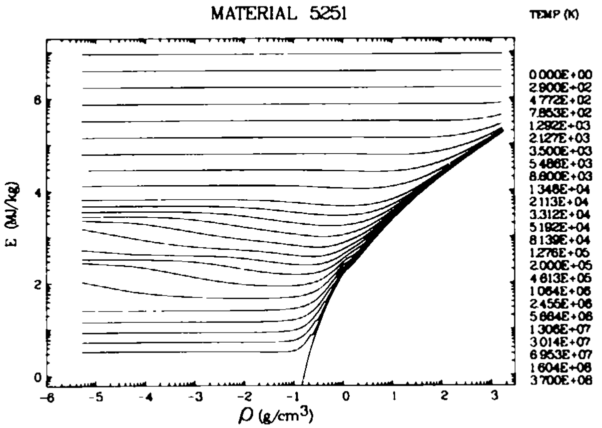
$P(T = 298.15\ \mathrm{K}, \rho_o) = 0.31349$ GPa
$E(T = 298.15\ \mathrm{K}, \rho_o) = 3.4055$ MJ/kg
$T(P = 10^{-6}\ \mathrm{GPa}, \rho_o) = 9.522 \times 10^{-4}$ K

DESCRIPTION OF PHYSICS

This EOS was created by isotopically scaling the deuterium EOS (SESAME #5263) to create a natural mix of hydrogen isotopes.



MATERIAL 5251
TEMP (K)
P (GPa)
10
8
6
4
2
0
-2
-4
-6
-6
-5
-4
-3
-2
-1
0
1
2
3
ρ (g/cm3)
0.000E+00
2.900E+02
4.772E+02
7.853E+02
1.292E+03
2.127E+03
3.500E+03
5.486E+03
8.600E+03
1.348E+04
2.113E+04
3.312E+04
5.192E+04
8.139E+04
1.276E+05
2.000E+05
4.613E+05
1.064E+06
2.456E+06
5.664E+06
1.306E+07
3.014E+07
6.953E+07
1.604E+08
3.700E+08


MATERIAL 5251
TEMP (K)
E (MJ/kg)
0
2
4
6
-6
-5
-4
-3
-2
-1
0
1
2
3
ρ (g/cm^3)
0.000E+00
2.900E+02
4.772E+02
7.853E+02
1.292E+03
2.127E+03
3.500E+03
5.486E+03
8.600E+03
1.346E+04
2.113E+04
3.312E+04
5.192E+04
8.139E+04
1.276E+05
2.000E+05
4.613E+05
1.064E+06
2.455E+06
5.664E+06
1.306E+07
3.014E+07
6.953E+07
1.604E+08
3.700E+08

SESAME #5263

Material: Deuterium [Ref. 1]
Composition: D_2
Originator: G. Kerley
Date of Origin: January 1972
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho < 3.5 \times 10^3$ g/cm^3
$0 < T < 3.7 \times 10^8$ K

BASIC PHYSICAL DATA

$\bar{A} = 2.014$
$\bar{Z} = 1$
$\rho_o = 0.1766$

$P(T = 298.15\text{ K}, \rho_o) = 0.31349$ GPa
$E(T = 298.15\text{ K}, \rho_o) = 1.7044$ MJ/kg
$T(P = 10^{-6}\text{ GPa}, \rho_o) = 8.2875 \times 10^{-4}$ K

DESCRIPTION OF PHYSICS

This is a wide-ranging equation of state for deuterium which treats the molecular solid, metallic solid, and fluid phases of the material. The various physical effects which are taken into account by this EOS are dissociation, ionization, vibrational-rotational effects, thermal electronic excitations, and phase transitions. The gas-liquid coexistence region is not treated because the critical temperature (33 K) is well below the range of the table.

The cold curve was calculated with an analytic expression which was derived by fitting compressibility experiments at low densities and band theory calculations at high densities.

Nuclear contributions in the metallic solid were calculated with Debye theory. The Lennard-Jones and Devonshire theory cell model was used to calculate the EOS of the solid molecular deuterium.

The CRIS model was used to calculate the thermodynamic properties of the fluid. This model uses the zero-temperature isotherm of the solid and a hard-sphere equation of state.

Because of dissociation and ionization, the fluid is a complicated mixture of molecules, atoms, protons, and electrons. To simplify the problem, separate equations of state were derived for the pure molecular gas and pure atomic gas. These results were combined by determining the fraction of dissociation using an equilibrium calculation.

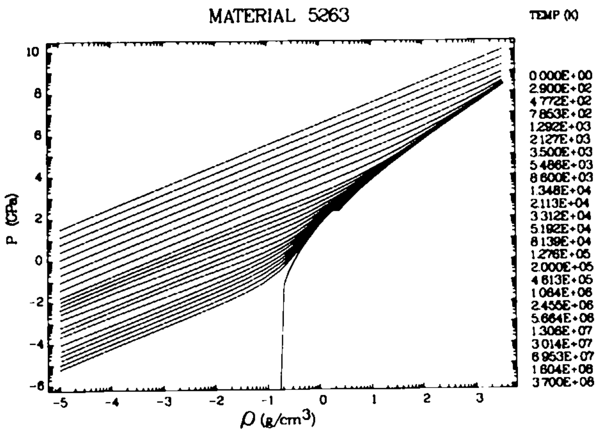
The contributions of excited electronic states and ionization to the EOS calculated with Saha theory at low densities and Thomas-Fermi-Dirac theory at high densities. Normally, a smooth transition between the two theories is impossible, but in this case, the Saha model was modified to join directly onto Thomas-Fermi-Dirac theory.

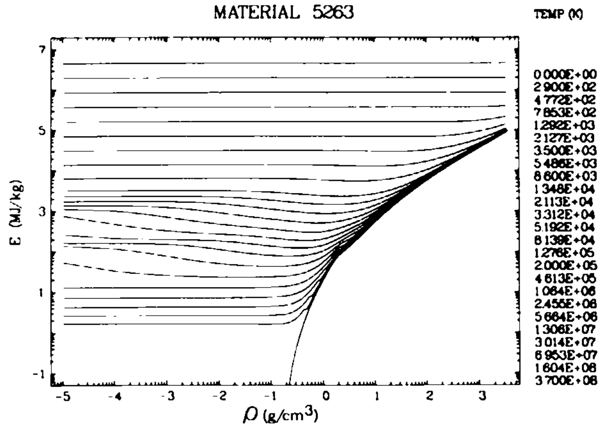
Separate equations of state were calculated for each of the three phases. The coexistence lines between the phases were determined by finding the pressures and temperatures at which two adjoining phases have equal Gibbs free energies.

Agreement between the calculated and experimental single-shock Hugoniots and between calculated and experimental reflected shock Hugoniots is very good.

REFERENCE

1. A complete description of this EOS is given in G. I. Kerley, "A Theoretical Equation of State for Deuterium," Los Alamos Scientific Laboratory report LA-4776 (January 1972).


MATERIAL 5263
TEMP (K)
0.000E+00
2.900E+02
4.772E+02
7.853E+02
1.292E+03
2.127E+03
3.500E+03
5.486E+03
8.600E+03
1.348E+04
2.113E+04
3.312E+04
5.192E+04
8.139E+04
1.276E+05
2.000E+05
4.613E+05
1.084E+06
2.455E+06
5.664E+06
1.306E+07
3.014E+07
6.953E+07
1.604E+08
3.700E+08
P (GPa)
10
8
6
4
2
0
-2
-4
-6
-5
-4
-3
-2
-1
0
1
2
3
ρ (g/cm3)


MATERIAL 5263
TEMP (K)
E (MJ/kg)
7
5
3
1
-1
-5
-4
-3
-2
-1
0
1
2
3
ρ (g/cm^3)
0.000E+00
2.900E+02
4.772E+02
7.853E+02
1.292E+03
2.127E+03
3.500E+03
5.486E+03
8.600E+03
1.348E+04
2.113E+04
3.312E+04
5.192E+04
8.139E+04
1.276E+05
2.000E+05
4.613E+05
1.064E+06
2.455E+06
5.664E+06
1.306E+07
3.014E+07
6.953E+07
1.604E+08
3.700E+08

SESAME #5271

Material: Deuterium-Tritium
Composition: D_2 50%
T_2 50%
Originators: R. C. Albers and J. D. Johnson
Date of Origin: September 1982
Type of Tables Included: 301, 303, 304
Limits: $0 \leq \rho \leq 4.3707 \times 10^3$ g/cm^3
$0 \leq T \leq 3.7 \times 10^8$ K

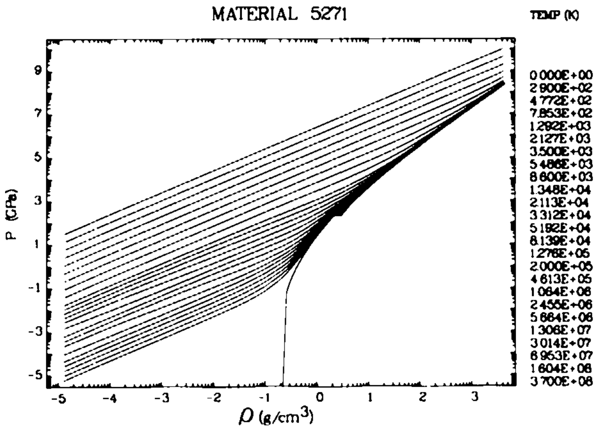
BASIC PHYSICAL DATA

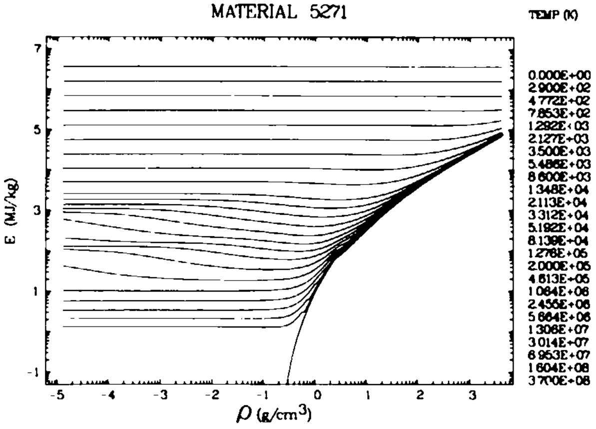
$\bar{A} = 2.515025$
$\bar{Z} = 1$
$\rho_o = 0.22053$ g/cm^3

$P(T = 298.15$ K, $\rho_o) = 0.31348$ GPa
$E(T = 298.15$ K, $\rho_o) = 1.3649$ MJ/kg
$T(P = 10^{-6}$ GPa, $\rho_o) = 3.479 \times 10^{-3}$ K

DESCRIPTION OF PHYSICS

This EOS was generated by isotopically scaling the deuterium EOS (SESAME #5263).


MATERIAL 5271
TEMP (K)
P (GPa)
9
7
5
3
1
-1
-3
-5
-5
-4
-3
-2
-1
0
1
2
3
ρ (g/cm3)
0.000E+00
2.900E+02
4.772E+02
7.853E+02
1.292E+03
2.127E+03
3.500E+03
5.486E+03
8.600E+03
1.348E+04
2.113E+04
3.312E+04
5.192E+04
8.139E+04
1.276E+05
2.000E+05
4.613E+05
1.064E+06
2.455E+06
5.664E+06
1.306E+07
3.014E+07
6.953E+07
1.604E+08
3.700E+08


MATERIAL 5271
TEMP (K)
0.000E+00
2.900E+02
4.772E+02
7.853E+02
1.292E+03
2.127E+03
3.500E+03
5.486E+03
8.600E+03
1.348E+04
2.113E+04
3.312E+04
5.192E+04
8.139E+04
1.276E+05
2.000E+05
4.613E+05
1.064E+06
2.455E+06
5.664E+06
1.306E+07
3.014E+07
6.953E+07
1.604E+08
3.700E+08
E (MJ/kg)
7
5
3
1
-1
-5
-4
-3
-2
-1
0
1
2
3
ρ (g/cm³)

SESAME #5280

Material: Ross-Aller Solar Mixture

Composition:

H	93.3926 at%
He	6.47554 at%
Z = 8.2856	0.131824 at%

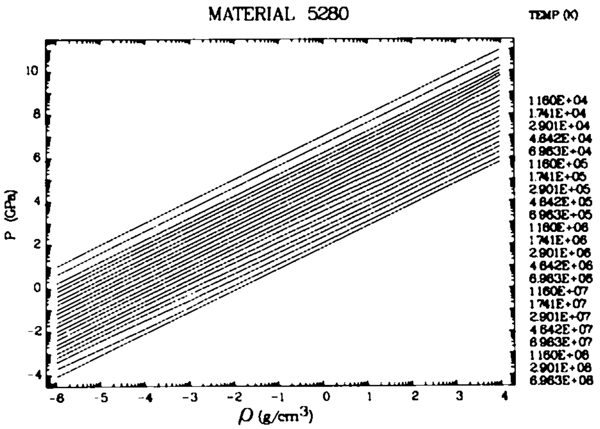
Originator: N. H. Magee
Date of Origin: April 1977
Type of Tables Included: 301
Limits: $10^{-6} \leq \rho \leq 10^{4}$ g/cm^3
1.16×10^{4} K $\leq T \leq 1.16 \times 10^{9}$ K

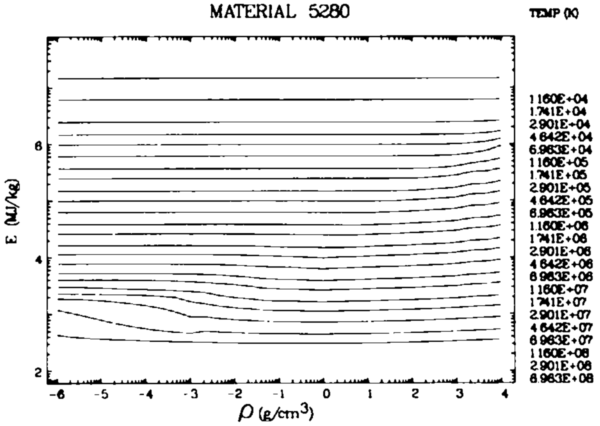
BASIC PHYSICAL DATA

$\bar{A} = 1.2226$
$\bar{Z} = 1.0744$
$\rho_0 = 0.$

DESCRIPTION OF PHYSICS

This equation of state was generated by the code MOOP in conjunction with a multifrequency opacity calculation for a mixture of elements which is known as the standard astrophysical mixture for the sun. The EOS of each element was calculated separately then mixed according to the number fraction above. The model used for the EOS was an ideal gas with plasma corrections. At temperatures greater than 100 eV, an average ion model was used; below 100 eV, the detailed configuration was calculated. Since MOOP is not used at low temperatures and high densities, that portion of the EOS was filled in with extrapolated values in order to obtain a rectangular grid of temperature and density.


MATERIAL 5280
TEMP (K)
P (GPa)
10
8
6
4
2
0
-2
-4
-6
-5
-4
-3
-2
-1
0
1
2
3
4
ρ (g/cm3)
1.160E+04
1.741E+04
2.901E+04
4.642E+04
6.963E+04
1.160E+05
1.741E+05
2.901E+05
4.642E+05
6.963E+05
1.160E+06
1.741E+06
2.901E+06
4.642E+06
6.963E+06
1.160E+07
1.741E+07
2.901E+07
4.642E+07
6.963E+07
1.160E+08
2.901E+08
6.963E+08


MATERIAL 5280
TEMP (K)
1.160E+04
1.741E+04
2.901E+04
4.642E+04
6.963E+04
1.160E+05
1.741E+05
2.901E+05
4.642E+05
6.963E+05
1.160E+06
1.741E+06
2.901E+06
4.642E+06
6.963E+06
1.160E+07
1.741E+07
2.901E+07
4.642E+07
6.963E+07
1.160E+08
2.901E+08
6.963E+08
E (MJ/kg)
2
4
6
ρ (g/cm³)
-6
-5
-4
-3
-2
-1
0
1
2
3
4

SESAME #5410

Material: Neon
Originator: J. Barnes and J. Rood
Date of Origin: November 1975
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho < 2.88 \times 10^4$ g/cm^3
$0 < T < 3.7 \times 10^8$ K

BASIC PHYSICAL DATA

$A = 20.183$
$Z = 10$
$\rho_o = 1.44$ g/cm^3

$P(T = 298.15\text{ K}, \rho_o) = 0.39128$ GPa
$E(T = 298.15\text{ K}, \rho_o) = 0.34022$ MJ/kg
$T(P = 10^{-6}\text{ GPa}, \rho_o) = 7.636 \times 10^{-4}$ K

$T_m = 24.55$ K [Ref. 1]

$T_c = 44.4$ K [Ref. 2]
$P_c = 2.65 \times 10^{-3}$ GPa [Ref. 2]
$\rho_c = 0.483$ g/cm^3 [Ref. 2]
The theoretical critical point that is actually in this EOS isunknown.

$\Theta_D = 67$ K [Ref. 3]

DESCRIPTION OF PHYSICS

This equation of state is undocumented. However, it was most likely generated with the standard Barnes-Cowan-Rood procedure. That is, above 1 eV the EOS was taken from an old MAPLE table in which the contributions due to the electrons are based on Thomas-Fermi-Dirac physics and the nuclear thermal part of the EOS is based on a model developed by R. D.

Cowan. Below 1 eV, the EOS consists of a cold curve calculated with the modified-Morse model and nuclear thermal contributions from a Debye model. (See Part II for a more detailed discussion of the Barnes-Cowan-Rood procedure.)

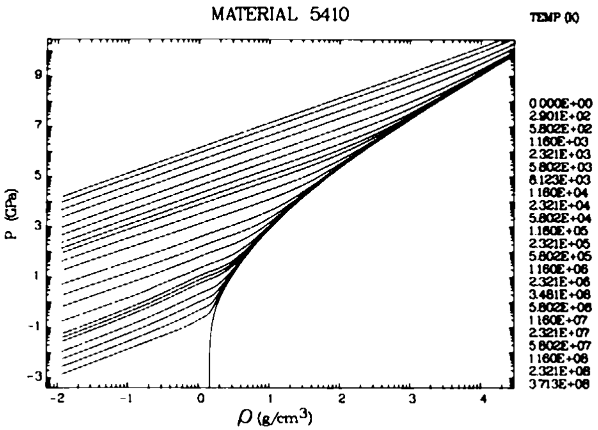
No Hugoniot experiments have been performed on neon.

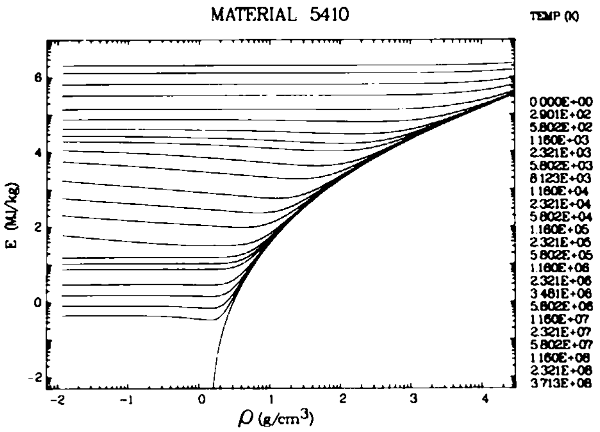
The EOS is thermodynamically consistent everywhere.

The two-temperature tables were derived by the code TWOTEMP and are noisy.

REFERENCES

1. Sargent-Welch Periodic Table of the Elements (1968).
2. N. B. Vargaftik, Tables on the Thermophysical Properties of Liquids and Gases 2nd Ed. (John Wiley and Sons, New York, 1975).
3. G. L. Pollack, "The Solid State of Rare Gases," Rev. Mod. Phys. 36, 748 (1964).


MATERIAL 5410
TEMP (K)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08
P (GPa)
9
7
5
3
1
-1
-3
-2
-1
0
1
2
3
4
ρ (g/cm³)


MATERIAL 5410
TEMP (K)
E (MJ/kg)
ρ (g/cm3)
-2
-1
0
1
2
3
4
6
4
2
0
-2
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08

SESAME #5411

Material: Neon [Ref. 1]
Originator: National Bureau of Standards
Date of Origin: 1965
Type of Tables Included: 301
Limits: $5.1028 \times 10^{-3} < \rho < 1.3406$ g/cm^3
$25 < T < 300$ K

BASIC PHYSICAL DATA

$A = 20.183$
$Z = 10$
$\rho_o = 1.2403$ g/cm^3

$P(T = 298.15\ \mathrm{K}, \rho_o) = 0.71818$ GPa
$E(T = 298.15\ \mathrm{K}, \rho_o) = 0.26968$ MJ/kg
$T(P = 10^{-4}\ \mathrm{GPa}, \rho_o) = 25.017$ K

$T_m = 24.55$ K [Ref. 2]

$T_c = *\ 44.40$ K (input)
$P_c = *\ 2.657086 \times 10^{-3}$ GPa (calculated)
$\rho_c = *\ 0.483$ g/cm^3 (input)

Triple Point Temperature: * 25 K (input)
Triple Point Pressure: * 5.102339×10^{-5} GPa (calculated)
Triple Point Density-Vapor: * 5.103×10^{-3} g/cm^3 (calculated)
Triple Point Density-Liquid: * 1.240 g/cm^3 (calculated)

DESCRIPTION OF PHYSICS

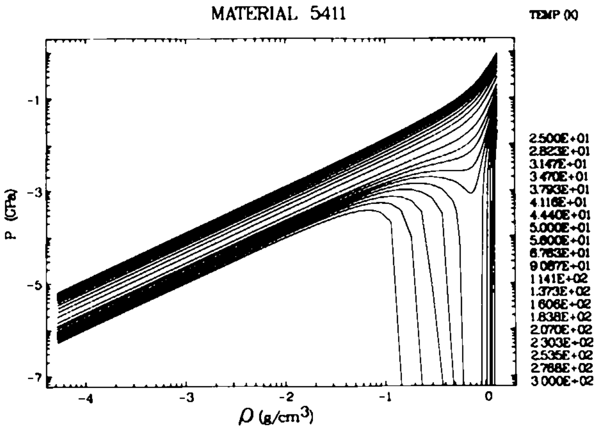
This neon equation of state was calculated from a series of computer routines developed by the National Bureau of Standards which describe the thermodynamic and transport properties of selected cryogens [Ref. 1]. The computer programs describe properties for the gaseous and liquid states starting at the triple point. The neon EOS is calculated from an 18-term empirical equation which was derived from a weighted, least squares fit of experimental data. The uncertainty in the pressure is 10% for the liquid at temperatures below the critical temperature and 0.5% everywhere else.

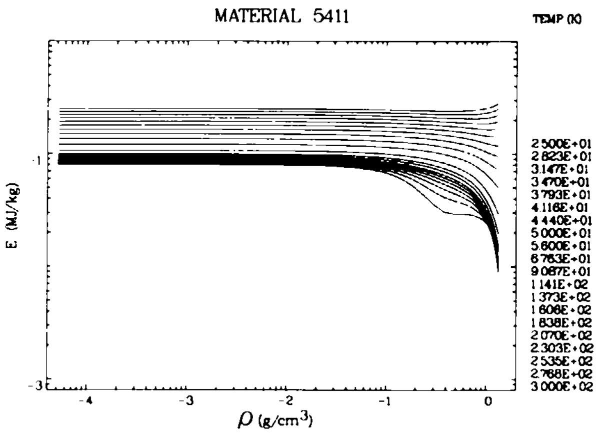
Beware that, although this EOS is very accurate, the temperature and density limits are restricted.

REFERENCES

1. R. D. McCarty, "Interactive FORTRAN IV Computer Programs for the Thermodynamic and Transport Properties of Selected Cryogens (Fluids Pack)," National Bureau of Standards Technical Note 1025 (US Government Printing Office, Washington, DC, October 1980).

2. Sargent-Welch Periodic Table of the Elements (1968).


MATERIAL 5411
TEMP (K)
P (GPa)
-1
-3
-5
-7
-4
-3
-2
-1
0
ρ (g/cm³)
2.500E+01
2.823E+01
3.147E+01
3.470E+01
3.793E+01
4.116E+01
4.440E+01
5.000E+01
5.600E+01
6.763E+01
9.087E+01
1.141E+02
1.373E+02
1.606E+02
1.838E+02
2.070E+02
2.303E+02
2.535E+02
2.768E+02
3.000E+02


MATERIAL 5411
TEMP (K)
E (MJ/kg)
-1
-3
-4
-3
-2
-1
0
ρ (g/cm³)
2.500E+01
2.823E+01
3.147E+01
3.470E+01
3.793E+01
4.116E+01
4.440E+01
5.000E+01
5.600E+01
6.763E+01
9.087E+01
1.141E+02
1.373E+02
1.606E+02
1.838E+02
2.070E+02
2.303E+02
2.535E+02
2.768E+02
3.000E+02

SESAME #5500

Material: Methane [Ref. 1]
Composition: CH_4
Originator: G. I. Kerley
Date of Origin: January 1980
Type of Tables Included: 301
Limits: $10^{-10} < \rho < 2.5$ g/cm^3
$20 < T < 10^4$ K

BASIC PHYSICAL DATA

$\bar{A} = 3.20852$
$\bar{Z} = 2.0$
$\rho_o = 0.45302$ g/cm^3

$P(T = 298.15$ K, $\rho_o) = 0.31719$ GPa
$E(T = 298.15$ K, $\rho_o) = 0.45689$ GPa
$T(P = 10^{-6}$ GPa, $\rho_o) = 75.628$ K

$T_m = 90.688$ K (at P = 0 bar) [Ref. 2]
$\quad$ * 90.688 K (theoretical value)

$T_c = 190.53$ K [Ref. 3]
$\quad$ * 200 K (calculated)
$P_c = 4.5957 \times 10^{-3}$ GPa [Ref. 3]
$\quad$ * 5.58×10^{-3} GPa (calculated)
$\rho_c = 0.1628$ g/cm^3 [Ref. 3]
$\quad$ * 0.145 g/cm^3 (calculated)

γ_o = * 2.97 (chosen by fitting solid EOS to thermal pressure measurements)

$E_{binding} = 0.65$ MJ/kg [Ref. 4]
(also used in calculation)

$\Theta_D = 112$ K [Ref. 4]

DESCRIPTION OF PHYSICS

The methane EOS was constructed over a wide range of temperatures and densities, primarily for the purpose of studying liquified natural gas technology. Both solid and fluid phases are covered by this equation of state.

At low densities, the cold curve of the solid was derived from the Buckingham exponential-6 intermolecular potential. At high densities, Thomas-Fermi-Dirac theory was used to calculate the cold curve. The density chosen to be the boundary between the two theories was determined by requiring a good match of theory to Hugoniot experiments.

The thermodynamic properties of the solid phase of methane were assumed to be the sum of several different contributions:

$$E(\rho,T) = E_c(\rho) + E_v(T) + E_R(T) + E_L(\rho,T)$$

$$P(\rho,T) = P_c(\rho) + P_L(\rho,T)$$

P_c and E_c are the cold curve pressures and energies. E_v and E_R are vibrational and rotational contributions to the EOS, which in this case were calculated using the rigid-rotator, harmonic oscillator approximation. P_L and E_L are lattice contributions to the pressure and energy which were derived by using the Debye model.

The following equations were used to calculate the thermodynamic properties of liquid methane:

$$E(\rho,T) = E_v(T) + E_R(T) + E_{TR}(\rho,T)$$

$$P(\rho,T) = P_{TR}(\rho,T)$$

P_{TR} and E_{TR} are the translational contributions which arise from the center-of-mass motion of the molecules in the intermolecular force field. These were calculated with the CRIS model which uses the solid cold curve to describe the forces.

Separate equation-of-state tables were calculated for the solid and fluid phases; then a composite table with a melting transition was constructed by determining where the pressures and Gibbs free energies of the two phases match at each temperature. In order to match experimental melting transition data, the solid energies were decreased by 0.016 MJ/kg relative to the fluid energies.

The zero of the energy of this table was set at the triple point for the liquid.

The theoretical methane EOS reproduces many different kinds of experiments well, including compressibility experiments, isothermal data, critical point data, measurements of saturation temperatures, heats of vaporization, and sound velocities. The theory also reproduces single-shock Hugoniot and reflected Hugoniot measurements.

This EOS, however, does not include dissociation effects, so it should be considered preliminary for temperatures above 3000 K.

There are Maxwell constructions in the two-phase region in expansion.

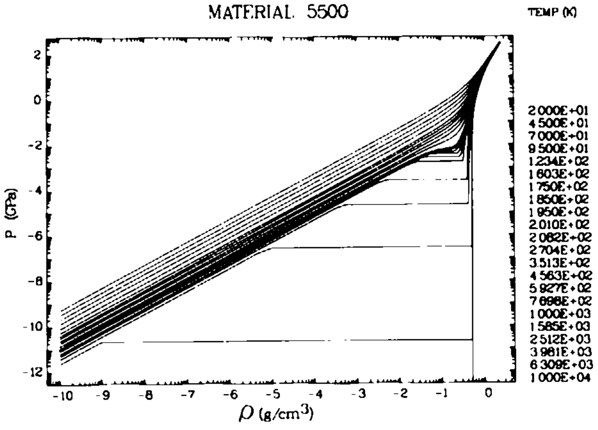
REFERENCES

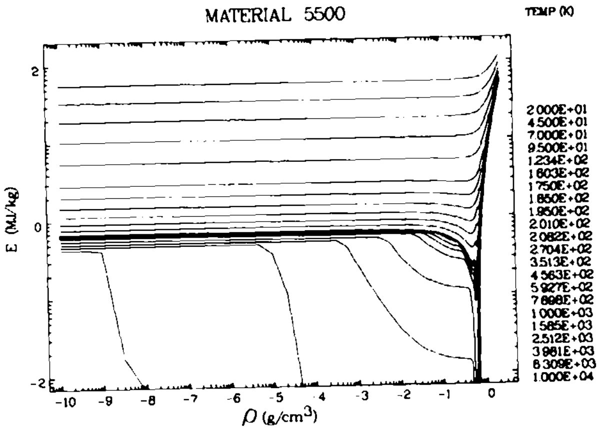
1. A complete description of the theoretical EOS for methane is given in G. I. Kerley, J. Appl. Phys. 51 (10), 5369 (1980).

2. V. M. Cheng, W. B. Daniels, and R. K. Crawford, Phys. Rev. B 11, 3972 (1975).

3. R. D. Goodwin, J. Res. Natl. Bur. Stand. Sec. A76, 81 (1972).

4. S. M. Breitlung, A. D. Jones and R. H. Boyd, J. Chem. Phys. 54, 3959 (1971).


MATERIAL 5500
TEMP (K)
P (GPa)
2
0
-2
-4
-6
-8
-10
-12
-10
-9
-8
-7
-6
-5
-4
-3
-2
-1
0
ρ (g/cm^3)
2.000E+01
4.500E+01
7.000E+01
9.500E+01
1.234E+02
1.603E+02
1.750E+02
1.850E+02
1.950E+02
2.010E+02
2.082E+02
2.704E+02
3.513E+02
4.563E+02
5.927E+02
7.698E+02
1.000E+03
1.585E+03
2.512E+03
3.981E+03
6.309E+03
1.000E+04


MATERIAL 5500
TEMP (K)
E (MJ/kg)
2
0
-2
-10
-9
-8
-7
-6
-5
-4
-3
-2
-1
0
ρ (g/cm3)
2.000E+01
4.500E+01
7.000E+01
9.500E+01
1.234E+02
1.603E+02
1.750E+02
1.850E+02
1.950E+02
2.010E+02
2.082E+02
2.704E+02
3.513E+02
4.563E+02
5.927E+02
7.698E+02
1.000E+03
1.585E+03
2.512E+03
3.981E+03
6.309E+03
1.000E+04

SESAME #5501

Material: Methane [Ref. 1]
Composition: CH_4
Originator: G. I. Kerley
Date of Origin: January 1980
Type of Tables Included: 301
Limits: $10^{-10} < \rho < 2.5$ g/cm^3
$20 < T < 10^4$ K

BASIC PHYSICAL DATA

$\bar{A} = 3.20852$
$\bar{Z} = 2.0$
$\rho_o = 0.45302$ g/cm^3

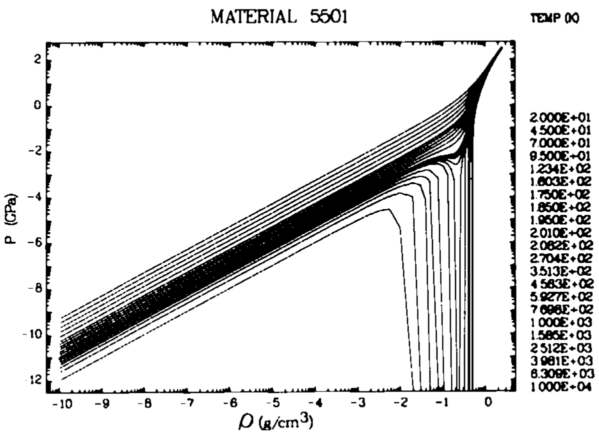
$P(T = 298.15\ K, \rho_o) = 0.31719$ GPa
$E(T = 298.15\ K, \rho_o) = 0.45689$ MJ/kg
$T(P = 10^{-6}\ GPa, \rho_o) = 93.544$ K

DESCRIPTION OF PHYSICS

This equation of state is identical to SESAME #5500 except that the vapor-liquid coexistence region has nonequilibrium van der Waals loops in order to define the superheated liquid and supercooled vapor states.

REFERENCE

1. A complete description of the methane EOS is given in G. I. Kerley, J. Appl. Phys. 51 (10), 5368 (1980).


MATERIAL 5501
TEMP (K)
P (GPa)
2
0
-2
-4
-6
-8
-10
-12
-10
-9
-8
-7
-6
-5
-4
-3
-2
-1
0
ρ (g/cm^3)
2.000E+01
4.500E+01
7.000E+01
9.500E+01
1.234E+02
1.603E+02
1.750E+02
1.850E+02
1.950E+02
2.010E+02
2.082E+02
2.704E+02
3.513E+02
4.563E+02
5.927E+02
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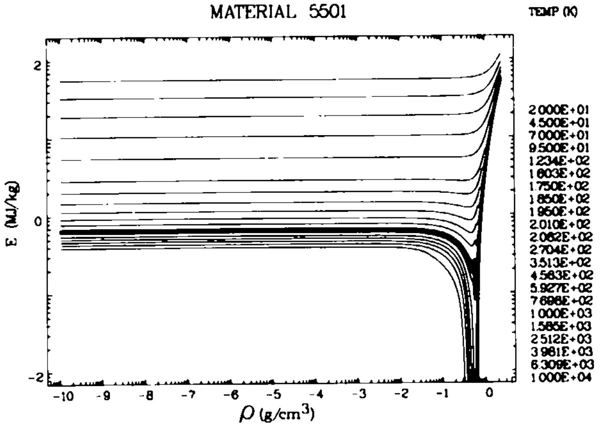
6.309E+03
1.000E+04


MATERIAL 5501
TEMP (K)
2.000E+01
4.500E+01
7.000E+01
9.500E+01
1.234E+02
1.603E+02
1.750E+02
1.850E+02
1.950E+02
2.010E+02
2.062E+02
2.704E+02
3.513E+02
4.563E+02
5.927E+02
7.696E+02
1.000E+03
1.585E+03
2.512E+03
3.981E+03
6.309E+03
1.000E+04
E (MJ/kg)
2
0
-2
-10
-9
-8
-7
-6
-5
-4
-3
-2
-1
0
ρ (g/cm³)

SESAME #5502

Material: Methane [Ref. 1]
Composition: CH_4
Originator: National Bureau of Standards
Date of Origin: 1974
Type of Tables Included: 301
Limits: $2.5173 \times 10^{-6} < \rho < 0.46972$ g/cm^3
$91 < T < 500$ K

BASIC PHYSICAL DATA

$\bar{A} = 3.20861$
$\bar{Z} = 2.0$
$\rho_o = 0.45163$ g/cm^3

$P(T = 298.15$ K, $\rho_o) = 0.3333$ GPa
$E(T = 298.15$ K, $\rho_o) = 0.69817$ MJ/kg
$T(P = 10^{-4}$ GPa, $\rho_o) = 90.724$ K

$T_m = 90.688$ K (at $P = 0$ bar) [Ref. 2]

$T_c = *\ 190.555$ K (input)
$P_c = *\ 4.598838 \times 10^{-3}$ GPa (calculated)
$\rho_c = *\ 0.1641$ g/cm^3 (input)

Triple Point Temperature: * 90.68 K (input)
Triple Point Pressure: * 1.17435×10^{-5} GPa (calculated)
Triple Point Density-Vapor: * 2.5173×10^{-4} g/cm^3 (calculated)
Triple Point Density-Liquid: * 0.45163 g/cm^3 (calculated)

DESCRIPTION OF PHYSICS

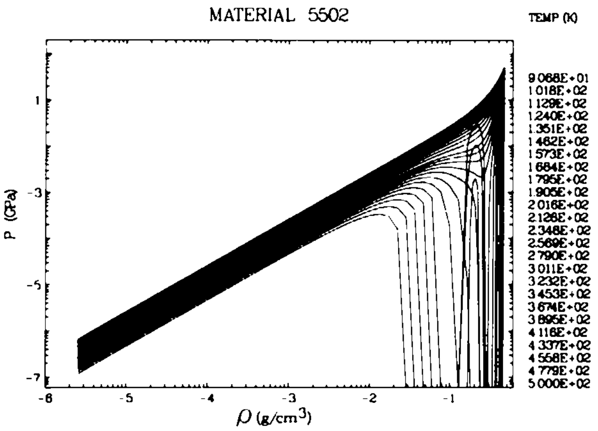
This methane equation of state was calculated from a series of computer routines developed by the National Bureau of Standards which describe the thermodynamic and transport properties of selected cryogens. The computer programs describe properties for gaseous and liquid states starting at the triple point. The methane EOS was calculated from a 32-term empirical equation which was derived from a weighted, least squares fit to experimental data. The uncertainty in the pressure is 5% for the liquid at temperatures below the critical temperature and 0.25% everywhere else.

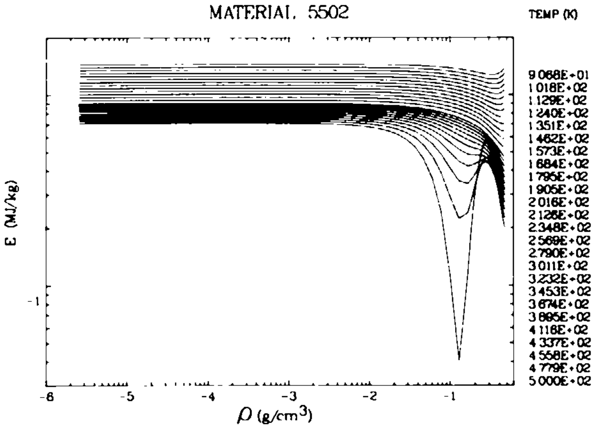
Beware that, although this EOS is very accurate, the temperature and density limits are restricted.

REFERENCES

1. R. D. McCarty, "Interactive FORTRAN IV Computer Programs for the Thermodynamic and Transport Properties of Selected Cryogens (Fluids Pack)," National Bureau of Standards Technical Note 1025 (US Government Printing Office, Washington, DC, October 1980).

2. V. M. Cheng, W. B. Daniels, and R. K. Crawford, Phys. Rev. B 11, 3972 (1975).


MATERIAL 5502
TEMP (K)
9.068E+01
1.018E+02
1.129E+02
1.240E+02
1.351E+02
1.462E+02
1.573E+02
1.684E+02
1.795E+02
1.905E+02
2.016E+02
2.126E+02
2.348E+02
2.569E+02
2.790E+02
3.011E+02
3.232E+02
3.453E+02
3.674E+02
3.895E+02
4.116E+02
4.337E+02
4.558E+02
4.779E+02
5.000E+02
P (GPa)
1
-3
-5
-7
-6
-5
-4
-3
-2
-1
ρ (g/cm³)


MATERIAL 5502
TEMP (K)
E (MJ/kg)
-1
-6
-5
-4
-3
-2
-1
ρ (g/cm³)
9.068E+01
1.018E+02
1.129E+02
1.240E+02
1.351E+02
1.462E+02
1.573E+02
1.684E+02
1.795E+02
1.905E+02
2.016E+02
2.126E+02
2.348E+02
2.569E+02
2.790E+02
3.011E+02
3.232E+02
3.453E+02
3.674E+02
3.895E+02
4.116E+02
4.337E+02
4.558E+02
4.779E+02
5.000E+02

SESAME #5520

Material: Ammonia [Ref. 1]
Composition: NH_3
Originator: National Bureau of Standards
Date of Origin: Unknown
Type of Tables Included: 301
Limits: $10^{-5} < \rho < 0.765\ g/cm^3$
$19.55 < T < 760\ K$

BASIC PHYSICAL DATA

$\bar{A} = 4.25757$
$\bar{Z} = 2.50$
$\rho_o = 0.73386\ g/cm^3$

$P(T = 298.15\ K, \rho_o) = 0.28434\ GPa$
$E(T = 298.15\ K, \rho_o) = -0.79939\ MJ/kg$
$T(P = 10^{-4}\ GPa, \rho_o) = 19.55\ K$

$T_c = *\ 405.4\ K$ (theoretical value)

DESCRIPTION OF PHYSICS

This equation of state for ammonia was derived by the National Bureau of Standards. It treats gaseous and liquid ammonia over a range of temperature that starts at the triple point and goes to twice the critical point temperature, and it extends to pressures of 500 GPa. The general approach was to construct a free energy surface in which the free energy for the ideal gas is combined with the free energy contribution for the temperature-density surface determined by a least-squares fit to P-ρ-T experimental data. (The analytic equation used was a 44-term, double power series function of temperature and density.) All other thermodynamic properties were calculated from the Helmholtz free energy surface by differentiation.

The tables of thermodynamic properties are thermodynamically consistent and agree with existing experimental data to within the assigned error tolerance of the data. Even though only P-ρ-T data were used in the least-squares fitting process, the derived thermodynamic surface also agrees with high-quality experimental calorimetric data and with data for the coexisting phases of the saturated liquid and vapor.

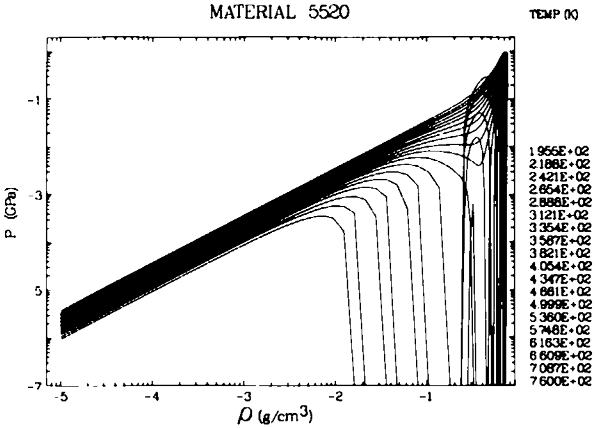
The melting transition (pressure vs temperature) was calculated with the Clapeyron equation. The liquid vapor saturation boundary was determined by finding the points where the Gibbs free energies for the two phases are equal. The reference state for the thermodynamic surface is defined to be the ideal gas at zero kelvin.

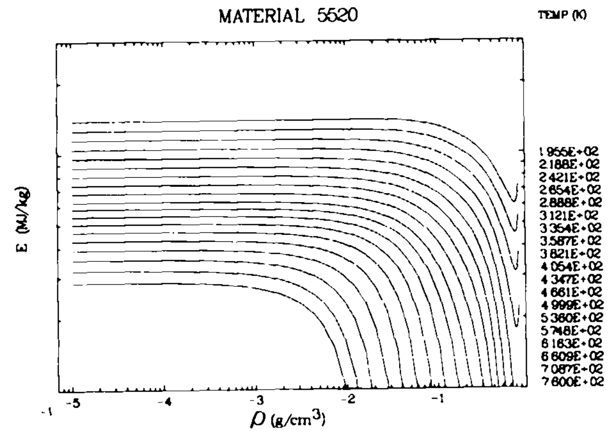
All chemical reactions such as dissociation are ignored. Dissociation is only important for the dilute gas at temperatures above 600 K.

Beware that, although this EOS is very accurate, the temperature-density limits are restricted.

REFERENCE

1. A complete description of the ammonia EOS is given in L. Haar and J. S. Gallagher, "Thermodynamic Properties of Ammonia," J. Phys. Chem. Ref. Data 7 (3), 635 (1978).


MATERIAL 5520
TEMP (K)
-1
-3
5
-7
P (GPa)
-5
-4
-3
-2
-1
ρ (g/cm3)
1.956E+02
2.188E+02
2.421E+02
2.654E+02
2.888E+02
3.121E+02
3.354E+02
3.587E+02
3.821E+02
4.054E+02
4.347E+02
4.661E+02
4.999E+02
5.360E+02
5.748E+02
6.163E+02
6.609E+02
7.087E+02
7.600E+02


MATERIAL 5520
TEMP (K)
E (MJ/kg)
ρ (g/cm^3)
-1
-5
-4
-3
-2
-1
1.955E+02
2.188E+02
2.421E+02
2.654E+02
2.888E+02
3.121E+02
3.354E+02
3.587E+02
3.821E+02
4.054E+02
4.347E+02
4.661E+02
4.999E+02
5.360E+02
5.748E+02
6.163E+02
6.609E+02
7.087E+02
7.600E+02

SESAME #5760

Material: Helium [Ref. 1]
Originator: H. C. Graboske (Lawrence Livermore National Laboratory)
Date of Origin: August 1974
Type of Tables Included: 301
Limits: $0 < \rho < 4.6784 \times 10^3$ g/cm^3
$0 < T < 1.16 \times 10^8$ K

BASIC PHYSICAL DATA

$A = 4.00260$
$Z = 2$
$\rho_o = 0.23392$ g/cm^3

$P(T = 298.15 \text{ K}, \rho_o) = 0.28858$ GPa
$E(T = 298.15 \text{ K}, \rho_o) = 1.0064$ MJ/kg
$T(P = 10^{-6} \text{ GPa}, \rho_o) = 8.995 \times 10^{-4}$ K

DESCRIPTION OF PHYSICS

This is a high-quality, wide-range equation of state for helium which incorporates several different theoretical models:

1) Perturbation theory - used in the low-temperature region which is characterized by short-range interatomic forces in a neutral fluid system. The free energy is computed by a perturbation relative to a reference system of hard spheres. The perturbation model is based on the Mansoori-Canfield method.

2) ACTEX - used in the low-density, intermediate-temperature region where the physical effects to be considered are partial ionization, partial degeneracy,

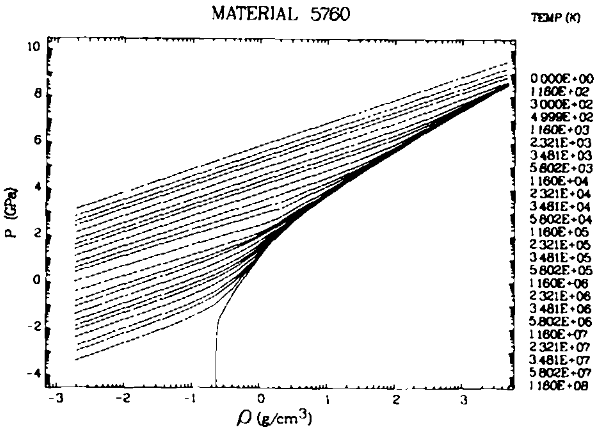
and weak-to-moderate Coulomb interactions. ACTEX is a rigorous quantum-statistical-mechanical theory based on a many-body perturbation expansion of the grand canonical partition function.

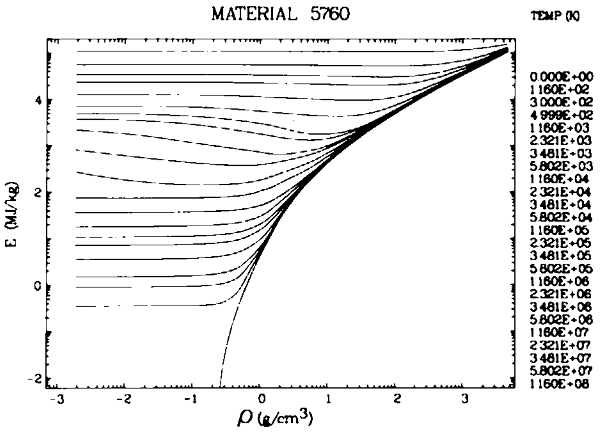
3) FMIN - used in the low-density, intermediate-temperature region in those areas where ACTEX does not converge. FMIN is based on a perturbation expansion in density. It includes effects of electron degeneracy and electron exchange interactions.

4) TFNUC - used in the high-density region. The electronic part of the EOS was generated with Thomas-Fermi theory. Effects of electron exchange and quantum correction terms are also included (based on a model by Kirzhnits). The ionic contributions to the EOS are based on plasma theory, Monte Carlo-Coulomb fluid calculations and solid Grüneisen theory at low temperatures.

REFERENCE

1. R. J. Olness, H. C. Graboske, K. W. Johnson, M. Ross, and F. J. Rogers, "The Equation of State of Helium in the Temperature Range 0.02585-10 eV," Lawrence Livermore Laboratory report UCIR-740 (December 1973).


MATERIAL 5760
TEMP (K)
0.000E+00
1.160E+02
3.000E+02
4.999E+02
1.160E+03
2.321E+03
3.481E+03
5.802E+03
1.160E+04
2.321E+04
3.481E+04
5.802E+04
1.160E+05
2.321E+05
3.481E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
3.481E+07
5.802E+07
1.160E+08
P (GPa)
10
8
6
4
2
0
-2
-4
-3
-2
-1
0
1
2
3
ρ (g/cm^3)


MATERIAL 5760
TEMP (K)
E (MJ/kg)
ρ (g/cm³)
4
2
0
-2
-3
-2
-1
0
1
2
3
0.000E+00
1.160E+02
3.000E+02
4.999E+02
1.160E+03
2.321E+03
3.481E+03
5.802E+03
1.160E+04
2.321E+04
3.481E+04
5.802E+04
1.160E+05
2.321E+05
3.481E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
3.481E+07
5.802E+07
1.160E+08

SESAME #5761

Material: Helium-4
Composition: Helium-4
Originator: R. C. Albers
Date of Origin: March 1981
Type of Tables Included: 301, 303, 304, 305, 306

Limits: $0 < \rho < 10^3$ g/cm^3
$0 < T < 1.16 \times 10^5$ K

BASIC PHYSICAL DATA

$A = 4.0026$
$Z = 2$
$\rho_o = 0.4$ g/cm^3

$P(T = 298.15\ \mathrm{K}, \rho_o) = 1.0713$ GPa
$E(T = 298.15\ \mathrm{K}, \rho_o) = 1.6464$ MJ/kg

$T_c = 5.2$ K [Ref. 1]
$P_c = 2.26 \times 10^{-4}$ GPa [Ref. 1]
$\rho_c = 0.0675$ g/cm^3 [Ref. 1]

$\gamma_o = 3.05758$ (at $\rho_{REF} = 0.14513$ g/cm^3 and $T_{REF} = 0$ K)

$E_{coh} = 1.48 \times 10^{-2}$ MJ/kg [Ref. 2]

$\theta_D = 10.15$ K (at $\rho_{REF} = 0.14513$ g/cm^3 and $T_{REF} = 0$ K)

Hugoniot Fit: (No data)

DESCRIPTION OF PHYSICS

The thermal electronic contributions to this EOS were calculated with three different models: Saha, Thomas-Fermi-Dirac, and INFERNO. INFERNO EOS's always exhibit metallic-like behavior, even at the lowest densities and temperatures where helium is actually an insulator. The electronic EOS was therefore massaged over an extensive region to force it to go smoothly from the metallic INFERNO model to the insulating Saha model.

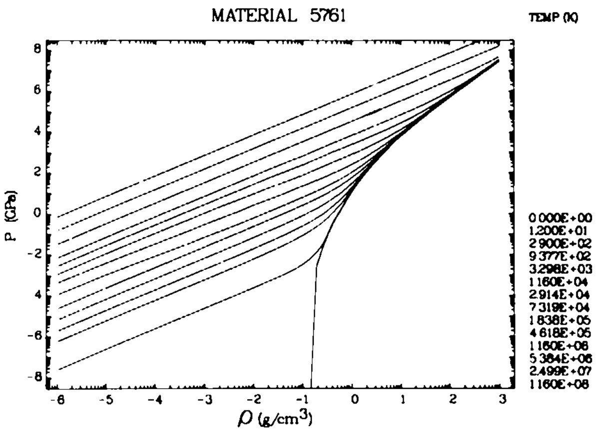
A modified PANDA code generated the total equation of state. The CRIS model with quantum corrections was used for the thermal ion component of the liquid EOS. A consistent set of Debye temperatures and Grüneisen parameters was generated from experimental data and reasonable extrapolations of the models. These were put into tables which PANDA could then interpolate on to find these quantities when required. The cold curve which is needed for the CRIS model was constructed in several stages. An initial cold curve was derived from experimental Hugoniot data and corrected for zero-point contributions. A Lennard-Jones tail was added to the low-density end, and a Thomas-Fermi-Dirac cold curve was merged onto the high-density end.

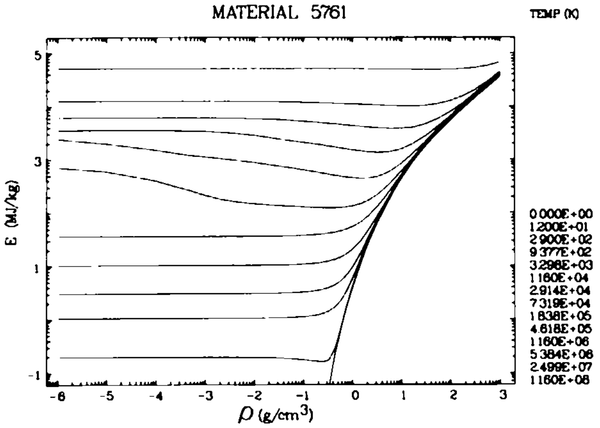
REFERENCES

1. J. Wilks, The Properties of Liquid and Solid Helium (Clarendon Press, Oxford, 1967).

2. P. R. Roach, J. B. Ketterson, and Chia-Wei Woo, Phys. Rev. A 2, 543 (1970).

5761-3


MATERIAL 5761
TEMP (K)
P (GPa)
8
6
4
2
0
-2
-4
-6
-8
-6
-5
-4
-3
-2
-1
0
1
2
3
ρ (g/cm³)
0.000E+00
1.200E+01
2.900E+02
9.377E+02
3.298E+03
1.160E+04
2.914E+04
7.319E+04
1.838E+05
4.618E+05
1.160E+06
5.384E+06
2.499E+07
1.160E+08


MATERIAL 5761
TEMP (K)
5
3
1
-1
E (MJ/kg)
-6
-5
-4
-3
-2
-1
0
1
2
3
ρ (g/cm³)
0.000E+00
1.200E+01
2.900E+02
9.377E+02
3.298E+03
1.160E+04
2.914E+04
7.319E+04
1.838E+05
4.618E+05
1.160E+06
5.384E+06
2.499E+07
1.160E+08

SESAME #5762

Material: Helium [Ref. 1]
Originator: National Bureau of Standards
Date of Origin: 1973
Type of Tables Included: 301
Limits: $1.1626 \times 10^{-3} < \rho < 0.3$ g/cm^3
$2.18 < T < 1.5 \times 10^3$ K

BASIC PHYSICAL DATA

$A = 4.0026$
$Z = 2$
$\rho_o = 0.14622$ g/cm^3

$P(T = 298.15\ \mathrm{K}, \rho_o) = 0.14451$ GPa
$E(T = 298.15\ \mathrm{K}, \rho_o) = 1.0002$ MJ/kg
$T(P = 10^{-4}\ \mathrm{GPa}, \rho_o) = 2.6081$ K

$T_m = 8.45$ K [Ref. 2]

$T_c = {}^*\ 5.2014$ K (input)
$P_c = {}^*\ 2.27464 \times 10^{-4}$ GPa (calculated)
$\rho_c = {}^*\ 0.06964$ g/cm^3 (input)

Lambda Temp: * 2.172 K (input)
Lambda Pressure: * 4.963285×10^{-5} GPa (calculated)
Lambda Density-Vapor: * 1.1625×10^{-3} g/cm^3 (calculated)
Lambda Density-Liquid: * 0.1462 g/cm^3 (calculated)

DESCRIPTION OF PHYSICS

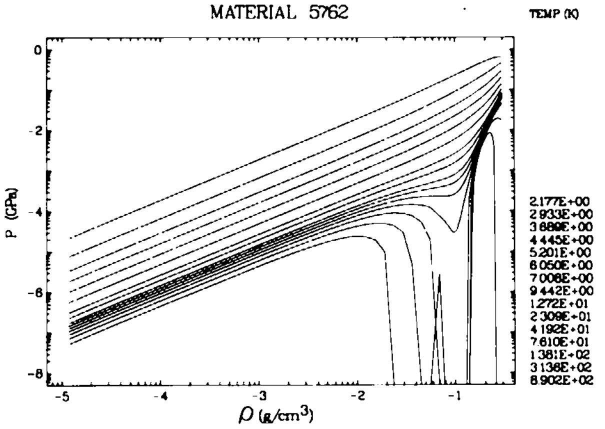
This helium equation of state was calculated from a series of computer routines developed by the National Bureau of Standards which describe the thermodynamic and transport properties of selected cryogens. The computer programs describe properties for the gaseous and liquid states starting at the triple point. The helium EOS was calculated from a 32-term empirical equation which was derived from a weighted, least-squares fit to experimental data. The uncertainty in the pressure is 10% for the liquid at temperatures below the critical temperature and 0.2% everywhere else.

Beware that, although this EOS is very accurate, the temperature and density limits are restricted.

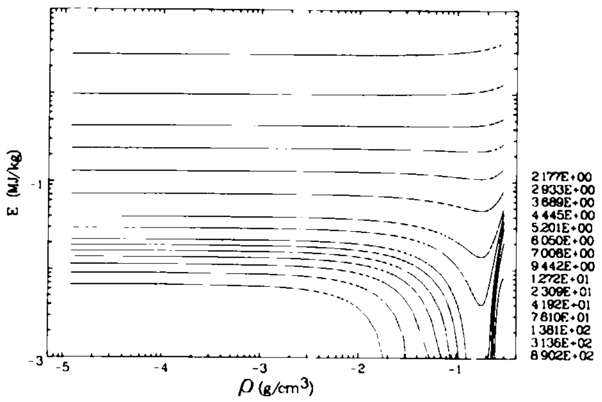
REFERENCES

1. R. D. McCarty, "Interactive FORTRAN IV Computer Programs for the Thermodynamic and Transport Properties of Selected Cryogens (Fluids Pack)," National Bureau of Standards Technical Note 1025 (US Government Printing Office, Washington, DC, October 1980).

2. Sargent-Welch Periodic Table of the Elements (1968).


MATERIAL 5762
TEMP (K)
0
-2
-4
-6
-8
P (GPa)
-5
-4
-3
-2
-1
ρ (g/cm³)
2.177E+00
2.933E+00
3.689E+00
4.445E+00
5.201E+00
6.050E+00
7.008E+00
9.442E+00
1.272E+01
2.309E+01
4.192E+01
7.610E+01
1.381E+02
3.138E+02
8.902E+02

5762-4



MATERIAL 5762

SESAME #7111

Material: Nevada Alluvium

Composition:

SiO_2	71.6 wt%
Al_2O_3	12.1 wt%
H_2O	4.0 wt%
K_2O	3.5 wt%
CaO	2.4 wt%

plus lesser amounts of other oxides

Originators: J. Barnes and J. Rood

Date of Origin: September 1975

Type of Tables Included: 301, 303, 304, 305, 306

Limits: $1.8359 \times 10^{-2} < \rho < 4.7 \times 10^{4}$ g/cm^3
$0 < T < 3.7 \times 10^{8}$ K

BASIC PHYSICAL DATA

$\bar{A} = 18.761$
$\bar{Z} = 9.3659$
$\rho_o = 2.35$ g/cm^3

$P(T = 298.15\ \text{K}, \rho_o) = 1.5646$ GPa
$E(T = 298.15\ \text{K}, \rho_o) = 0.33733$ MJ/kg
$T(P = 10^{-6}\ \text{GPa}, \rho_o) = 1.913 \times 10^{-4}$ K

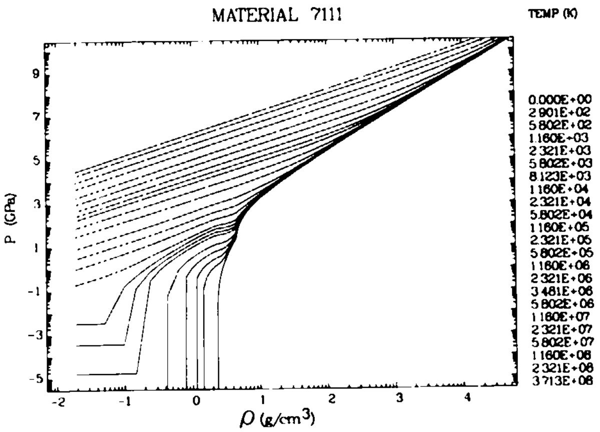
DESCRIPTION OF PHYSICS

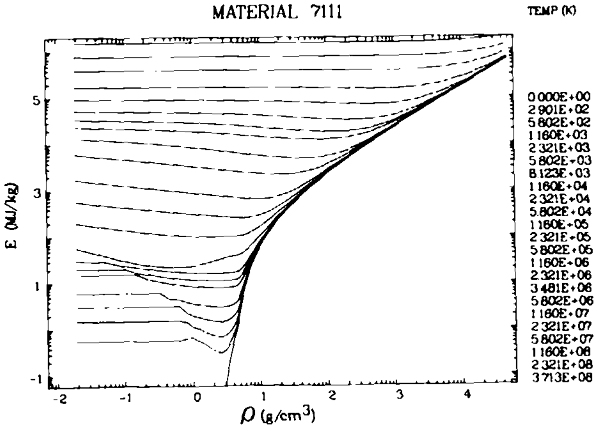
This equation of state is undocumented. However, it was most likely generated with the Barnes-Cowan-Rood procedure. That is, above 1 eV, the electronic part of the EOS was calculated with Thomas-Fermi-Dirac theory using an average atomic weight of 18.761 and an average atomic number of 9.3659. The nuclear thermal and cold curve contributions above 1 eV are based on a model by R. D. Cowan. Below 1 eV, the EOS consists of a cold curve calculated with a modified-Morse model and nuclear thermal contributions from a Debye model. (See Part II for a more detailed discussion of this procedure of EOS generation.)

The EOS is thermodynamically consistent everywhere.

Hugoniot experiments have been performed by R. G. McQueen for Nevada tuff starting at initial densities of 1.8 g/cm^3 and 1.54 g/cm^3. (These densities are porous relative to the reference density of this EOS.) Agreement with these experiments is fair.

The two-temperature tables were derived by using the code TWOTEMP and are noisy.


MATERIAL 7111
TEMP (K)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08
P (GPa)
9
7
5
3
1
-1
-3
-5
-2
-1
0
1
2
3
4
ρ (g/cm^3)


MATERIAL 7111
TEMP (K)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08
E (MJ/kg)
5
3
1
-1
-2
-1
0
1
2
3
4
ρ (g/cm³)

SESAME #7150

<u>Material</u>: Water [Ref. 1]
<u>Composition</u>: H_2O
<u>Originator</u>: F. H. Ree (Lawrence Livermore National Laboratory)
<u>Date of Origin</u>: June 1977
<u>Type of Tables Included</u>: 301
<u>Limits</u>: 2×10^{-6} g/cm^3 $< \rho \leq 400$ g/cm^3
$300 < T < 1.74 \times 10^8$ K

BASIC PHYSICAL DATA

$\bar{A} = 6.0053$
$\bar{Z} = 3.3333$
$\rho_o = 0.9982$ g/cm^3

$P(T = 298.15\ K, \rho_o) = 3.092 \times 10^{-3}$ GPa
$E(T = 298.15\ K, \rho_o) = 1.942 \times 10^{-2}$ MJ/kg
$T(P = 10^{-6}\ GPa, \rho_o) = 295.29$ K

$T_c = {}^*\ 647.3$ K (from theoretical EOS calculation)
$P_c = {}^*\ 21.408$ MPa (calculated)
$\rho_c = {}^*\ 0.305$ g/cm^3 (calculated)

Hugoniot Fit: * $U_s = 1.4829 + 2.1057\ U_p - 0.1744\ U_p^2 + 0.010085\ U_p^3$ km/s (used in calculation of EOS)

DESCRIPTION OF PHYSICS

This is a wide-range, high-quality equation of state for water. Several different theoretical models were used to generate it:

1) <u>TIGER</u> - calculates the EOS of a heterogeneous mixture containing gaseous components (H, H_2, O, O_2, OH, and H_2O) and

liquid components (H_2O) using the Becker-Kistiakowsky-Wilson equation. Ionization is assumed to be negligible. The TIGER region extends in density from 2×10^{-6} g/cm^3 to 2.5×10^{-2} g/cm^3, and in temperature from 0.1 eV to 1.0 eV.

2) OCCIPITAL - used in the high-temperature, low-density region in which H_2O is completely dissociated into electrons, ions, and neutral atomic hydrogen and oxygen. The concentrations of each of these species is obtained with the Saha equation, and the thermodynamic properties are calculated assuming that each component of the mixture behaves like an ideal gas.

3) TFCMIX - uses Thomas-Fermi theory to calculate an electronic EOS. The Kirzhnits correction is added to account for the wave nature of electrons and the electron exchange contribution. Nuclear contributions to the EOS are based on plasma theory, Monte Carlo- Coulomb fluid calculations, and solid Grüneisen-Debye theory at low temperatures. The TFCMIX region covers high densities at temperatures greater than 40 eV.

4) MASTER - Below temperatures of 40 eV and at pressures below 15 GPa on the cold curve, MASTER was used to phenomenologically correct the EOS for atomic shell structure and electronic correlations. This is to ensure that the experimental Hugoniot data will be reproduced.

5) Experimental Region - covers temperatures of 0.08 eV to 0.1 eV and densities less than 1.25 g/cm^3. Analytic fits to three different experimental sources were used to generate the EOS in this area: Schmidt's steam table [Ref. 2], Burnham's static compression data [Ref. 3], and Bridgman's data [reported in Refs. 4 and 5].

Hugoniot data are reproduced well by this EOS.

REFERENCES

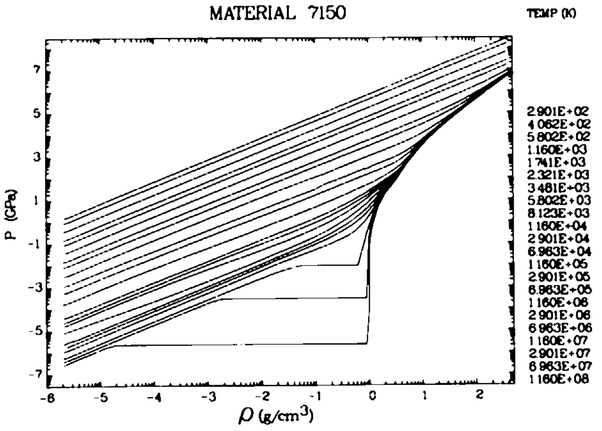
1. A complete description of this EOS is given in F. H. Ree, "Equation of State of Water," Lawrence Livermore Labortory report UCRL-52190 (December 1976).

2. E. Schmidt, Properties of Water and Steam SI-Units, (ClarendonPress, Oxford, 1969).

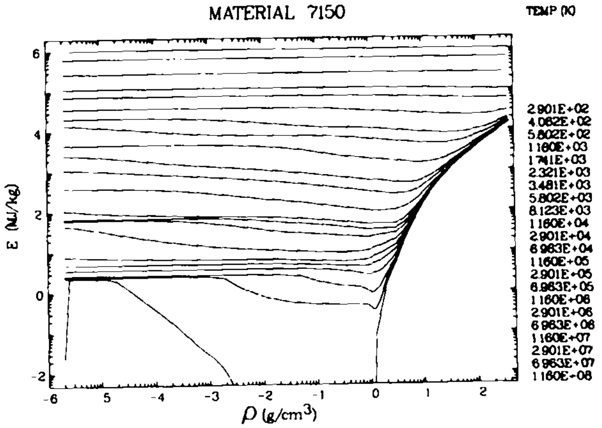
3. C. W. Burnham, J. R. Holloway, and N. F. Davis, "Thermodynamic Properties of H_2O to 1000 C and 1 kbar," The Geological Society of America Special Paper No. 132 (1969).

4. M. H. Rice and J. M. Walsh, J. Chem. Phys. 26, 824 (1957).

5. G. A. Gurtman, J. W. Kirsch, and C. R. Hastings, J. Appl. Phys. 42, 851 (1971).


MATERIAL 7150
TEMP (K)
2.901E+02
4.062E+02
5.802E+02
1.160E+03
1.741E+03
2.321E+03
3.481E+03
5.802E+03
8.123E+03
1.160E+04
2.901E+04
6.963E+04
1.160E+05
2.901E+05
6.963E+05
1.160E+06
2.901E+06
6.963E+06
1.160E+07
2.901E+07
6.963E+07
1.160E+08
P (GPa)
7
5
3
1
-1
-3
-5
-7
-6
-5
-4
-3
-2
-1
0
1
2
ρ (g/cm³)

7150-6


MATERIAL 7150
TEMP (K)
E (MJ/kg)
6
4
2
0
-2
-6
5
-4
-3
-2
-1
0
1
2
ρ (g/cm³)
2.901E+02
4.062E+02
5.802E+02
1.160E+03
1.741E+03
2.321E+03
3.481E+03
5.802E+03
8.123E+03
1.160E+04
2.901E+04
6.963E+04
1.160E+05
2.901E+05
6.963E+05
1.160E+06
2.901E+06
6.963E+06
1.160E+07
2.901E+07
6.963E+07
1.160E+08

SESAME #7152

Material: Water [Ref. 1]
Composition: H_2O
Originator: National Bureau of Standards
Date of Origin: May 1981
Type of Tables Included: 301
Limits: $10^{-8} < \rho < 1.4$ g/cm^3
$250 < T < 4000$ K

BASIC PHYSICAL DATA

$\bar{A} = 6.00511$
$\bar{Z} = 3.33333$
$\rho_o = 0.99978$ g/cm^3

$P(T = 298.15 \text{ K}, \rho_o) = 6.1643 \times 10^{-3}$ GPa
$E(T = 298.15 \text{ K}, \rho_o) = 0.10423$ MJ/kg
$T(P = 10^{-6} \text{ GPa}, \rho_o) = 281.8$ K

DESCRIPTION OF PHYSICS

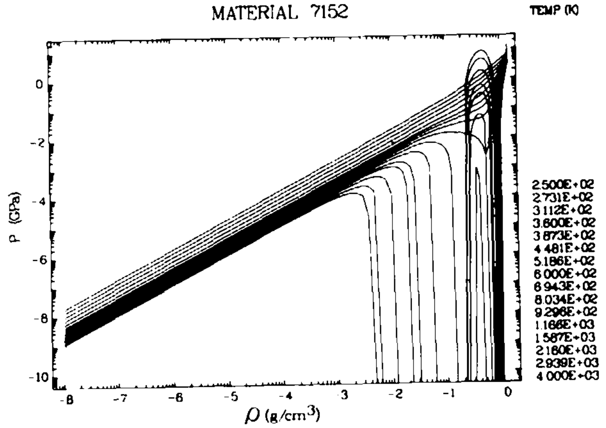
This EOS for water was calculated from analytic equations which were derived by the National Bureau of Standards from fitting experimental data. The data selected for the derivation of the thermodynamic surface were primarily P-ρ-T data, but they also used data for the enthalpy of the saturated liquid and for the isothermal compressibility of the liquid below 100°C. The thermodynamic surface covers a range from the freezing point to 4000 K and from the dilute gas to well in excess of 1 GPa. The liquid and gaseous states for undissociated water are described. The reference state is defined to be the liquid at the triple point, for which state the internal energy and entropy are zero.

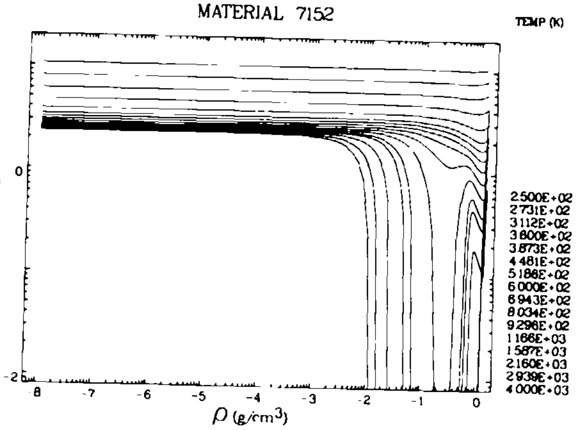
Beware that, although this equation of state is very accurate, the range of temperature and density covered is limited.

REFERENCE

1. L. Haar and J. S. Gallagher, "A Thermodynamic Surface for Water: The Formulation and Computer Programs," National Bureau of Standards internal report 81-2253 (May 1981).

MATERIAL 7152




MATERIAL 7152
TEMP (K)
E (MJ/kg)
0
-2
-8
-7
-6
-5
-4
-3
-2
-1
0
ρ (g/cm3)
2.500E+02
2.731E+02
3.112E+02
3.800E+02
3.873E+02
4.481E+02
5.186E+02
6.000E+02
6.943E+02
8.034E+02
9.296E+02
1.166E+03
1.587E+03
2.160E+03
2.939E+03
4.000E+03

SESAME #7160

Material: Deutero-polyethylene (branched, completely deuterated)
Composition: CD_2
Originator: F. Dowell
Date of Origin: September 1982
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho < 2.0949 \times 10^3$ g/cm^3
$0 < T < 1.16 \times 10^9$ K

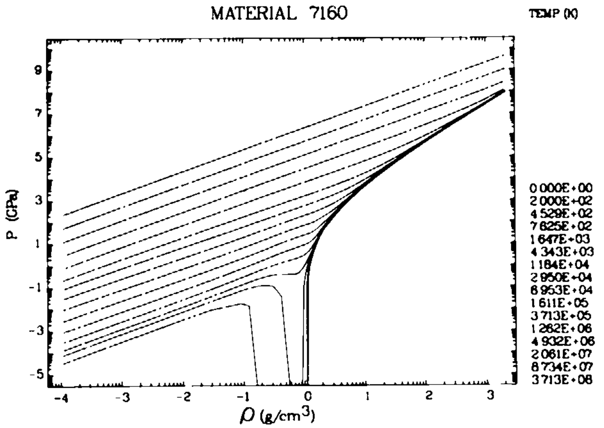
BASIC PHYSICAL DATA

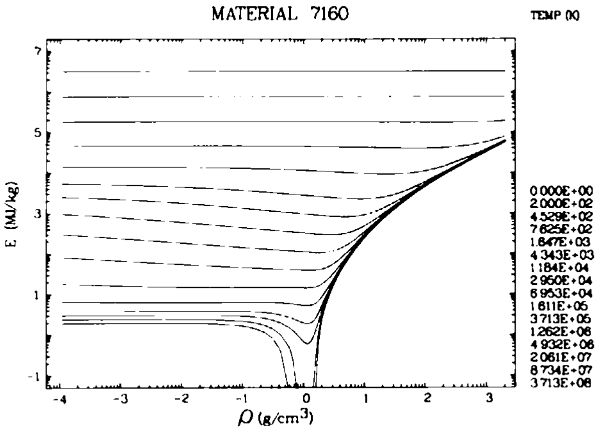
$\bar{A} = 5.3468$
$\bar{Z} = 2.666667$
$\rho_o = 1.0475$ g/cm^3

$P(T = 298.15 \text{ K}, \rho_o) = 2.36$[illegible]$5 \times 10^{-4}$ GPa
$E(T = 298.15 \text{ K}, \rho_o) = -6.3649 \times 10^{-5}$ MJ/kg
$T(P = 10^{-6} \text{ GPa}, \rho_o) = 298$ K

DESCRIPTION OF PHYSICS

This EOS is an isotopic scaling of SESAME #7171.


MATERIAL 7160
TEMP (K)
P (GPa)
9
7
5
3
1
-1
-3
-5
-4
-3
-2
-1
0
1
2
3
ρ (g/cm3)
0 000E+00
2 000E+02
4 529E+02
7 625E+02
1 647E+03
4 343E+03
1 184E+04
2 950E+04
6 953E+04
1 611E+05
3 713E+05
1 262E+06
4 932E+06
2 061E+07
8 734E+07
3 713E+08


MATERIAL 7160
TEMP (K)
E (MJ/kg)
7
5
3
1
-1
-4
-3
-2
-1
0
1
2
3
ρ (g/cm^3)
0 000E+00
2 000E+02
4 529E+02
7 625E+02
1.647E+03
4 343E+03
1 184E+04
2 950E+04
6 953E+04
1 611E+05
3 713E+05
1 262E+06
4 932E+06
2 061E+07
8 734E+07
3 713E+08

SESAME #7171

Material: Polyethylene (branched, low-density) [Ref. 1]
Composition: CH_2
Originator: F. Dowell
Date of Origin: September 1982
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho < 1.832 \times 10^3$ g/cm^3
$0 < T < 1.16 \times 10^9$ K

BASIC PHYSICAL DATA

$\bar{A} = 4.6757$
$\bar{Z} = 2.6667$
$\rho_o = 0.916$ g/cm^3

$P(T = 298.15 \text{ K}, \rho_o) = 9.0859 \times 10^{-5}$ GPa
$E(T = 298.15 \text{ K}, \rho_o) = -5.1977 \times 10^{-5}$ MJ/kg
$T(P = 10^{-6} \text{ GPa } \rho_o) = 298$ K

$\gamma_o =$ * 0.561 (used in calculation)
(calculated from experimental values for the constant pressure heat capacity, the isentropic bulk modulus, and the thermal expansion coefficient at ρ_o)

$E_{coh} = 1.03$ MJ/kg [estimated from Ref. 2]
* 3.35 MJ/kg (used in calculation)

$E_{binding} = -1.6323$ MJ/kg
(set so that zero of energy is at $P=0$ and $T=298.15$ K)

Hugoniot Fit: $U_S = 2.5331 + 1.7648\ U_p - 0.0469\ U_p^2$ km/s for $0.7 < U_p < 4.9$ km/s (Ref. 3)
(used in calculation of cold curve)

DESCRIPTION OF PHYSICS

This is an equation of state for branched (low-density) polyethylene. The models used to generate this EOS do not explicity treat polyethylene as a polymer; however, since experimental data are used in the models, the polymeric nature is implicitly included in parts of the EOS.

The EOS for polyethylene is treated as the sum of three contributions: zero kelvin, thermal electronic, and solid lattice vibrations. The cold curve was calculated at low densities in compression from experimental Hugoniot data assuming a Mie-Grüneisen model. This was smoothly joined onto high-density Thomas-Fermi-Dirac calculations. For $\rho < 0.911\ g/cm^3$, the cold curve was calculated with an analytic Lennard-Jones formula with an r^{-6} attractive term.

The thermal electronic contributions to the EOS were calculated with Thomas-Fermi-Dirac theory assuming an average atomic weight of 4.6757 and an average atomic number of 2.666667.

The solid lattice vibrations were described by a Debye model which was modified to extrapolate to an ideal gas at high temperatures or low densities. At densities below reference density, a virial expression was used.

This EOS does not include effects for the glass transitions or melting. Also, it has van der Waals loops in expansion instead of a Maxwell construction.

Hugoniot data are reproduced very well by this EOS. Static measurements of pressure-volume-temperature data were also compared with theory, and agreement was within 0.12% to 2.91%, except for one data point in the liquid state.

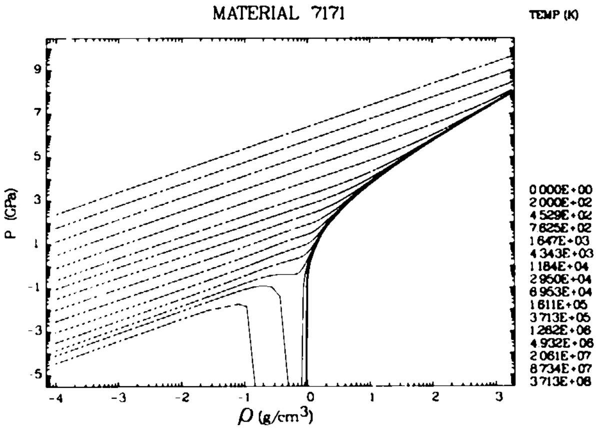
This EOS is thermodynamically consistent everywhere.

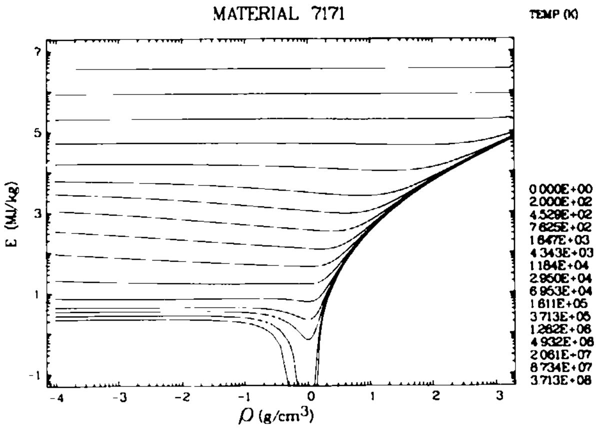
REFERENCES

1. A complete description of this EOS is given in F. Dowell, "A Simple EOS for Branched (Low-Density) Polyethylene," Los Alamos National Laboratory report LA-9559-MS (October 1982).

2. C. W. Bunn, "The Melting Points of Chain Polymers," J. Polym. Sci. 16, 323 (1955).

3. S. P. Marsh, LASL Shock Hugoniot Data, (University of California Press, Berkeley, 1980).


MATERIAL 7171
TEMP (K)
P (GPa)
9
7
5
3
1
-1
-3
-5
-4
-3
-2
-1
0
1
2
3
ρ (g/cm³)
0 000E+00
2 000E+02
4 529E+02
7 625E+02
1 647E+03
4 343E+03
1 184E+04
2 950E+04
6 953E+04
1 611E+05
3 713E+05
1 262E+06
4 932E+06
2 061E+07
8 734E+07
3 713E+08


MATERIAL 7171
TEMP (K)
E (MJ/kg)
ρ (g/cm3)
7
5
3
1
-1
-4
-3
-2
-1
0
1
2
3
0.000E+00
2.000E+02
4.529E+02
7.625E+02
1.647E+03
4.343E+03
1.184E+04
2.950E+04
6.953E+04
1.611E+05
3.713E+05
1.282E+06
4.932E+06
2.061E+07
8.734E+07
3.713E+08

SESAME #7180

Material: Polyethylene (Marlex) [Ref. 1]
Composition: CH_2
Originator: F. Dowell
Date of Origin: September 1982
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho < 1.908 \times 10^3$ g/cm^3
$0 < T < 1.16 \times 10^9$ K

BASIC PHYSICAL DATA

$\bar{A} = 4.6757$
$\bar{Z} = 2.6667$
$\rho_o = 0.954$ g/cm^3

$P(T = 298.15\ \text{K}, \rho_o) = 7.8334 \times 10^{-5}$ GPa
$E(T = 298.15\ \text{K}, \rho_o) = -5.200 \times 10^{-5}$ MJ/kg
$T(P = 10^{-6}\ \text{GPa}, \rho_o) = 298$ K

$\gamma_o =$ * 0.739 (used in calculation)
(calculated from experimental values for isentropic bulk modulus, thermal expansion coefficient, and constant pressure heat capacity at ρ_o)

$B_o = 4.48$ GPa [Ref. 2]

$E_{coh} =$ * 4.00 MJ/kg (used in calculation)
(This is higher than the estimated experimental value.)

Hugoniot Fit: * $U_S = 2.8233 + 1.6810\ U_p - 0.0339\ U_p^2$ km/s for $0.7 < U_p < 5.4$ km/s [Ref. 2] (used in calculation of EOS)

DESCRIPTION OF PHYSICS

This is an equation of state for "linear", high-density polyethylene (Marlex). The models used to generate this EOS do not explicitly treat Marlex as a polymer; however, since experimental data are used in the models, the polymeric nature of Marlex is implicitly included in parts of the EOS.

The cold curve of this EOS was calculated at low densities from experimental Hugoniot data assuming a Mie-Grüneisen model. This low-pressure part of the cold curve was smoothly joined onto high-density Thomas-Fermi-Dirac zero-degree calculations. At $\rho < 0.949$ g/cm^3, the cold curve was calculated with an analytic Lennard-Jones formula with an r^{-6} attractive term.

The thermal electronic contributions to the EOS were calculated with Thomas-Fermi-Dirac theory assuming an average atomic weight of 4.6757 and an average atomic number of 2.666667.

The solid lattice vibrations were calculated with a Debye model which was modified to extrapolate to an ideal gas at high temperatures or low densities. At densities below reference density, a virial expression was used.

The solid binding energy was set to -1.6836 MJ/kg in order for the zero of energy to be at $P = 0$ and $T = 298.15$ K.

This EOS does not include effects for the glass transitions or melting. It has van der Waals loops in expansion instead of a Maxwell construction.

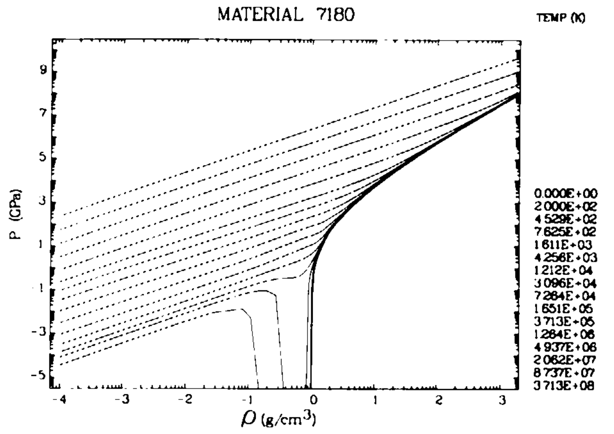
Hugoniot data are reproduced very well by this EOS. Static measurement pressure-volume-temperature data were also compared with theory, and agreement was within 0-5% in density, except for one data point in the liquid state.

The thermodynamic consistency of this EOS is good everywhere.

REFERENCES

1. A complete description of this EOS is given in F. Dowell, "A Simple EOS for "Linear" (High Density) Polyethylene (Marlex)," Los Alamos National Laboratory report LA-9564-MS (November 1982).

2. S. P. Marsh, LASL Shock Hugoniot Data (University of California Press, Berkeley, 1980).


MATERIAL 7180
TEMP (K)
P (GPa)
9
7
5
3
1
-1
-3
-5
-4
-3
-2
-1
0
1
2
3
ρ (g/cm3)
0.000E+00
2.000E+02
4.529E+02
7.625E+02
1.611E+03
4.256E+03
1.212E+04
3.096E+04
7.264E+04
1.651E+05
3.713E+05
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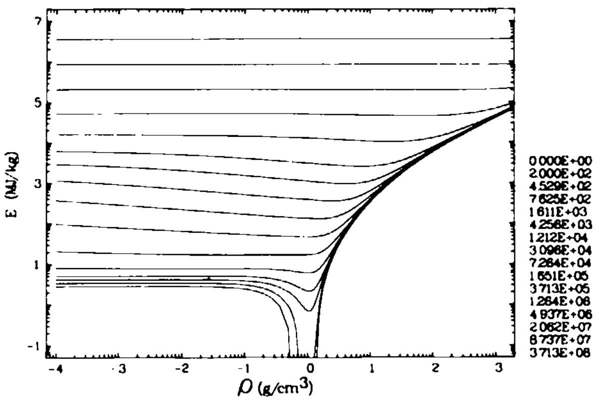
4.937E+06
2.062E+07
8.737E+07
3.713E+08



MATERIAL 7180

SESAME #7190

Material: Teflon (Polytetrafluoroethylene) [Ref. 1]
Composition: CF_2
Originator: F. Dowell and J. D. Johnson
Date of Origin: August 1982
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho < 4.304 \times 10^3$ g/cm^3
$0 < T < 1.16 \times 10^9$ K

BASIC PHYSICAL DATA

$\bar{A} = 16.669$
$\bar{Z} = 8.0$
$\rho_o = 2.152$ g/cm^3

$P(T = 298.15\ \text{K}, \rho_o) = 1.0574 \times 10^{-4}$ GPa
$E(T = 298.15\ \text{K}, \rho_o) = -1.5399 \times 10^{-5}$ MJ/kg
$T(P = 10^{-6}\ \text{GPa}, \rho_o) = 298$ K

$\gamma_o = {}^*\ 0.455$ (used in calculation)
(calculated from experimental values for the constant pressure heat capacity, the isentropic bulk modulus, and the thermal expansion coefficient at ρ_o)

$E_{coh} = 0.324$ MJ/kg [estimated from Ref. 2]
$\quad {}^*\ 1.150$ MJ/kg (used in calculation)

$E_{binding} = {}^*\ -0.44658$ MJ/kg
(set so that zero of energy is at P=0 and T=298.15 K)

Hugoniot Fit: $U_S = 1.571 + 1.961\ U_p - 0.0537\ U_p^2$
km/s for $0.6 < U_p < 4.4$ km/s
(used in calculation of
cold curve) [Ref. 3]

DESCRIPTION OF PHYSICS

Teflon is a polymer which is a chain of CF_2 molecules. The models used to generate this EOS do not explicitly treat teflon as a polymer; however, since experimental data are used in the models, the polymeric nature is implicitly included in parts of the EOS.

The EOS for teflon is treated as the sum of three contributions: zero kelvin, thermal electronic, and solid lattice vibrations. The cold curve was calculated at low densities in compression from experimental Hugoniot data assuming a Mie-Grüneisen model. This was smoothly joined onto high-density Thomas-Fermi-Dirac calculations. For $\rho < 2.140\ g/cm^3$, the cold curve was calculated with an analytic Lennard-Jones formula with an r^{-6} attractive term.

The thermal electronic contributions to the EOS were calculated with Thomas-Fermi-Dirac theory assuming an average atomic weight of 16.669 and an average atomic number of 8.

The solid lattice vibrations were calculated with a Debye model which was modified to extrapolate to an ideal gas at high temperatures or low densities. At densities below reference density, a virial expression was used.

This EOS does not include effects for structural transitions, the glass transition, or melting. Also, it has van der Waals loops in expansion instead of a Maxwell construction.

Hugoniot data are reproduced very well by this EOS. Static measurements of pressure-volume-temperature data were also compared with theory, and agreement was within 3-8% in density.

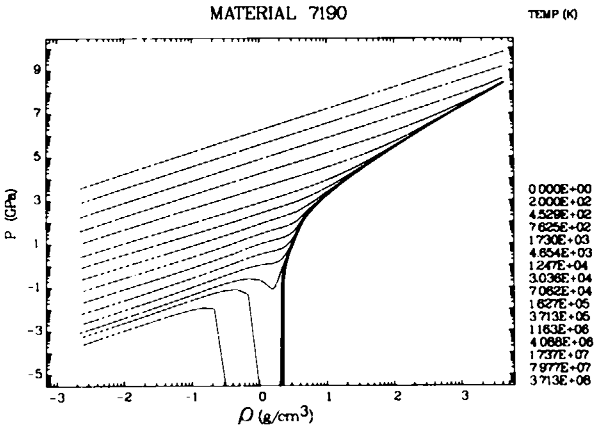
This EOS is thermodynamically consistent everywhere.

REFERENCES

1. A complete description of this EOS is given in F. Dowell and J. D. Johnson, "A Simple EOS for Polytetrafluoroethylene (Teflon)," Los Alamos National Laboratory report LA-9439-MS (August 1982).

2. C. W. Bunn, "The Melting Points of Chain Polymers," J. Poly. Sci. 16, 323 (1955).

3. S. P. Marsh, LASL Shock Hugoniot Data (University of California Press, Berkeley, 1980).


MATERIAL 7190
TEMP (K)
P (GPa)
9
7
5
3
1
-1
-3
-5
-3
-2
-1
0
1
2
3
ρ (g/cm³)
0.000E+00
2.000E+02
4.529E+02
7.625E+02
1.730E+03
4.654E+03
1.247E+04
3.036E+04
7.062E+04
1.627E+05
3.713E+05
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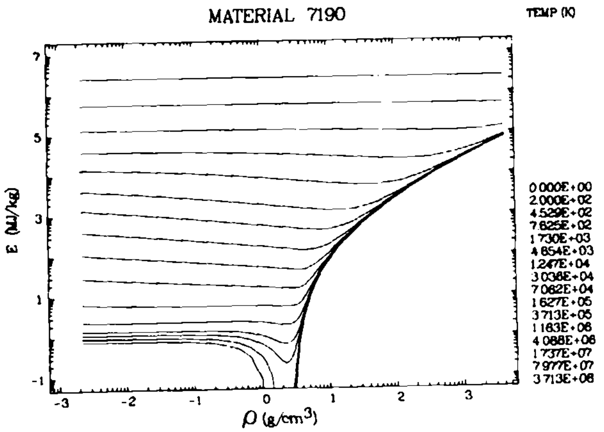
4.088E+06
1.737E+07
7.977E+07
3.713E+08


MATERIAL 7190
TEMP (K)
0.000E+00
2.000E+02
4.529E+02
7.625E+02
1.730E+03
4.654E+03
1.247E+04
3.036E+04
7.062E+04
1.627E+05
3.713E+05
1.163E+06
4.088E+06
1.737E+07
7.977E+07
3.713E+08
E (MJ/kg)
7
5
3
1
-1
-3
-2
-1
0
1
2
3
ρ (g/cm3)

SESAME #7242

Material: Lithium Deuteride
Composition: Li^6D
Originators: J. Abdallah and J. D. Johnson
Date of Origin: September 1981
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho < 1.564 \times 10^4$ g/cm^3
$0 < T < 3.7 \times 10^8$ K

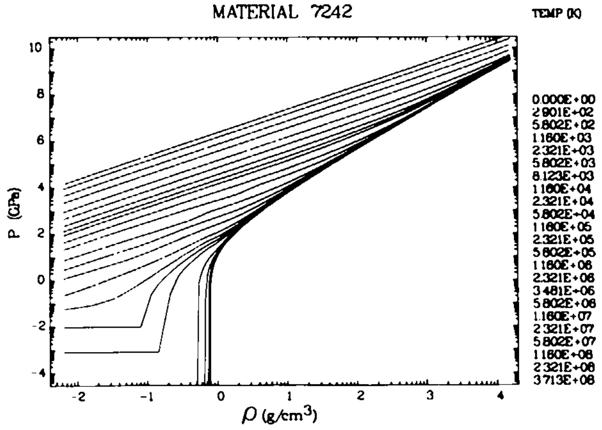
BASIC PHYSICAL DATA

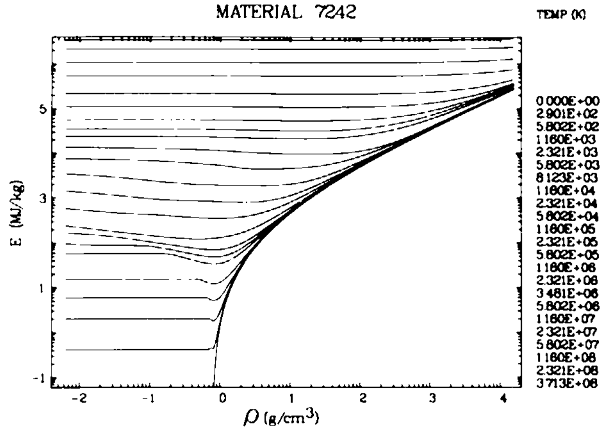
$\bar{A} = 4.041397$
$\bar{Z} = 2.0$
$\rho_o = 0.78201$ g/cm^3

$P(T = 298.15\ K, \rho_o) = 0.35756$ GPa
$E(T = 298.15\ K, \rho_o) = 0.45727$ MJ/kg
$T(P = 10^{-6}\ GPa, \rho_o) = 25.50$ K

DESCRIPTION OF PHYSICS

This EOS for lithium deuteride was created by isotopically scaling SESAME #7370 (lithium hydride). The original lithium hydride EOS was calculated with the standard Barnes-Cowan-Rood method.


MATERIAL 7242
TEMP (K)
P (GPa)
10
8
6
4
2
0
-2
-4
-2
-1
0
1
2
3
4
ρ (g/cm³)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08


MATERIAL 7242
TEMP (K)
E (MJ/kg)
5
3
1
-1
-2
-1
0
1
2
3
4
ρ (g/cm^3)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08

SESAME #7243

Material: Lithium Deuteride
Composition: Li^6D
Originator: K. Trainor
Date of Origin: February 1983
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $10^{-4} < \rho < 10^4$ g/cm^3
$0 < T < 2.3 \times 10^8$ K

BASIC PHYSICAL DATA

$\bar{A} = 4.0$
$\bar{Z} = 2.0$
$\rho_o = 0.802$ g/cm^3

$P(T = 298.15\ K, \rho_o) = 1.4195$ GPa
$E(T = 298.15\ K, \rho_o) = 1.5232$ MJ/kg
$T(P = 10^{-6}\ GPa, \rho_o) = 2.24605 \times 10^{-4}$ K

$B_o = 32.2$ GPa [Ref. 1]
* 30 GPa (used in calculation)

DESCRIPTION OF PHYSICS

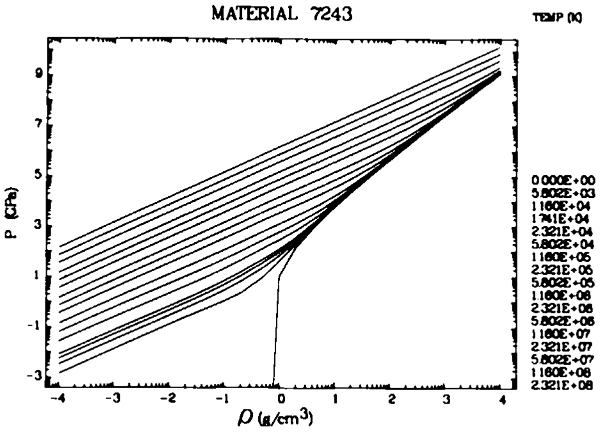
This equation of state for Li^6D was generated with a fast-response method. First, an electronic EOS was calculated with Thomas-Fermi-Dirac theory. Two corrections were added to that basis: an ion correction based on a model by R. D. Cowan and an empirical correction which forces the experimental zero-pressure density and bulk modulus to be reproduced. In the case of this EOS, however, a bulk modulus of 30 GPa was used instead of the experimental value of 32.2 GPa in order for the experimental Hugoniot data to be reproduced. The theoretical EOS was tweaked to match a series of Hugoniot experiments by S. P. Marsh [Ref. 1]. (There are six sets of data, five of which start at initially porous densities.) The reference density used for this EOS (0.802 g/cm^3) is based on measurements by S. P. Marsh and assumes that the Li^{6}D sample is contaminated with 2 wt% of water.

This EOS is not designed to be accurate at low temperature (<0.5 eV), particularly in the vapor-liquid coexistence region in expansion. Also, zero pressure is at the reference density on the cold curve, not at room temperature.

The EOS is thermodynamically consistent everywhere.

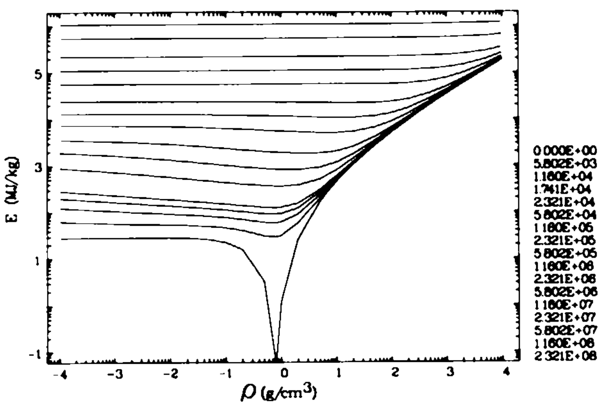
REFERENCE

1. S. P. Marsh, "Hugoniot Equations of State for Li^{6}H, Li^{6}D, Li^{n}H, and Li^{n}D," Los Alamos Scientific Laboratory report LA-4942 (July, 1972).


MATERIAL 7243
TEMP (K)
P (GPa)
9
7
5
3
1
-1
-3
-4
-3
-2
-1
0
1
2
3
4
ρ (g/cm^3)
0.000E+00
5.802E+03
1.160E+04
1.741E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08

7243-4

MATERIAL 7243



SESAME #7252

Material: Lithia-Boria Glass [Ref. 1]
Composition: Li_2O 27.7 at%
B_2O_2 72.3 at%
Originator: G. I. Kerley
Date of Origin: November 1978
Type of Tables Included: 301
Limits: $10^{-10} < \rho < 4.5 \times 10^3$ g/cm^3
$0 < T < 3.7\ 10^8$ K

BASIC PHYSICAL DATA

$\bar{A} = 13.074$
$\bar{Z} = 6.401$
$\rho_o = 2.215$ g/cm^3 (at T=298.15K)

$P(T = 298.15\ K, \rho_o) = -0.61824$ GPa
$E(T = 298.15\ K, \rho_o) = 8.2511 \times 10^{-3}$ MJ/kg
$T(P = 10^{-6}\ GPa, \rho_o) = 435.46$ K

$\gamma_o = * 1.2$ (used in calculation)
$B_o = 56.04$ GPa (measured in shock wave experiments)

$E_{coh} = 40.7$ MJ/kg
(estimated from cohesive energies of separate components)

DESCRIPTION OF PHYSICS

Hugoniot data for lithia-boria glass and for Lindeman glass show a solid-solid phase transition at approximately 9 GPa. Two separate EOS tables were computed for the two phases and then merged to create a multiphase EOS. The phase transition on each isotherm is located at the point at which the pressures and Gibbs free energies of the two phases are equal.

The cold curves for each of the equations of state were computed from the shock wave data assuming a Mie-Grüneisen model. The Grüneisen parameter was assumed to be of the form:

$$\gamma(\rho) = \gamma_o(\rho_o/\rho) + \frac{2}{3}(1 - \rho_o/\rho)^2 \quad .$$

For the low density phase,

$$\rho_o = 2.215 \text{ g/cm}^3 \quad ,$$

$$\gamma_o = 1.2 \quad , \text{ and}$$

$$U_S = 5.03 + 1.4\ U_p \text{ km/s} \quad .$$

The slope of the Hugoniot relation was chosen on the assumption that the phase transition occurs at 9.2 GPa.
For the high density phase,

$$\rho_o = 2.7 \text{ g/cm}^3 \quad ,$$

$$\gamma_o = 1.2 \quad , \text{ and}$$

$$U_S = 5.4 + 1.38\ U_p \text{ km/s} \quad .$$

The reference density of the high-density phase was estimated by extrapolating the Hugoniot data to zero pressure.

The calculation of the EOS for both phases also included nuclear vibration and electronic excitation contributions. The nuclear term was calculated with a Debye model which was modified to go to an ideal gas at high temperatures. The electronic contributions were calculated with the Thomas-Fermi-Dirac model.

Above temperatures of 0.22 eV, a Maxwell construction was performed in the vapor-liquid coexistence region. Below 0.22 eV, van der Waals loops (negative pressures) were retained in order to have a tension region for spall models.

The agreement of this EOS with experimental Hugoniot data is very good (including modeling of the phase transition).

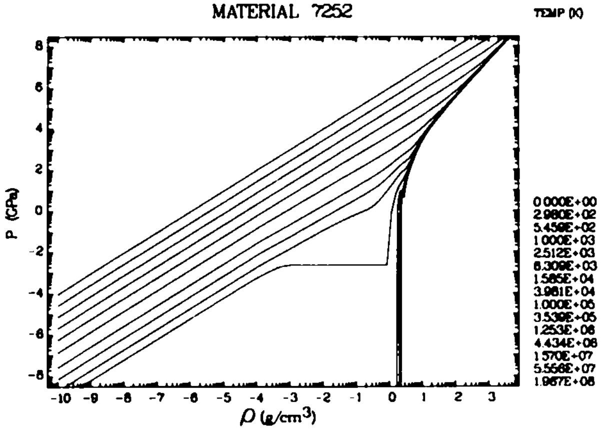
The lithia-boria glass equation of state is most accurate near the Hugoniot and at high temperatures (due to inclusion of Thomas-Fermi-Dirac electronic excitations). The vapor dome region is reasonable.

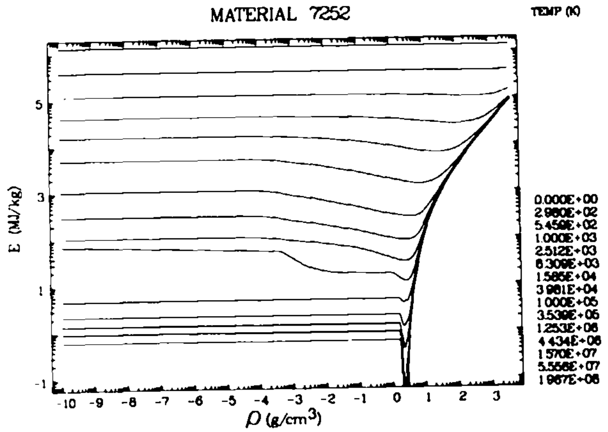
The EOS is thermodynamically consistent everywhere.

REFERENCE

1. G. I. Kerley, "An EOS for Lithia-Boria Glass," Los Alamos Scientific Laboratory memorandum T-4-SL-5 to Distribution (December 11, 1978).

7252-5


MATERIAL 7252
TEMP (K)
P (GPa)
8
6
4
2
0
-2
-4
-6
-8
-10
-9
-8
-7
-6
-5
-4
-3
-2
-1
0
1
2
3
ρ (g/cm³)
0.000E+00
2.980E+02
5.459E+02
1.000E+03
2.512E+03
6.309E+03
1.585E+04
3.981E+04
1.000E+05
3.539E+05
1.253E+06
4.434E+06
1.570E+07
5.558E+07
1.967E+08


MATERIAL 7252
TEMP (K)
E (MJ/kg)
5
3
1
-1
-10
-9
-8
-7
-6
-5
-4
-3
-2
-1
0
1
2
3
ρ (g/cm3)
0.000E+00
2.980E+02
5.459E+02
1.000E+03
2.512E+03
6.309E+03
1.585E+04
3.981E+04
1.000E+05
3.539E+05
1.253E+06
4.434E+06
1.570E+07
5.558E+07
1.967E+08

SESAME #7281

Material: Salt [Ref. 1]
Composition: NaCl
Originator: A. Merts and N. Magee
Date of Origin: November 1981
Type of Tables Included: 301
Limits: $0 < \rho < 2.16 \times 10^4$ g/cm^3
$116 < T < 5.8 \times 10^8$ K

BASIC PHYSICAL DATA

$\bar{A} = 29.2214$
$\bar{Z} = 14$
$\rho_o = 2.165$ g/cm^3

$P(T = 298.15\ \text{K}, \rho_o) = 0.26335$ GPa
$E(T = 298.15\ \text{K}, \rho_o) = 8.4061 \times 10^{-2}$ MJ/kg
(There is no zero-pressure point in this table.)

DESCRIPTION OF PHYSICS

The equation of state for salt was calculated with a code developed by A. Merts which produces an EOS which is similar in spirit to those generated with the Barnes-Cowan-Rood procedure. The zero-degree isotherm was calculated from an analytic expression which was adjusted to reproduce experimental Hugoniot data, the cohesive energy, and the tensile strength. The analytic formula ensures that the experimental zero-pressure density and bulk modulus are reproduced. The thermal electronic contributions to the EOS at finite temperatures were calculated with Thomas-Fermi theory. The thermal nuclear contributions are based on a model by Thompson and are embodied in the following formulas:

$$P_n = \rho N_o kT \left[\frac{3\Gamma + \phi}{1 + \phi}\right]$$

$$E_n = 1.5 N_o kT \left[\frac{2 + \phi}{1 + \phi}\right]$$

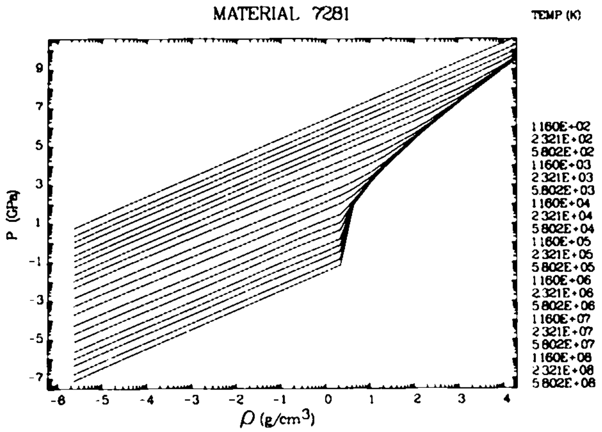
Γ is the Grüneisen ratio, and ϕ is an interpolation function of density and temperature which allows the equations to smoothly transit from low to high temperature.

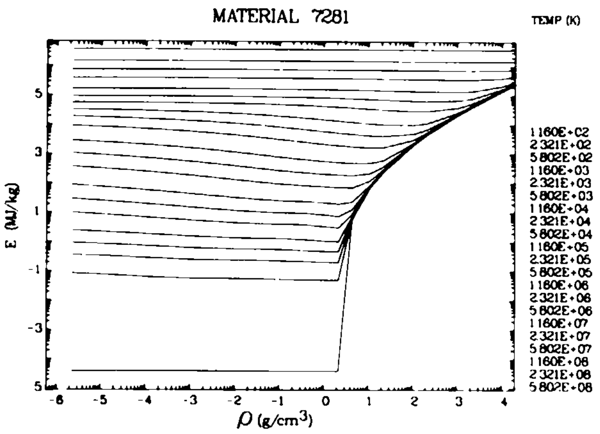
The boundary of the liquid-vapor coexistence region is found by determining at what pressure for a given temperature that the Gibbs free energy is equal at the upper and lower densities. Inside the two-phase region, the pressure is made constant (equal to the value on the boundary), whereas the energy is a linear interpolation between the values at the upper and lower densities.

This EOS is thermodynamically consistent everywhere. It is fairly good throughout most of the solid and vapor regions, though inaccurate in the vicinity of the critical point.

REFERENCE

1. The method of generating this EOS is described in A. L. Merts and N. H. Magee, Jr., "Low Temperature Equation of State for Metals," Los Alamos Scientific Laboratory report LA-5068 (January 1973).


MATERIAL 7281
TEMP (K)
P (GPa)
9
7
5
3
1
-1
-3
-5
-7
-6
-5
-4
-3
-2
-1
0
1
2
3
4
ρ (g/cm³)
1.160E+02
2.321E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
5.802E+08


MATERIAL 7281
TEMP (K)
E (MJ/kg)
5
3
1
-1
-3
5
-6
-5
-4
-3
-2
-1
0
1
2
3
4
ρ (g/cm3)
1 160E+02
2 321E+02
5 802E+02
1 160E+03
2 321E+03
5 802E+03
1 160E+04
2 321E+04
5 802E+04
1 160E+05
2 321E+05
5 802E+05
1 160E+06
2 321E+06
5 802E+06
1 160E+07
2 321E+07
5 802E+07
1 160E+08
2 321E+08
5 802E+08

SESAME #7330

Material: Calcium Carbonate [Ref. 1]
Composition: $CaCO_3$
Originator: F. H. Ree (Lawrence Livermore
National Laboratory, H-Division)
Date of Origin: 1981
Type of Tables Included: 301
Limits: $0.25 < \rho < 1000$ g/cm^3
$300 < T < 2.9 \times 10^8$ K

BASIC PHYSICAL DATA

$\bar{A} = 20.0179$
$\bar{Z} = 10.$
$\rho_o = 2.71$ g/cm^3

$P(T = 298.15\ \mathrm{K}, \rho_o) = 1.501 \times 10^{-2}$ GPa
$E(T = 298.15\ \mathrm{K}, \rho_o) = 1.200 \times 10^{-2}$ MJ/kg
$T(P = 10^{-6}\ \mathrm{GPa}, \rho_o) = 290.11$ K

$T_m = {*}\ 1612$ K (used in calculation) [Ref. 2]

$\gamma_o = {*}\ 0.55$ (used in calculation)

$\theta_D = {*}\ 900$ K (used in calculation)

Hugoniot Fit: * $U_S = 4.2 + 1.85\ U_p - 0.1\ U_p^2$
km/s
(used in calculation)

DESCRIPTION OF PHYSICS

This is a high-quality, wide-range, multiphase EOS which incorporates several different physical models:

1) GRAY - A semi-empirical model which uses the Grüneisen model to calculate the EOS for the solid (assumed to be harmonic).

The solid is also assumed to be in the aragonite phase, except for the room temperature isotherm which includes a metastable phase transition from aragonite to calcite. The liquid state is calculated by modifying the solid free energy by an entropy correction associated with loss of order. The GRAY region extends from densities of 2.71 g/cm^3 to 8.0 g/cm^3 and from temperatures of 0.025 eV to 1.0 eV.

2) TIGER/CHEQ - These models were used in the low-temperature, low- density region which is sensitive to the chemical equilibrium between $CaCO_3$ and the dissociated species of $CaCO_3$. TIGER calculates gaseous EOS properties of the mixture using a Becker-Kistiakowsky-Wilson model. CHEQ was used in the vapor-solid region to determine the equilibrium concentrations of the chemical species by the extent-of-reaction variable method.

3) OCCIPITAL - This model covers the high-temperature, low-density region in which $CaCO_3$ is assumed to be completely dissociated into electrons, ions, and neutral atoms. The concentrations of each of these species are obtained from the Saha equation, and the thermodynamic properties are calculated assuming that each component of the mixture behaves like an ideal gas.

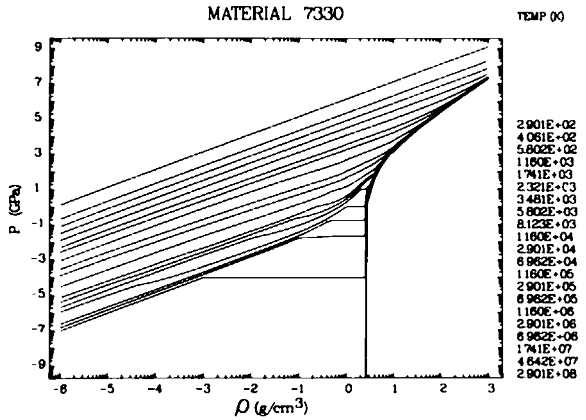
4) TFNUC - calculates electronic contributions to the EOS using Thomas-Fermi theory with Kirzhnits corrections for the wave nature of electrons and the electron exchange

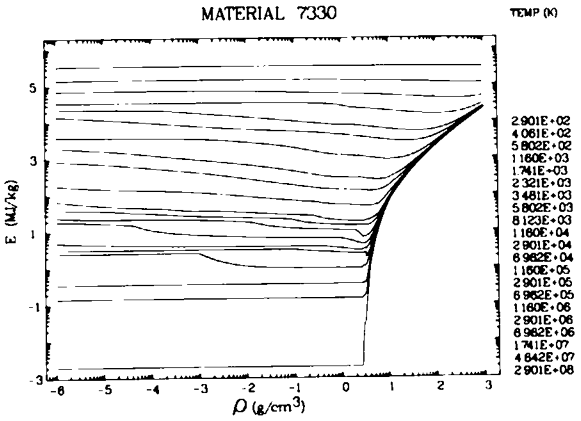
contribution. Nuclear contributions are calculated with a Grüneisen model at low temperature and the one-component-plasma model at high temperature.

Agreement between the theoretical Hugoniot and experiments is good above pressures of 20 GPa.

REFERENCES

1. A complete description of this EOS is given in F. H. Ree, "Equations of State of $CaCO_3$ and Its Mixtures with H_2O," Lawrence Livermore National Laboratory report UCRL-53113 (March 1981).
2. R. C. Weast, CRC Handbook of Chemistry and Physics (CRC Press, Inc., Cleveland, Ohio, 1977-1978).


MATERIAL 7330
TEMP (K)
2.901E+02
4.061E+02
5.802E+02
1.160E+03
1.741E+03
2.321E+C3
3.481E+03
5.802E+03
8.123E+03
1.160E+04
2.901E+04
6.962E+04
1.160E+05
2.901E+05
6.962E+05
1.160E+06
2.901E+06
6.962E+06
1.741E+07
4.642E+07
2.901E+08
P (GPa)
9
7
5
3
1
-1
-3
-5
-7
-9
-6
-5
-4
-3
-2
-1
0
1
2
3
ρ (g/cm³)


MATERIAL 7330
TEMP (K)
E (MJ/kg)
5
3
1
-1
-3
-6
-5
-4
-3
-2
-1
0
1
2
3
ρ (g/cm3)
2.901E+02
4.061E+02
5.802E+02
1.160E+03
1.741E+03
2.321E+03
3.481E+03
5.802E+03
8.123E+03
1.160E+04
2.901E+04
6.962E+04
1.160E+05
2.901E+05
6.962E+05
1.160E+06
2.901E+06
6.962E+06
1.741E+07
4.642E+07
2.901E+08

SESAME #7371

Material: Lithium Hydride
Composition: Li^nH
Originator: K. Trainor
Date of Origin: September 1981
Type of Tables Included: 301
Limits: $10^{-4} < \rho < 10^4$ g/cm^3
$116 < T < 1.86 \times 10^8$ K

BASIC PHYSICAL DATA

$\bar{A} = 4.0$
$\bar{Z} = 2.0$
$\rho_o = 0.775$ g/cm^3

$P(T = 298.15\ K, \rho_o) = 0.8315$ GPa
$E(T = 298.15\ K, \rho_o) = 0.84589$ MJ/kg
$T(P = 10^{-6}\ GPa, \rho_o) = 13.55$ K

$B_o = 31.4$ GPa [Ref. 1]
* 28 GPa (input into calculation)

Hugoniot Fit: $U_S = 6.426 + 1.167\ U_p$ km/s
[Ref. 1]

DESCRIPTION OF PHYSICS

The equation of state for Li^nH assumes that natural lithium (92.5% Li^7 and 7.5% Li^6) is in the compound. It was generated with Thomas-Fermi theory for the electronic part of the EOS and with a Cowan model for the ion EOS. An empirical correction was also added to ensure that the zero-pressure experimental density is reproduced. In order to match the Hugoniot experiments, a bulk modulus of 28 GPa (instead of the experimental value of 31.4 GPa) was used in the empirical correction package.

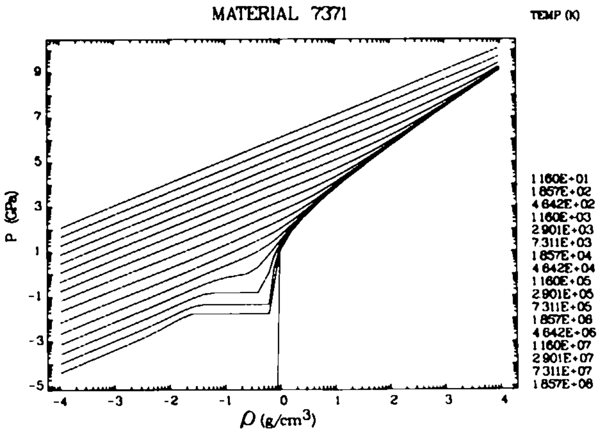
The LiH zero-degree isotherm compares moderately well with APW band theory calculations by F. Perrot [Ref. 2], although at 19 g/cm^3, the APW zero-degree pressure is approximately 20% lower.

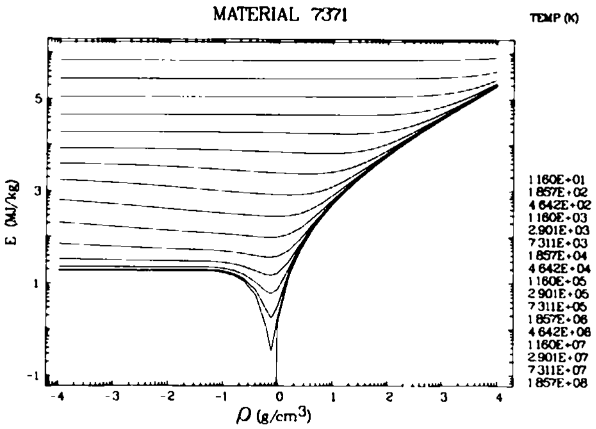
Thermodynamic consistency is good everywhere except in the two-phase region.

REFERENCES

1. S. P. Marsh, "Hugoniot Equations of State of $\mathrm{Li}^6\mathrm{H}$, $\mathrm{Li}^6\mathrm{D}$, $\mathrm{Li}^n\mathrm{H}$, $\mathrm{Li}^n\mathrm{D}$," Los Alamos Scientific Laboratory report LA-4942 (July 1972).

2. F. Perrot, Phys. Stat. Sol. (B) 77, 517 (1976).


MATERIAL 7371
TEMP (K)
P (GPa)
9
7
5
3
1
-1
-3
-5
-4
-3
-2
-1
0
1
2
3
4
ρ (g/cm^3)
1.160E+01
1.857E+02
4.642E+02
1.160E+03
2.901E+03
7.311E+03
1.857E+04
4.642E+04
1.160E+05
2.901E+05
7.311E+05
1.857E+06
4.642E+06
1.160E+07
2.901E+07
7.311E+07
1.857E+08


MATERIAL 7371
TEMP (K)
E (MJ/kg)
5
3
1
-1
-4
-3
-2
-1
0
1
2
3
4
ρ (g/cm3)
1.160E+01
1.857E+02
4.642E+02
1.160E+03
2.901E+03
7.311E+03
1.857E+04
4.642E+04
1.160E+05
2.901E+05
7.311E+05
1.857E+06
4.642E+06
1.160E+07
2.901E+07
7.311E+07
1.857E+08

SESAME #7380

Material: Quartz
Composition: SiO_2
Originators: J. Barnes and J. Rood
Date of Origin: August 1973
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho < 4.408 \times 10^4$ g/cm^3
$0 < T < 3.7 \times 10^8$ K

BASIC PHYSICAL DATA

$\bar{A} = 20.028$
$\bar{Z} = 10.0$
$\rho_o = 2.204$ g/cm^3

$P(T = 298.15 \text{ K}, \rho_o) = 0.82538$ GPa
$E(T = 298.15 \text{ K}, \rho_o) = 0.18958$ MJ/kg
$T(P = 10^{-6} \text{ GPa}, \rho_o) = 3.662 \times 10^{-4}$ K

$B_o = *\ 37.05$ GPa (used in calculation)

$E_{coh} = 28.6$ MJ/kg (used in calculation) (calculated by adding cohesive energies of each compound)

$\theta_D = *\ 494$ K (used in calculation)

Hugoniot Fit: $U_S = 1.3 + 1.56\ U_p$ km/s [Ref. 1] (for high-pressure phase)

DESCRIPTION OF PHYSICS

This equation of state is undocumented. However, it was most likely generated with the Barnes-Cowan-Rood procedure. Above 1 eV, the electronic part of the EOS was calculated with Thomas-Fermi-Dirac theory using an average atomic weight of 20.028 and an average atomic number of 10. The nuclear thermal and cold curve contributions are based on a model by R. D. Cowan.

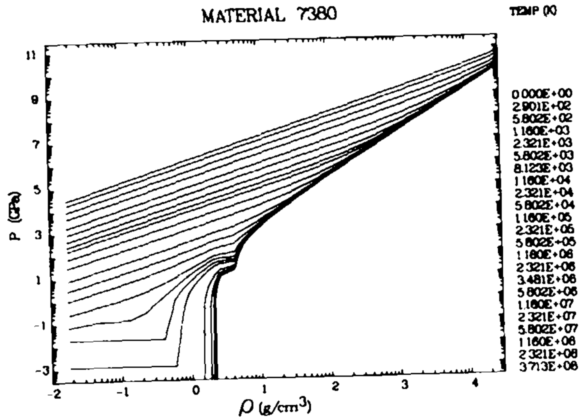
The low-temperature EOS was treated in a special manner since quartz has a solid-solid phase transition. The reference density of quartz is 2.204 g/cm^3 with a bulk modulus of 37.05 GPa. But the high-density phase has an apparent density of 4.285 g/cm^3 and bulk modulus of 560 GPa. So for the cold curve, two separate calculations using the modified-Morse model were performed. These were joined at a point determined by the phase transition shown in the Hugoniot data. The thermal nuclear contributions to the EOS below 1 eV were based on a Debye model.

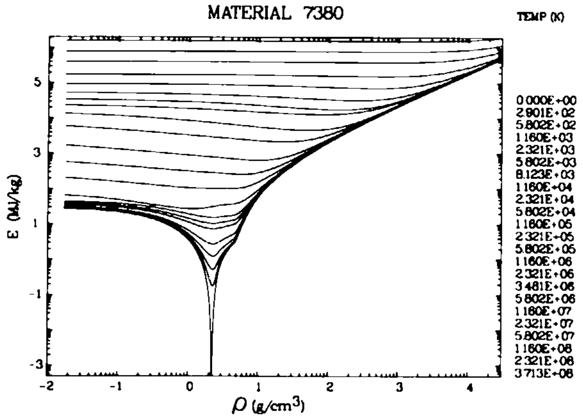
The EOS is thermodynamically consistent everywhere.

The two-temperature tables were derived by the code TWOTEMP and are noisy.

REFERENCE

1. S. P. Marsh, LASL Shock Hugoniot Data (University of California Press, Berkeley, 1980).


MATERIAL 7380
TEMP (K)
P (GPa)
11
9
7
5
3
1
-1
-3
-2
-1
0
1
2
3
4
ρ (g/cm³)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08


MATERIAL 7380
TEMP (K)
E (MJ/kg)
5
3
1
-1
-3
-2
-1
0
1
2
3
4
ρ (g/cm3)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08

SESAME #7381

Material: Quartz
Composition: SiO_2
Originator: R. C. Albers
Date of Origin: February 1981
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho < 2.204 \times 10^4$ g/cm^3
$0 < T < 10^5$ eV

BASIC PHYSICAL DATA

$\bar{A}$ = 20.028
$\bar{Z}$ = 10.0
ρ_o = 2.204 g/cm^3

$P(T = 298.15\ K, \rho_o) = 1.692 \times 10^{-2}$ GPa
$E(T = 298.15\ K, \rho_o) = 0.4241$ MJ/kg
$T(P = 10^{-8}\ GPa, \rho_o) = 292.66$ K

γ_o = * 0.036 (used in calculation)
B_o = * 36.6 GPa (used in calculation)

Poisson ratio = 0.167

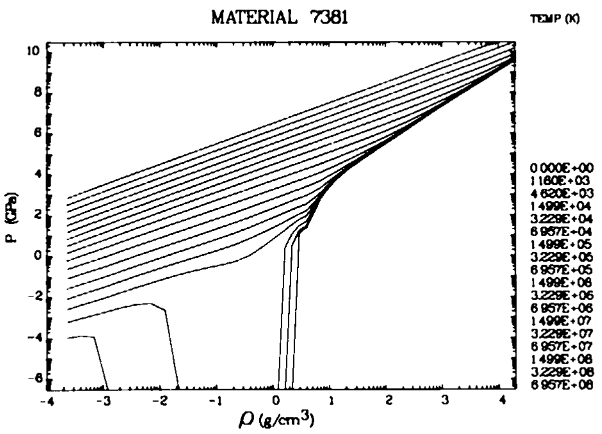
E_{coh} = * 30.57 MJ/kg (used in calculation)

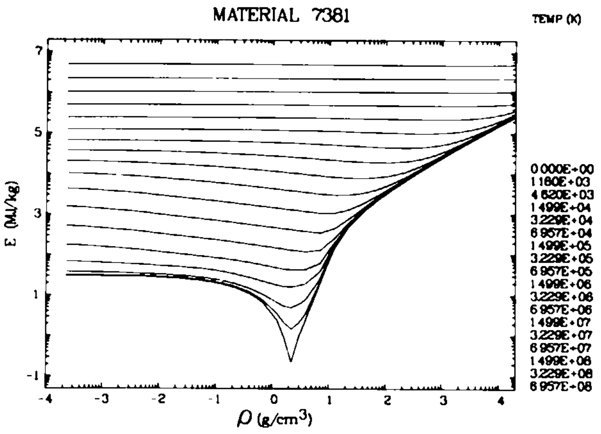
Hugoniot Fit: $U_S = 4.075 + 1.606\ U_p$ km/s for $U_p < 0.708$ km/s
$U_S = 5.212$ km/s for $0.708 < U_p < 2.61$ km/s
$U_S = 0.801 + 1.69\ U_p$ for $U_p > 2.61$ km/s

DESCRIPTION OF PHYSICS

The cold curve at low density was generated from a special kinked Hugoniot (to simulate the effect of a phase transition).

This was matched onto a Thomas-Fermi-Dirac cold curve at very high pressures. The thermal electronic component of the EOS was calculated by mixing Thomas-Fermi-Dirac EOS's for silicon and oxygen. A Cowan model was used for the thermal ionic component. Hence, this EOS is very good for two-temperature applications that subtract off a Cowan model for the ionic degrees of freedom.


MATERIAL 7381
TEMP (K)
P (GPa)
10
8
6
4
2
0
-2
-4
-6
-4
-3
-2
-1
0
1
2
3
4
ρ (g/cm3)
0.000E+00
1.160E+03
4.620E+03
1.499E+04
3.229E+04
6.957E+04
1.499E+05
3.229E+05
6.957E+05
1.499E+06
3.229E+06
6.957E+06
1.499E+07
3.229E+07
6.957E+07
1.499E+08
3.229E+08
6.957E+08


MATERIAL 7381
TEMP (K)
0.000E+00
1.160E+03
4.620E+03
1.499E+04
3.229E+04
6.957E+04
1.499E+05
3.229E+05
6.957E+05
1.499E+06
3.229E+06
6.957E+06
1.499E+07
3.229E+07
6.957E+07
1.499E+08
3.229E+08
6.957E+08
E (MJ/kg)
7
5
3
1
-1
-4
-3
-2
-1
0
1
2
3
4
ρ (g/cm³)

SESAME #7382

Material: Quartz [Ref. 1]
Composition: SiO_2
Originator: F. H. Ree (Lawrence Livermore
National Laboratory, H-Division)
Date of Origin: 1976
Type of Tables Included: 301
Limits: $1.6 \times 10^{-6} < \rho < 150$ g/cm^3
$116 < T < 2.9 \times 10^8$ K

BASIC PHYSICAL DATA

$\bar{A} = 20.0283$
$\bar{Z} = 10$
$\rho_o = 2.65$ g/cm^3

$P(T = 298.15\text{ K}, \rho_o) = 1.520 \times 10^{-2}$ GPa
$E(T = 298.15\text{ K}, \rho_o) = 0.3379$ MJ/kg
$T(P = 10^{-8}\text{ GPa}, \rho_o) = 185.67$ K

$T_m = {}^*$ 1996 K (α-quartz) (used in calculation)

$T_c \gtrsim 1.0$ eV (Actually, no true critical point exists in the SiO_2 system because a large amount of liquid silicon is present above 0.8 eV, and this distorts the character of the vapor-liquid equilibrium.)

$\gamma_o = {}^*$ 0.6 (used in calculation)

Hugoniot Fit: * $U_S = 3.69 + 1.85\, U_p - 0.6374\, U_p^2 + 0.16695\, U_p^3 - 1.1893 \times 10^{-2}\, U_p^4 - 9.0375 \times 10^{-5}\, U_p^5$
km/s
(used in calculation)

DESCRIPTION OF PHYSICS

This is a wide-range, multiphase EOS which incorporates five different theoretical models:

1) TIGER - calculates the EOS for a heterogeneous system of mixtures containing several gaseous, liquid, and solid components using a Becker-Kistiakowsky-Wilson model. Ionization is assumed to be negligible.

2) GRAY - calculates the thermodynamic properties of the alpha-quartz, stishovite, and liquid phases using the Grüneisen model. The solid is assumed to be harmonic. No internal rotation, vibration, or electronic contributions are taken into account because the model is only used below 1 eV.

3) OCCIPITAL - used in the region where the SiO_2 molecule is completely dissociated into electrons, ions, and neutral atoms. The concentrations of each of these species is obtained with the Saha equation, and the thermodynamic properties are calculated assuming that the mixture behaves like an ideal gas.

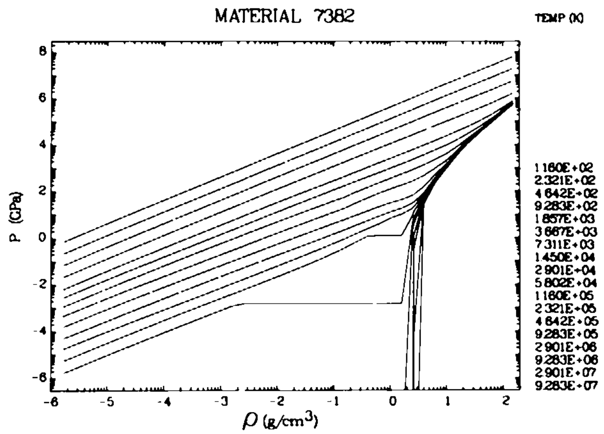
4) TFCMIX - uses Thomas-Fermi theory to calculate an electronic EOS. The Kirzhnits correction is added to account for the wave nature of electrons and the electron exchange contribution. A nuclear correction based on a model by Warren is also added.

5) MASTER - phenomenologically corrects the EOS at low temperature, low compression for atomic shell structure, and electronic correlations.

Agreement between the theoretical Hugoniots and the experimental data is good below 100 GPa. At higher pressures, however, the theoretical Hugoniots lie below the experiments.

REFERENCE

1. A complete description of the EOS is given in F. H. Ree, "Equation of State of the Silicon Dioxide Systems," Lawrence Livermore Laboratory report UCRL-52153 (November 1976).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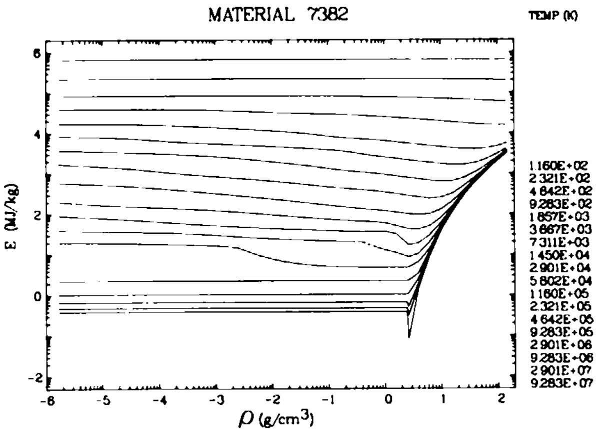

MATERIAL 7382
TEMP (K)
6
4
2
0
-2
E (MJ/kg)
-6
-5
-4
-3
-2
-1
0
1
2
ρ (g/cm³)
1.160E+02
2.321E+02
4.642E+02
9.283E+02
1.857E+03
3.667E+03
7.311E+03
1.450E+04
2.901E+04
5.802E+04
1.160E+05
2.321E+05
4.642E+05
9.283E+05
2.901E+06
9.283E+06
2.901E+07
9.283E+07

SESAME #7390

Material: Westerly Granite

Composition:

SiO_2	73.9 wt%
Al_2O_3	14.9 wt%
K_2O	4.5 wt%
CaO	3.3 wt%
FeO	2.0 wt%

plus trace amounts of other oxides

Originators: J. Barnes and J. Rood

Date of Origin: March 1975

Type of Tables Included: 301, 303, 304, 305, 306

Limits: $2.0523 \times 10^{-2} < \rho < 5.254 \times 10^{4}$ g/cm^3
$0 < T < 3.7 \times 10^{8}$ K

BASIC PHYSICAL DATA

$\bar{A} = 20.669$
$\bar{Z} = 10.272$
$\rho_o = 2.627$ g/cm^3

$P(T = 298.15\ \text{K}, \rho_o) = 0.84726$ GPa
$E(T = 298.15\ \text{K}, \rho_o) = 0.16352$ MJ/kg
$T(P = 10^{-6}\ \text{Gpa}, \rho_o) = 3.578 \times 10^{-4}$ K

$\gamma_o =$ * 1.9756823 (calculated)
$B_o =$ * 53.2 GPa (used in calculation)
(calculated from $C_o = 4.5$ km/s)

$E_{coh} =$ * 27.7 MJ/kg (used in calculation)

$\theta_D =$ * 574 K (used in calculation)

Hugoniot Fit: $U_S = 4.93 + 0.372\ U_p$ km/s for $1 < U_p < 2.1$
$U_S = 2.103 + 1.629\ U_p$ km/s for $2.5 < U_p < 4.1$ [Ref. 1]

DESCRIPTION OF PHYSICS

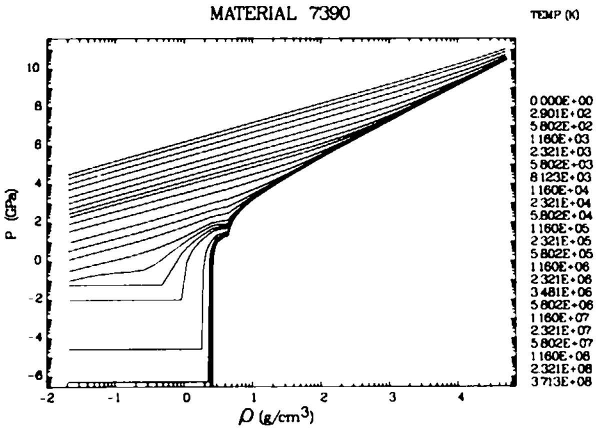
No formal documentation exists for the EOS for westerly granite. However, from piecing together the notes made during the calculation, it seems that the EOS was generated with the Barnes-Cowan-Rood method. At high temperatures, the EOS was calculated by mixing four MAPLE tables: oxygen, silicon, aluminum, and a chlorine-like element. (The silicon EOS was actually a Z-scaled aluminum.) The MAPLE tables are based on Thomas-Fermi-Dirac theory for the electronic part of the EOS, and the nuclear thermal and cold curve contributions in the MAPLE tables are from a model by R. D. Cowan.

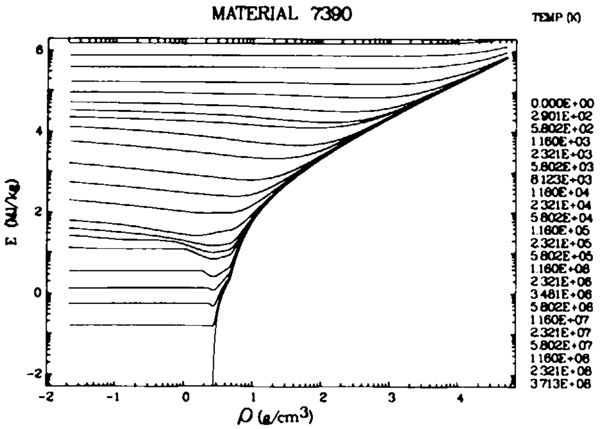
The cold curve of the granite EOS was calculated with a modified-Morse model. At low temperature, nuclear thermal contributions based on a Debye model were added to the cold curve component of the EOS.

The two-temperature tables for this EOS were derived by the code TWOTEMP and are noisy.

REFERENCE

1. M. van Thiel, "Compendium of Shock Wave Data," Lawrence Livermore Laboratory report UCRL-50108, Rev. 1 (1977).


MATERIAL 7390
TEMP (K)
P (GPa)
10
8
6
4
2
0
-2
-4
-6
-2
-1
0
1
2
3
4
ρ (g/cm³)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08


MATERIAL 7390
TEMP (K)
E (MJ/kg)
ρ (g/cm³)
6
4
2
0
-2
-2
-1
0
1
2
3
4
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08

SESAME #7410

Material: Alumina
Composition: Al_2O_3
Originator: J. Barnes and J. Rood
Date of Origin: November 1972
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $3.1016 \times 10^{-2} < \rho < 3.97 \times 10^3$ g/cm^3
$0 < T < 3.7 \times 10^8$ K

BASIC PHYSICAL DATA

$\bar{A} = 20.392$
$\bar{Z} = 10.$
$\rho_o = 3.97$ g/cm^3

$P(T = 298.15\ \mathrm{K}, \rho_o) = 0.56333$ GPa
$E(T = 298.15\ \mathrm{K}, \rho_o) = 9.3022 \times 10^{-2}$ MJ/kg
$T(P = 10^{-6}\ \mathrm{GPa}, \rho_o) = 5.4567 \times 10^{-4}$ K

$T_c =$ * 16014 K (calculated)

$\gamma_o =$ * 1.5273 (calculated)
$B_o =$ 250 GPa [Ref. 1]
* 240 GPa (used in calculation)

$E_{coh} =$ * 29.75 MJ/kg (used in calculation)

$\theta_D =$ * 960 K (used in calculation)
(determined from measured value of specific heat at room temperature)

Hugoniot Fit: $U_S = 7.916 + 1.897\ U_p - 0.195\ U_p^2$ km/s [Ref. 2]

DESCRIPTION OF PHYSICS

No formal documentation exists for the aluminum oxide equation of state. However, it was most likely generated with the Barnes-Cowan-Rood procedure. At high temperature, the thermal electronic part of the EOS was generated with Thomas-Fermi-Dirac theory using an average atomic weight of 20.392 and an average atomic number of 10. The nuclear thermal and cold curve contributions at high temperature are based on a model by R. D. Cowan.

At low temperature, the EOS consists of two contributions: a cold curve calculated with a modified-Morse model and a nuclear thermal part based on a Debye model.

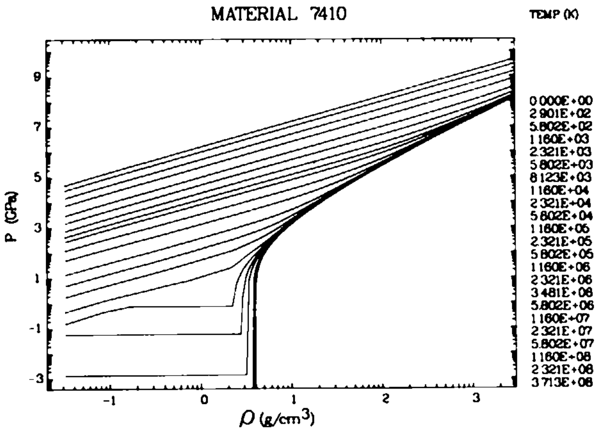
The EOS is thermodynamically consistent everywhere.

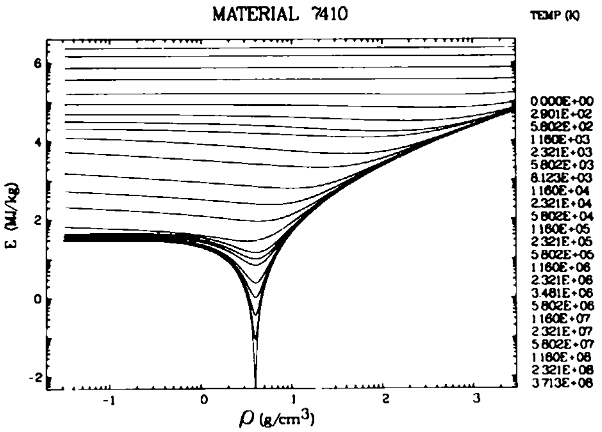
The two-temperature tables were derived with the code TWOTEMP and are noisy.

REFERENCES

1. S. P. Marsh, LASL Shock Hugoniot Data (University of California Press, Berkeley, 1980).

2. M. van Thiel, "Compendium of Shock Wave Data," Lawrence Livermore Laboratory report UCRL-50108, Rev. 1 (1977).


MATERIAL 7410
TEMP (K)
P (GPa)
9
7
5
3
1
-1
-3
-1
0
1
2
3
ρ (g/cm³)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08


MATERIAL 7410
TEMP (K)
E (MJ/kg)
6
4
2
0
-2
-1
0
1
2
3
ρ (g/cm³)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08

SESAME #7520

Material: Mica

Composition:

O	56.1 wt%
Si	16.7 wt%
Mg	12.6 wt%
Al	7.6 wt%
Fe	4.5 wt%
H	2.4 wt%

Originators: J. Barnes and J. Rood
Date of Origin: May 1974
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $2.1094 \times 10^{-2} < \rho < 5.4 \times 10^{4}$ g/cm^3
$0 < T < 3.7 \times 10^{8}$ K

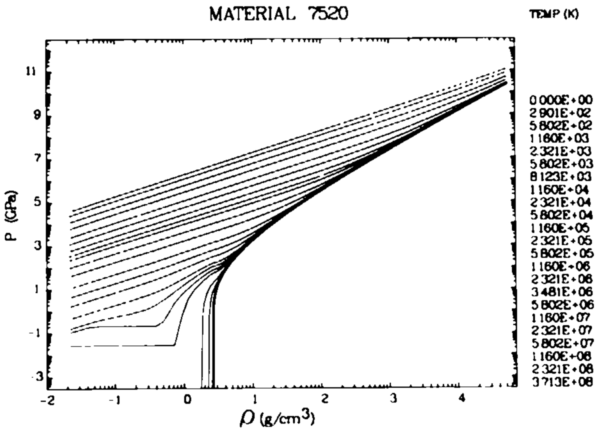
BASIC PHYSICAL DATA

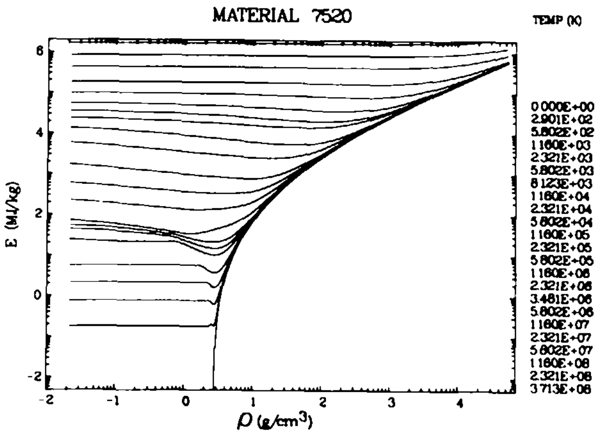
$\bar{A} = 13.524$
$\bar{Z} = 6.8697$
$\rho_o = 2.7$ g/cm^3

$P(T = 298.15\ \mathrm{K}, \rho_o) = 1.0820$ GPa
$E(T = 298.15\ \mathrm{K}, \rho_o) = 0.19713$ MJ/kg
$T(P = 10^{-6}\ \mathrm{GPa}, \rho_o) = 2.8180 \times 10^{-4}$ K

DESCRIPTION OF PHYSICS

No documentation at all exists for the mica EOS. However, it was probably generated with the standard Barnes-Cowan-Rood method. See Part II for a more detailed description of this method of EOS generation.


MATERIAL 7520
TEMP (K)
P (GPa)
11
9
7
5
3
1
-1
-3
-2
-1
0
1
2
3
4
ρ (g/cm^3)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08


MATERIAL 7520
TEMP (K)
E (MJ/kg)
6
4
2
0
-2
-2
-1
0
1
2
3
4
ρ (g/cm³)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08

SESAME #7541

Material: Carbon Phenolic [Ref. 1]

Composition:	C	64.18 at%
	H	29.50 at%
	O	5.98 at%
	N	0.34 at%

Originator: J. D. Johnson
Date of Origin: April 1981
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho < 1.516 \times 10^3$ g/cm^3
$0 < T < 3.7 \times 10^8$ K

BASIC PHYSICAL DATA

$\bar{A} = 9.0105$
$\bar{Z} = 4.648$
$\rho_o = 1.45$ g/cm^3

$P(T = 298.15 \text{ K}, \rho_o) = -2.2470 \times 10^{-3}$ GPa
$E(T = 298.15 \text{ K}, \rho_o) = 1.2573 \times 10^{-4}$ MJ/kg
$T(P = 10^{-6} \text{ GPa}, \rho_o) = 299$ K

$\gamma_o = * \, 0.5$ (used in calculation)

$E_{coh} = * \, 100$ kcal/mole (used in calculation)

Hugoniot Fit: $U_s = 3.05 + 1.0 \, U_p$ km/s
(produced best fit to Hugoniot data in calculation)

DESCRIPTION OF PHYSICS

The thermal electronic part of this EOS was calculated with Thomas-Fermi-Dirac theory using an average atomic weight of 9.0105 and an average atomic number of 4.648. The thermal nuclear model used was CHART D, and the cold curve was calculated from Hugoniot data in the experimental range and Thomas-Fermi-Dirac theory at high pressures. For the expanded part of the cold curve, a Lennard-Jones potential was joined smoothly to the derived cold curve used in the compressed region.

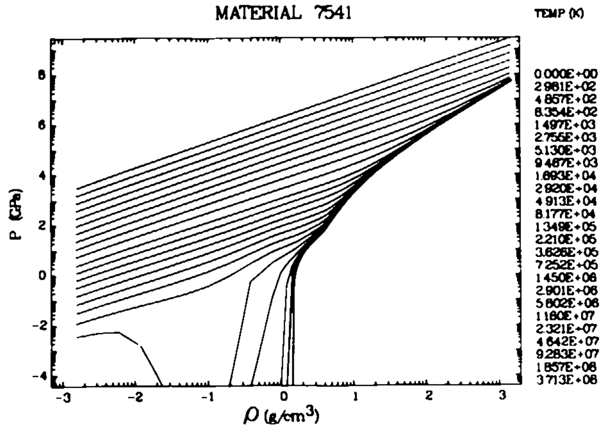
The code EOSLTS merged the various components of the EOS: nuclear thermal, electron thermal, and cold curve.

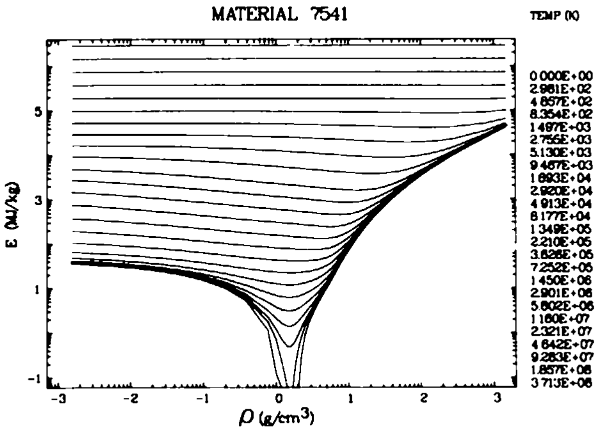
The fit of the theoretical EOS to Hugoniot data is good. The user should beware, however, that there is great variability between one sample of this substance and another. In the expanded region, the vapor dome region is very approximate.

This EOS has van der Waals loops instead of a Maxwell construction. Thermodynamic consistency is good everywhere.

REFERENCE

1. J. D. Johnson and B. Bennett, "An EOS for Carbon Phenolic," Los Alamos National Laboratory report LA-9176-MS (March 1982).


MATERIAL 7541
TEMP (K)
0.000E+00
2.981E+02
4.857E+02
8.354E+02
1.497E+03
2.756E+03
5.130E+03
9.487E+03
1.693E+04
2.920E+04
4.913E+04
8.177E+04
1.349E+05
2.210E+05
3.626E+05
7.252E+05
1.450E+06
2.901E+06
5.802E+06
1.160E+07
2.321E+07
4.642E+07
9.283E+07
1.857E+08
3.713E+08
P (GPa)
8
6
4
2
0
-2
-4
-3
-2
-1
0
1
2
3
ρ (g/cm³)


MATERIAL 7541
TEMP (K)
E (MJ/kg)
5
3
1
-1
-3
-2
-1
0
1
2
3
ρ (g/cm³)
0.000E+00
2.981E+02
4.857E+02
8.354E+02
1.497E+03
2.755E+03
5.130E+03
9.467E+03
1.693E+04
2.920E+04
4.913E+04
8.177E+04
1.349E+05
2.210E+05
3.626E+05
7.252E+05
1.450E+06
2.901E+06
5.802E+06
1.160E+07
2.321E+07
4.642E+07
9.283E+07
1.857E+08
3.713E+08

SESAME #7560

Material: Polyurethane
Composition: C 62.3 wt%
O 23.3 wt%
N 7.3 wt%
H 7.1 wt%
Originators: J. Barnes and J. Rood
Date of Origin: October 1974
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho < 2.53 \times 10^4$ g/cm^3
$0 < T < 3.7 \times 10^8$ K

BASIC PHYSICAL DATA

$\bar{A} = 7.0384$
$\bar{Z} = 3.7629$
$\rho_o = 1.265$ g/cm^3

$P(T = 298.15\ \mathrm{K}, \rho_o) = 0.83376$ GPa
$E(T = 298.15\ \mathrm{K}, \rho_o) = 0.6592$ MJ/kg
$T(P = 10^{-6}\ \mathrm{GPa}, \rho_o) = 3.6097 \times 10^{-4}$ K

$B_o = 5.4$ GPa [Ref. 1]

Hugoniot Fit: $U_S = 1.999 + 2.101\, U_p - 1.351\, U_p^2$ km/s [Ref. 2]

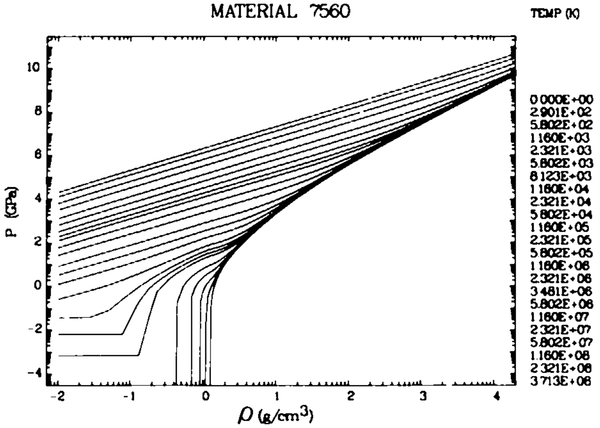
DESCRIPTION OF PHYSICS

This equation of state is completely undocumented. However, it was probably generated with the standard Barnes-Cowan-Rood method. See Part II for a more detailed description of the procedure.

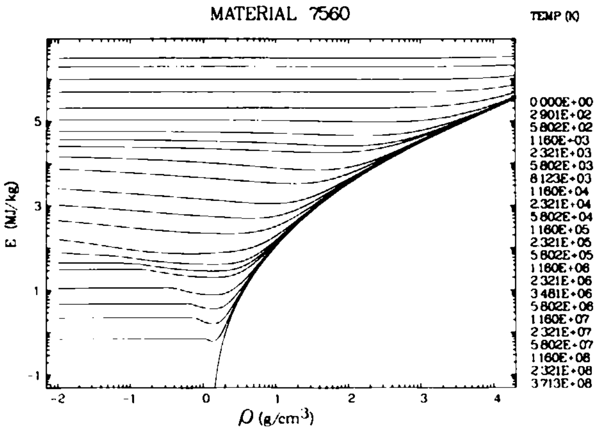
REFERENCE

1. S. P. Marsh, LASL Shock Hugoniot Data (University of California Press, Berkeley, 1980).

2. M. van Thiel, "Compendium of Shock Wave Data," Lawrence Livermore Laboratory report UCRL-50108, Rev. 1 (1977).


MATERIAL 7560
TEMP (K)
P (GPa)
ρ (g/cm³)
10
8
6
4
2
0
-2
-4
-2
-1
0
1
2
3
4
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08

7560-L


MATERIAL 7560
TEMP (K)
E (MJ/kg)
5
3
1
-1
-2
-1
0
1
2
3
4
ρ (g/cm-3)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08

SESAME #7590

Material: Polystyrene
Composition: CH
Originators: J. Barnes and A. Lindstrom
Date of Origin: January 1976
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $0 < \rho < 2.088 \times 10^4$ g/cm^3
$0 < T < 3.7 \times 10^8$ K

BASIC PHYSICAL DATA

$\bar{A} = 6.51$
$\bar{Z} = 3.5$
$\rho_o = 1.044$ g/cm^3

$P(T = 298.15\ \text{K}, \rho_o) = 1.0008$ GPa
$E(T = 298.15\ \text{K}, \rho_o) = 0.81249$ MJ/kg
$T(P = 10^{-6}\ \text{GPa}, \rho_o) = 3.0028 \times 10^{-4}$ K

$T_c = {*}\ 13860$ K (calculated)
$P_c = {*}\ 3.2295 \times 10^{-2}$ GPa (calculated)

$\gamma_o = {*}\ 1.18$ (used in calculation)
$B_o = 3.77$ GPa [Ref. 1]
4.08 GPa [Ref. 2]

$\theta_D = {*}\ 258$ K (used in calculation)

Hugoniot Fit: $U_S = 2.746 + 1.319\ U_p$ km/s
[Ref. 3]

DESCRIPTION OF PHYSICS

The polystyrene equation of state was generated with the standard Barnes-Cowan-Rood procedure. At higher temperatures (probably above 1 eV), the EOS was generated by scaling MAPLE table #18. The MAPLE table consists of an electronic EOS calculated with Thomas-Fermi-Dirac theory and cold curve and nuclear thermal contributions based on a model by R. D. Cowan.

Below 1 eV, the EOS is the sum of two contributions: a cold curve based on a modified-Morse model and nuclear thermal contributions calculated with a Debye model. See Part II for a more detailed description of this method of EOS generation.

The EOS is thermodynamically consistent everywhere.

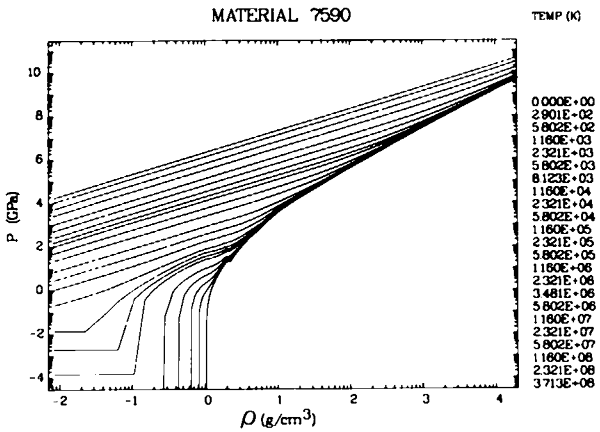
The two-temperature tables were derived with the code TWOTEMP and are noisy.

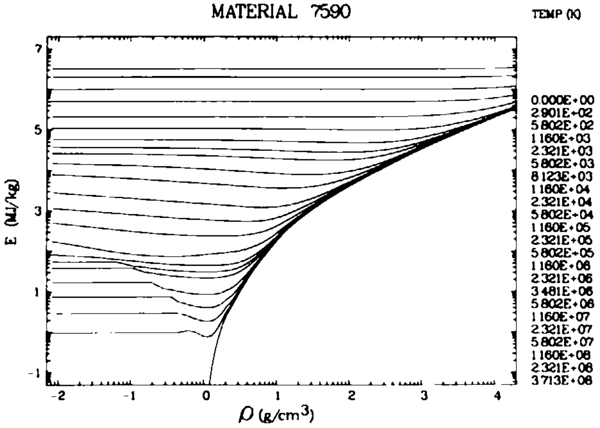
REFERENCES

1. S. P. Marsh, LASL Shock Hugoniot Data (University of California Press, Berkeley, 1980).

2. Handbook of Chemistry and Physics, R. C. Weast, Ed. (CRC Press, Cleveland, Ohio, 1976).

3. M. van Thiel, "Compendium of Shock Wave Data," Lawrence Livermore National Laboratory report UCRL-50108, Rev. 1 (1977).


MATERIAL 7590
TEMP (K)
P (GPa)
10
8
6
4
2
0
-2
-4
-2
-1
0
1
2
3
4
ρ (g/cm^3)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08


MATERIAL 7590
TEMP (K)
7
5
3
1
-1
E (MJ/kg)
-2
-1
0
1
2
3
4
ρ (g/cm3)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08

SESAME #7831

Material: Carbon Liquid
Originator: G. I. Kerley
Date of Origin: October 1981
Type of Tables Included: 301
Limits: $0.23 < \rho < 100\ \mathrm{g/cm^3}$
$0 < T < 10^7\ \mathrm{K}$

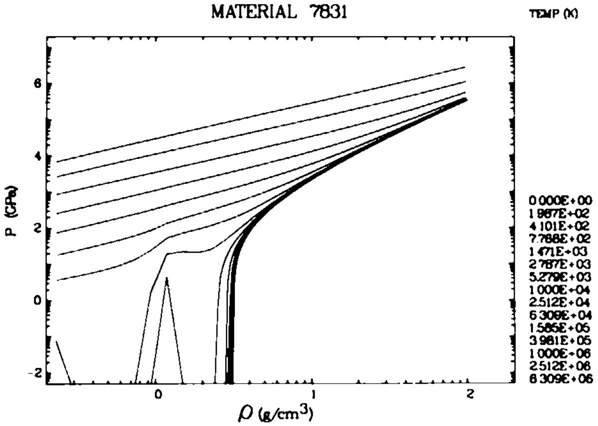
BASIC PHYSICAL DATA

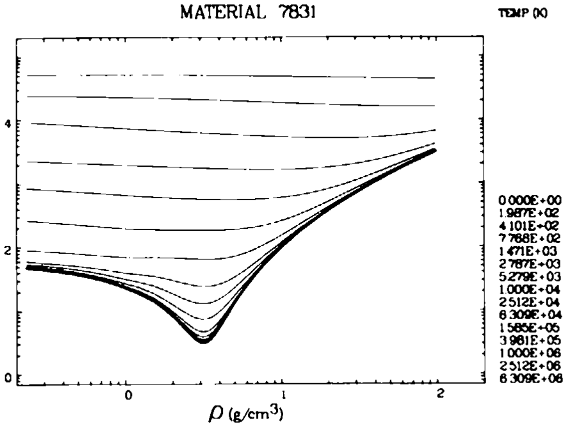
$A = 12.011$
$Z = 6$
$\rho_o = 3.6878\ \mathrm{g/cm^3}$

$P(T = 298.15\ \mathrm{K},\ \rho_o) = 47.251\ \mathrm{GPa}$
$E(T = 298.15\ \mathrm{K},\ \rho_o) = 4.2909\ \mathrm{MJ/kg}$

DESCRIPTION OF PHYSICS

This equation of state describes the metallic fluid phase of carbon. Its purpose is to aid in the design and interpretation of high-pressure, shock wave experiments based on the impedance-matching techniques. The zero-kelvin isotherm (cold curve) was calculated with electron band theory based on the self-consistent, linear-muffin-tin-orbital (LMTO) method. The contributions from the center-of-mass motion of the molecules (nuclear thermal contributions) were computed with the CRIS hard-sphere perturbation theory for fluids. The thermal electronic part of the EOS was calculated with the INFERNO code. INFERNO solves the Dirac equation for an atom embedded in an electron gas. Wave functions and energies are obtained for both bound states and the continuum.


MATERIAL 7831
TEMP (K)
P (GPa)
6
4
2
0
-2
0
1
2
ρ (g/cm³)
0.000E+00
1.987E+02
4.101E+02
7.788E+02
1.471E+03
2.787E+03
5.279E+03
1.000E+04
2.512E+04
6.309E+04
1.585E+05
3.981E+05
1.000E+06
2.512E+06
6.309E+06


MATERIAL 7831
TEMP (K)
E (MJ/kg)
0
2
4
0
1
2
ρ (g/cm³)
0.000E+00
1.987E+02
4.101E+02
7.768E+02
1.471E+03
2.787E+03
5.279E+03
1.000E+04
2.512E+04
6.309E+04
1.585E+05
3.981E+05
1.000E+06
2.512E+06
6.309E+06

SESAME #8180

Material: PBX-9502 (high explosive)

Composition:

C	25.245 at%
H	24.491 at%
N	24.148 at%
O	24.148 at%
F	1.474 at%
Cl	0.494 at%

Originators: C. Mader and J. Rood
Date of Origin: July 1981
Type of Tables Included: 301, 303, 304, 305, 306
Limits: $1.4797 \times 10^{-2} < \rho < 3.788 \times 10^{4}$ g/cm^3
$0 < T < 3.7 \times 10^{8}$ K

BASIC PHYSICAL DATA

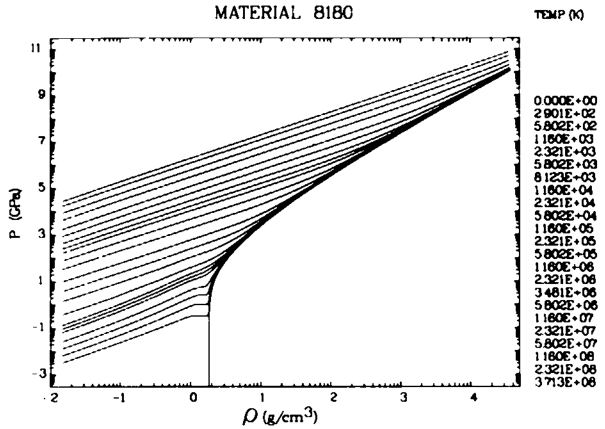
$\bar{A} = 10.980013$
$\bar{Z} = 5.598417$
$\rho_o = 1.894$ g/cm^3

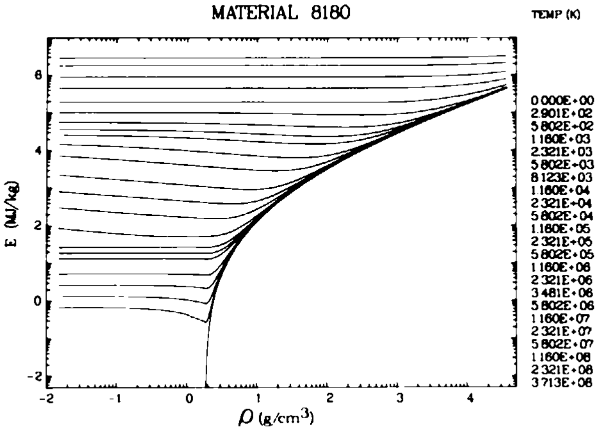
$P(T = 298.15\ K,\ \rho_o) = 0.5061$ GPa
$E(T = 298.15\ K,\ \rho_o) = 0.2674$ MJ/kg
$T(P = 10^{-6}\ GPa,\ \rho_o) = 3.6779 \times 10^{-3}$ K

DESCRIPTION OF PHYSICS

No documentation exists for this EOS, and the models used in the calculation are unknown.

The densities and energies of the original EOS were sealed by a factor of 1.029348 in order to bring the reference density in line with the experimentally measured value.


MATERIAL 8180
TEMP (K)
P (GPa)
11
9
7
5
3
1
-1
-3
-2
-1
0
1
2
3
4
ρ (g/cm³)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08


MATERIAL 8180
TEMP (K)
E (MJ/kg)
6
4
2
0
-2
-2
-1
0
1
2
3
4
ρ (g/cm^3)
0.000E+00
2.901E+02
5.802E+02
1.160E+03
2.321E+03
5.802E+03
8.123E+03
1.160E+04
2.321E+04
5.802E+04
1.160E+05
2.321E+05
5.802E+05
1.160E+06
2.321E+06
3.481E+06
5.802E+06
1.160E+07
2.321E+07
5.802E+07
1.160E+08
2.321E+08
3.713E+08

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