Bound and estimate for the maximum compression of single shocks

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(Received 16 September 1998)

We derive that the compression for any single shock has an upper bound of 7. This is in the case of shocking from any initial state except gaseous densities with temperatures such that a significant fraction of the electrons are bound. For shocks in condensed material initially near ambient, we present a simple analytic estimate for the maximum compression as a function of ρ_0 (initial density), A (atomic weight), Z (atomic number), and ΔE (the sum of cohesion, dissociation, and total ionization energies). [S1063-651X(99)07803-4]

PACS number(s): 62.50.+p, 52.35.Tc, 51.30.+i

INTRODUCTION

For any material that is compressed by a shock wave, one might suppose that increasing the pressure of the shock wave to arbitrarily high values will produce an arbitrarily large compression. This is not true, and in particular one can show that for infinitely strong shock waves in any substance there is a compression of exactly fourfold from the initial density in front of the shock to the final density behind the shock. Thus, in defiance of the high pressure, the compression is limited by the high temperatures produced by shocks. For condensed materials shocked from near ambient, the maximum possible compression attainable by a single shock is greater than 4 and occurs at some finite pressure, the particular values depending on the specific material and on the initial density and temperature. This overshot of the fourfold limit is caused by the ''softening'' of the material when energy is drained into internal degrees of freedom such as in ionization.

In this Brief Report we derive from general arguments an upper bound on the maximum compression attainable by a single shock in any material from any initial state except those with gaseous densities and a significant number of bound electrons. We also obtain an estimate of the maximum compression in the case of condensed materials shocked from near ambient.

UPPER BOUND

A Hugoniot curve is a curve in thermodynamic parameter space that is the collection of final states behind a shock as the strength of a shock is varied for fixed initial state. Hugoniot curves, along with isotherms, isobars, and isentropes, for example, are curves specified on the equation-of-state surface by constraints such as requiring that the temperature, pressure, or entropy be constant. It is just that the constraint for the Hugoniot curve is not as simple as keeping a standard thermodynamic variable fixed. For weaker shocks with little entropy production, the Hugoniot curve is approximately an isentrope. For shocks with significant entropy production, the Hugoniot curve in pressure-density space is stiffer than an isentrope. The principal Hugoniot curve is that one with ambient as the initial state [1].

Any Hugoniot curve is determined from the hydrodynamic equation of state $P(\rho,E)$ and the energy jump constraint

$$E-E_0=\frac{1}{2}(P+P_0)(1/\rho_0-1/\rho). \tag{1}$$

Here P is the pressure, ρ is the density, and E is the internal energy per gram. P_0, ρ_0, and E_0 represent the same, but are for the initial state of the Hugoniot curve. We define the compression as $\eta=\rho/\rho_0$ and rewrite Eq. (1) as

$$\eta=4+[2\rho(E-E_0)-3(P+P_0)]/(P+P_0). \tag{2}$$

We now assume that the virial theorem is exact for the equation of state [2]; i.e., if $E=K+U$, where K is the average kinetic energy per gram and U is the average potential energy per gram, then $P/\rho=2K/3+U/3$. (We are considering here the case of physical interest, namely, the charge-neutral, quantum Coulomb system.) Substituting into Eq. (2), we get

$$\eta=\eta_b-3P_0(1+\eta)/(P+P_0)\leqslant\eta_b, \tag{3}$$

where $\eta_b=4+\rho(U-U_0)/(P+P_0)$. If $U\leqslant U_0$, then $\eta\leqslant\eta_b\leqslant 4$. If $U\geqslant U_0$, then we rewrite Eq. (3) as

$$\eta\leqslant\eta_b=4+3/[1+2K_s/U_s+3P_0(1/\rho+1/\rho_0)/U_s], \tag{4}$$

where $K_s=K-K_0$ and $U_s=U-U_0$.

For classical systems, $K_s\geqslant 0$ because the average kinetic energy is linear in temperature T. This is not the case in general for a quantum, charge-neutral, bare Coulomb system. For low densities where atomic states are a good approximation for the electrons, the electrons ionize from localized high-kinetic-energy states to low-kinetic-energy extended free states. Thus the average kinetic energy drops as the temperature rises as long as there is a significant fraction of electrons remaining to be ionized. This is nothing more than the uncertainty principle with the electrons going from a small to a big box. The situation just discussed is not the case for densities higher than gaseous. There, the electrons do not have an extreme change in localization in going from low to high temperatures. Thus, for quantum systems, it is *very* reasonable that $K_s\geqslant 0$ when $U_s\geqslant 0$ if $\eta\geqslant 7-\varepsilon$ $(\varepsilon>0)$ for a material shocked from densities greater than gaseous. (Models support this position.) Then, from Eq. (4), $\eta\leqslant\eta_b\leqslant 7$.

Thus we conclude that the compression along a single-shock Hugoniot curve for any material cannot exceed 7 for a broad class of initial shock states.

ESTIMATE FOR THE PRINCIPAL HUGONIOT CURVE

We now look to the principal Hugoniot curve, where $P_0=0$. We assume that we are shocking from $T=0$. (The difference between zero and room temperature is small when we are looking for estimates of the maximum compression.) From Eqs. (3) and (4), we find that

$$\eta=4+3/(1+2K_s/U_s). \tag{5}$$

It is convenient to define $Y=U_s/(2\Delta E)$, where, for the principal Hugoniot curve, $\Delta E=-E_0$ and is the sum of cohesive, dissociation, and total ionization energies. Then

$$\eta=(7Y+4K_s/\Delta E)/(Y+K_s/\Delta E). \tag{6}$$

From the exact high-temperature series for the equation of state of any elemental material [3], we obtain Y as an exact series in $1/K_s$. (We are thinking of K_s as the independent variable.) All that we need is

$$Y=1+a\alpha^{1/2}+\cdots, \tag{7a}$$

with

$$a=-e^3(1+Z)^2(L/A)^2/\Delta E \tag{7b}$$

and

$$\alpha=3\pi Z^3\rho_0/(2K_s). \tag{7c}$$

In these equations, L is Avogadro's number and e is the electron charge. The $a\alpha^{1/2}$ originates from the Debye-Hückel term in the high-T expansion.

We substitute Eqs. (7a)–(7c) into Eq. (6) and solve for the maximum compression η_m. The result is

$$\eta_m=4(1+7C)/(1+4C), \tag{8a}$$

with

$$C=2(\Delta E/Z)^3A^4/[81e^6\pi(1+Z)^4L^4\rho_0]. \tag{8b}$$

This is our estimate for the maximum compression along the principal Hugoniot curve.

Equation (8b) can be simplified further if one neglects cohesive and dissociation energies. We fit to the total ionization energies of Moore (through Ca) [4] to estimate that $\Delta E\cong 13.6Z^{2.4}$ eV per atom. Thus

$$C\cong 0.011AZ^{4.2}/[\rho_0(1+Z)^4]. \tag{8c}$$

CONCLUSIONS

The estimates of Eqs. (8a)–(8c) and an upper bound of 7 are our results. The only existing data that are a strong test of our η_m expression are for Al [5]. In that case, $\eta_m\sim 5$ and that value agrees well with Eqs. (8). One has available more terms in the expansion, Eq. (7a). We have extensively studied these terms and found that they do not influence our estimates at all. We have also extensively worked with the series, Eq. (7a), using Padé approximants. Again, there was no significant influence. We feel Eqs. (8a)–(8c) are quite a good approximation of η_m.

In a previous discussion of the high-pressure Hugoniot curve [6], we presented the relations $s=1+\gamma/2$ and $\eta_m=1+2/\gamma$, where s is the derivative of the shock velocity with respect to the particle velocity and $\gamma=1/\rho\,\partial P/\partial E|_\rho$ is the Grüneisen parameter. These relations are exact at any point on the Hugoniot curve where the density derivative of the pressure is infinite. The first is also approximately true for any given material over a very large region of the Hugoniot curve, including particle velocities from about 10 to 100 km/s. In such a region it is universal that $s\approx 1.2$ and thus $\gamma\approx 0.4$. It is above this very linear region that the Hugoniot curve becomes steeper and in pressure-density space attains maximum compression. There, s will be a little larger than its value in the linear region. (We should clarify that there are two linear regions in the shock-velocity–particle-velocity Hugoniot curve. One is from 0 to about 3 km/s for the particle velocity, and the other, which is the one of interest, is from about 10 to 100 or more km/s.) From our approximation of the maximum compression and the above two relations, we can obtain estimates of s and γ at the maximum compression point. The ultimate limiting values for shocks of infinite strength are $\eta=4$, $s=4/3$, and $\gamma=2/3$.

[1] For more discussion, see, for example, J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, *Molecular Theory of Gases and Liquids* (Wiley, New York, 1954), p. 398.

[2] We especially prefer the physics derivation of J. Yvon, Acad. Sci., Paris **227**, 763 (1948).

[3] See, for example, A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971), p. 267.

[4] C. E. Moore, *Ionization Potentials and Ionization Limits Derived from the Analysis of Optical Spectra*, Natl. Bur. Stand. Ref. Data Series, Natl. Bur. Stand. (U.S.) Circ. No. NSRDS-NBS 35 (U.S. GPO, Washington, D.C., 1970).

[5] A. S. Vladimirov, N. P. Voloshin, V. N. Nogin, A. V. Petrovtsev, and V. A. Simonenko, JETP Lett. **39**, 85 (1984).

[6] J. D. Johnson, in *Shock Compression of Condensed Materials—1997*, edited by S. C. Schmidt, AIP Conf. Proc. No. **429** (AIP, New York, 1998), pp. 27–30; *General Features of Hugoniots—II*, Los Alamos Report No. LA-13217-MS, 1997.