STATE OF ARGON BEHIND A SHOCK WAVE AT MACH NUMBERS FROM 20 TO 50, WITH ALLOWANCE FOR EXCITATION, MULTIPLE IONIZATION, AND COULOMB INTERACTION

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The following seven equations describe the incident shock wave in the laboratory coordinate system, with allowance for ionization up to Ar^{3+}

conservation of matter

$$\rho_1 V = \rho_2(V - u_2);$$

conservation of momentum

$$p_1 + \rho_1 V^2 = p_2 + \rho_2(V - u_2)^2;$$

conservation of energy

$$h_1 + {}^1/_2\ V^2 = h_2 + {}^1/_2(V - u_2)^2;$$

law of mass action

$$x_1 = \left[1 + \frac{n_e}{K'} + \frac{K''}{n_e}\left(1 + \frac{K'''}{n_e}\right)\right]^{-1},$$

$$x_2 = \frac{K''}{n_e} x_1, \quad x_3 = \frac{K'''}{n_e} x_2\,;$$

equation of state with allowance for Coulomb interaction [1]

$$p = \frac{\rho}{m} kT\,(1 + x_1 + 2x_2 + 3x_3) -$$

$$- \frac{e^3 \rho}{3m^{3/2}} \left(\frac{\pi\rho}{kT}\right)^{1/2} (2x_1 + 6x_2 + 12x_3)^{3/2}.$$

Here V is shock-wave speed, u_2 is the speed of the flow behind the shock wave, ρ is density, p is pressure, T is temperature, and h is enthalpy, subscripts 1 and 2 denote the conditions ahead of and behind the shock wave, K' is the equilibrium constant for production of Ar^+, K" and K"' are the same for Ar^{2+} and Ar^{3+}, and x_1, x_2, and x_3 represent the degrees of ionization:

$$x_j = \frac{n_j}{n_0 + n_1 + n_2 + n_3} \qquad (j = 1,\ 2,\ 3).$$

Here n_j is the number of Ar^{+j} ions per cm^3, n_e is the number of electrons per cm^3, m is the mass of an argon atom, e is electronic charge, and k is Boltzmann's constant.

The following is the expression for h including excitation, multiple ionization, and Coulomb interaction:

$$h = \frac{5}{2}\,\frac{kT}{m}\,(1 + x_1 + 2x_2 + 3x_3) -$$

$$- \frac{4}{3}\,\frac{e^3}{m^{3/2}} \left(\frac{\pi\rho}{kT}\right)^{1/2} (2x_1 + 6x_2 + 12x_3)^{3/2} +$$

$$\frac{1}{m}\,[J_1\,(x_1 + x_2 + x_3) + J_2\,(x_2 + x_3) + J_3 x_3] +$$

$$+ \frac{1}{m}\,(1 - x_1 - x_2 - x_3)\,\frac{X^{(0)}}{Z^{(0)}} + \sum x_j\,\frac{X^{(j)}}{Z^{(j)}},$$

$$X^{(j)} = \sum_i g_i^{(j)} \varepsilon_i^{(j)} \exp\left(-\frac{\varepsilon_i^{(j)}}{kT}\right),$$

$$Z^{(j)} = \sum_i g_i^{(j)} \exp\left(-\frac{\varepsilon_i^{(j)}}{kT}\right).$$

Here $X^{(j)}$ is the excitation energy of state j, $Z^{(j)}$ is the statistical sum, $g_i^{(0)}, \ldots, g_i^{(3)}$ are the statistical weights of the energy states, $\varepsilon_i^{(0)}, \ldots, \varepsilon_i^{(3)}$ are the energies of the levels reckoned from the lowest level, and J_1, J_2, and J_3 are the corresponding ionization potentials. Here the first term takes account of the translational energy, the second of the Coulomb interaction, the third of the energy used in ionization, and the last of the excitation.

The equilibrium constants are defined by the formulas of statistical physics with allowance for the excitation and the reduction in the ionization potentials by Coulomb interaction:

$$K' = 2\,\frac{Z^{(1)}}{Z^{(0)}}\,\frac{(2\pi m_e kT)^{3/2}}{h^3} \exp\left(-\frac{J_1 - \Delta E_1}{kT}\right),$$

$$K'' = 2\,\frac{Z^{(2)}}{Z^{(1)}}\,\frac{(2\pi m_e kT)^{3/2}}{h^3} \exp\left(-\frac{J_2 - \Delta E_2}{kT}\right),$$

$$K''' = 2\,\frac{Z^{(3)}}{Z^{(2)}}\,\frac{(2\pi m_e kT)^{3/2}}{h^3} \exp\left(-\frac{J_3 - \Delta E_3}{kT}\right).$$

Here m_e is electron mass and h is Planck's constant, while E_j is the reduction in the ionization potential, which is given by the Debye-Hückel method as

$$\Delta E_j = \frac{e^3}{3} \left(\frac{\pi\rho}{mkT}\right)^{1/2} (2x_1 + 6x_2 + 12x_3)^{1/2} \left(6j - \frac{2x_1 + 6x_2 + 12x_3}{1 + x_1 + 2x_2 + 3x_3}\right),$$

while h_e is

$$n_e = \rho/m(x_1 + 2x_2 + 3x_3).$$

This system of equations is closed with respect to the unknowns. Parameters p_1 and M were varied in the calculations. In the first sim-

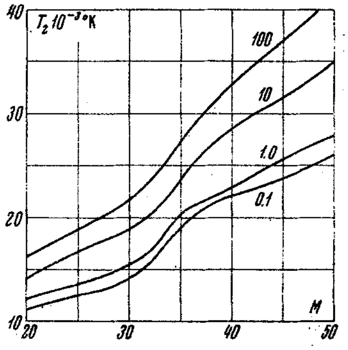

Fig. 1

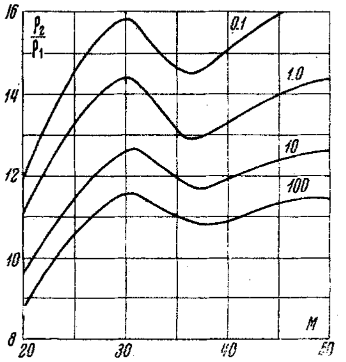

Fig. 2

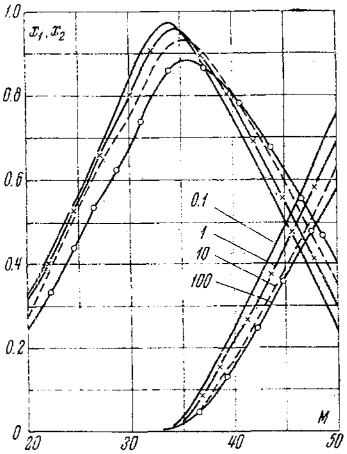

Fig. 3

plified scheme (without allowance for Coulomb interaction), the system was solved by the method of steepest descent [2]. The results were then used as the first approximation in Seidel's method, with special attention to the conditions of convergence. A BESM-3M computer was used.

The atomic constants for argon were taken from [3]. The calculations were performed for M from 20 to 50 for initial pressures of 0.1, 0.3, 1.0, 3.0, 10, 25, 50, and 100 mm Hg. Figures 1-3 show T_2, ρ_2/ρ_1, and the degree of ionization behind the shock wave as functions of M for four initial pressures; only x_1 and x_2 are shown in the last case, because x_3 was small and was only $2 \cdot 10^{-3}$ for M = 50 and an initial pressure of 0.1 mm Hg.

The peak x_1 is nearly 1, but x_2 near that peak is small, and in this region most of the shock-wave energy goes to raising T_2, which reduces the density. Subsequently, x_2 becomes substantial, which shows the increase in T_2 and results in an increase in density.

In calculating the excitation energy we encounter the question of the number of levels to be incorporated, since the upper levels are cut off in a plasma of finite density, while the energy of electronic excitation is proportional to the number of levels. Unfortunately, there is presently no agreed view on this, and the various possible estimates give different results. For example, the summation over the levels may be truncated at a value n^* of the principal quantum number such that the size of the orbit for a hydrogen-type ion becomes comparable with the Debye screening radius:

$$n^* = \left(\frac{Z^2kT}{4\pi n_e e^2 a_0^2}\right)^{1/4}.$$

Here Z is nuclear charge and $a_0 = 0.53 \cdot 10^{-8}$ cm is the Bohr radius. This means that the limit is $n^* = 8$ for a gas initially at room temperature and a pressure of 100 mm Hg after exposure to M = 20.

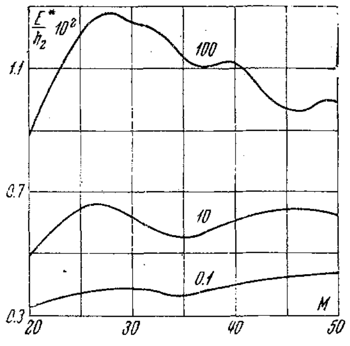

Fig. 4

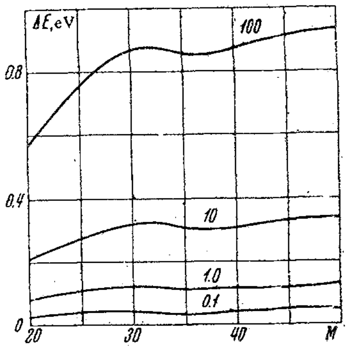

Fig. 5

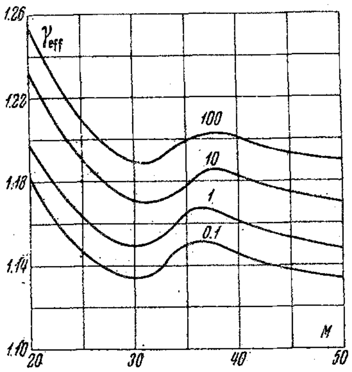

Fig. 6

The summation can be stopped at the level where the electron binding energy is kT, since then every collision with a free electron will eject a bound electron from the atom [4]. The binding energy E_n for an electron in level n of a hydrogen-type ion is equal to the Coulomb energy in the nuclear field:

$$E_n = \frac{J_H Z^2}{n^2}.$$

Here $J_H = 13.5$ eV is the ionization potential of hydrogen. We equate this energy to kT to get that $n^* = 3$ for the above conditions. This shows that the uncertainty in the number of levels to be incorporated is too great and certainly exceeds the temperature dependence for n^*. It was therefore decided to incorporate the first five levels. The Inglis-Teller theory leads also to this result.

Figure 4 shows the ratio of E^* to h_2 as a function of M for initial pressures of 1, 10, and 100 mm Hg. It is clear that the electronic excitation must be considered in calculating the gas parameters for high M and gas pressures.

The quantity ΔE_j was calculated above via the Debye-Hückel theory. Figure 5 shows ΔE_1 as a function of M for various initial pressures. For pressures of the order of 100 mm Hg, the condition $\Delta E \ll kT$ (slight deviation from ideal behavior) is not met strictly.

It is also of interest to derive γ_{eff} (effective adiabatic parameter), especially when this is nearly constant, since then we can use exact solutions for various gasdynamic problems. This quantity was derived via the above calculations from

$$\gamma_{eff} = 1 + p/\rho H$$

in which H is specific internal energy. Figure 6 shows γ_{eff} as a function of M, and it is clear that the variation is very substantial except in the range 25–50 in M, where it is around ±0.01 for each initial pressure.

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