An Experimental Verification of the Thomas-Fermi Model for Metals under High Pressure

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The densities of iron, copper, and cadmium compressed by shock waves with pressure amplitudes of ~51, ~38, and ~33 Mbar, respectively, are determined experimentally by comparative measurements. The results are 21.7 g/cm^3 for iron, 23.6 g/cm^3 for copper, and 26.6 g/cm^3 for cadmium. The experimental results are compared with calculated adiabats based on the Thomas-Fermi model. It is shown that the calculations are consistent with the experimental shock adiabat parameters. For the investigated metals the Thomas-Fermi model is applicable above 150–200 Mbar.

THE Thomas-Fermi model is widely used as a basis for calculating the shock-compressed states of materials under ultra-high pressures. For heavy metals with high atomic numbers the reliability of quantum-statistical solutions at $P \geq 500-1000$ Mbar is not questioned. However, uncertainty has existed regarding the minimum pressures at which these solutions become admissible. In the present work we have attempted to determine these limits experimentally by investigating the comparative compressibility of metals using strong shock waves.

In the absolute method of determining dynamic compressibility (the "deceleration technique"[1]) two independent parameters are determined experimentally: the velocity of the striker, $W = 2U$, (where U is the mass velocity of matter behind the shock wave front), and the velocity D of the shock wave that is created in the target by the impact of the striker. When the target and striker are made of the same material, the known values of D and U in conjunction with the conservation of mass and momentum yield the density of the material, $\rho = \rho_0 D(D-U)^{-1}$, and the shock pressure $P = \rho_0 DU$. This technique and the similar reflection technique[2] have been used[3-5] with striker velocities $W \approx 14$ km/sec to measure the dynamic compressibility of certain metals at ~10 Mbar. The main difficulty, which has heretofore not been overcome, that arises when still higher pressures are created lies in the necessity of accelerating the striker extremely symmetrically and without causing heating. Therefore in recent work[6-8] performed with the reflection technique dynamic compressibility under extremely high pressures has been determined by a comparison procedure. One measures the velocities of shock waves passing through successive layers of the test materials, one of which is taken as a standard.

For the standard material the dynamic compression curve is obtained from a very reliable interpolation formula that connects the experimental portion of its adiabat (to ~10 Mbar) with calculated values based on quantum-statistical models[9] ($P > 100$ Mbar). The materials used as standards should be metals with high atomic numbers, for which the quantum-statistical solutions are most reliable.

The comparison technique was used in[6,7] to obtain the shock compression parameters of iron at 31, copper at 16, and cadmium at 14 Mbar. In the present work we have greatly extended the experimental pressure range for these three metals. As in[6], where the experimental conditions were similar, the shock wave velocities were recorded in relatively long samples (of the order of 10 cm) in order to attain the requisite accuracy.

Our standard material was lead. From known states in the standard material[1)] and the wave velocity in the investigated material we are enabled by the method of P – U diagrams[2] to determine the other compression parameters of the latter, which are the mass velocity, pressure, and density. Shock wave velocities were recorded in three systems: iron-lead, lead-copper, and copper-cadmium. The thicknesses of the pairs of samples were, respectively, 100–80, 70–80, and 80–70 mm; their diameters were ~600 mm. Shock wave velocities in the samples were recorded by means of four groups of diametrically positioned electric-contact pickups located at the interfaces of the metals. The analysis of the oscillograms showed that the time intervals registered by the pickups did not differ by more than 0.7%. This indicates quite high symmetry of shock wave passage through the samples.

Because the velocity of the shock waves changed slightly during their propagation through the samples, we had to compare the wave velocities at the common interfaces of the metals. The calculations accordingly included corrections allowing for these velocity changes.

In the first system (iron-lead) the initial data used to determine the iron compression parameters were

$$U_{Pb} = 19.12 \text{ km/sec} \quad P_{Pb} = 56.60 \text{ Mbar} \quad D_{Pb} = 26.12 \text{ km/sec}$$

which correspond to the intersection point of the wave ray, $\rho_{0Pb} D_{Pb}$ ($D_{Pb} = 26.12$ km/sec), and its dynamic adiabat. For the latter we used the dynamic adiabat of lead with parameters close to those given in[6]. The pressure region (10 Mbar < P < 60 Mbar) can be represented by the analytic expression

$$P = \frac{\rho_0 C_0'^2}{(\lambda-1)^2}\sigma(\sigma-1)\left[\frac{\lambda}{\lambda-1}-\sigma\right]^2; \quad \sigma = \frac{\rho}{\rho_0}, \quad D = C_0' + \lambda U$$

with the coefficients $\rho_0 = 11.34$ g/cm^3, $C_0' = 2.8$ km/sec, and $\lambda = 1.22$.

The state that is sought on the adiabat of iron must

1) The initial state parameters of the standard are determined, according to the known wave velocity, from its dynamic compression curve.

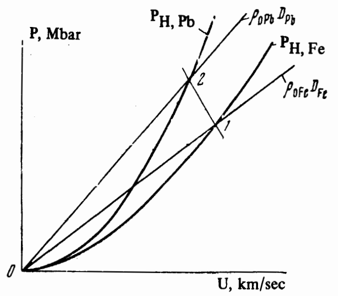

FIG. 1. Schematic diagram for determining the shock compression parameters of iron.

fulfill two requirements: 1) It must be located on the wave ray $\rho_0 Fe D_{Fe}$ (D_{Fe} = 31.90 km/sec at the iron-lead interface), and 2) it must belong to the dynamic adiabat of iron, whose "twofold-compression" adiabat with the initial values at point 1 in Fig. 1 corresponds to point 2 on the adiabat of lead.

The twofold-compression adiabat of iron, which passes exactly through point 2, was selected from a family of curves having a branching point on the wave ray $\rho_0 Fe D_{Fe}$. As in[6] these adiabats were constructed from the equation

$$P = P_{Fe_1} + \rho_{Fe_1}[C_{Fe} + \lambda(U_{Fe} - U)](U_{Fe} - U),$$

where $C_{Fe} = \rho_{Fe}^{-1}(\partial P/\partial U)_{Fe}$ is the velocity of sound in iron, which determines the slope of the adiabat 1–2; $\lambda \approx 1$; P_{Fe}, ρFe, and U_{Fe} are the pressure, density, and mass velocity on the wave ray in iron. C_{Fe_1} lies within a narrow range, from C_{Fe} = 0.85 D[10] to $C_{Fe} \approx 0.5$ D (the limiting value). The variation of this quantity from 0.8 D to 0.7 D was shown to have little effect upon the position of point 1 on the adiabat of iron. Also, the position of the two-fold-compression adiabat 1–2 calculated in this way for iron is close to the mirror image of its compression curve from state 1. Therefore, in subsequent plots we shall identify the twofold-compression adiabat and (also because of the small differences) the expansion isentropes of the standard materials with the mirror images of their dynamic adiabats.

We obtained the following parameters for the compression of iron: D = 31.90 km/sec, U = 20.35 km/sec, P = 50.96 Mbar, ρ = 21.67 g/cm^3, and relative compression $\sigma = \rho/\rho_0 = 2.761$.

The second and third systems (lead-copper and copper-cadmium) corresponded to the graphically calculated P – U diagram of the reflection method. From the initial parameters of the screen material (lead) at its interface with copper: D_{Pb} = 22.17 km/sec, U_{Pb} = 15.87 km/sec, and P_{Pb} = 39.85 Mbar, we determined the parameters in copper: D = 26.18 km/sec (interface), U - 16.26 km/sec, P = 38.0 Mbar, ρ = 23.58 g/cm^3; and σ = 2.64. Using copper as the standard (in the third system), with the initial parameters D_{Cu} = 25.3 km/sec, U_{Cu} = 16.11 km/sec, and P_{Cu} = 36.40 Mbar we determined the parameters of cadmium compression: D = 23.88 km/sec (Cu–Cd interface), U = 16.12 km/sec, P - 33.25 Mbar, ρ = 26.60 g/cm^3, and σ = 3.08.

In the graphs the dynamic adiabat of copper corresponding to the foregoing experimental parameters is described by the relations $P(\rho)$ and $D(U)$ with the

Table I

Test material	Parameters in the relation $D = C_0' + \lambda U$		Limits of applicability, km/sec
	C_0', km/sec	λ	
Fe	5.30	1.320	14< D <27
Cd	3.70	1.250	9< D <25
Cu	4.92	1.307	10< D <27
Pb	2.80	1.220	9< D <27

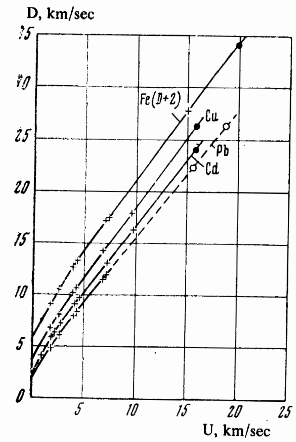

FIG. 2

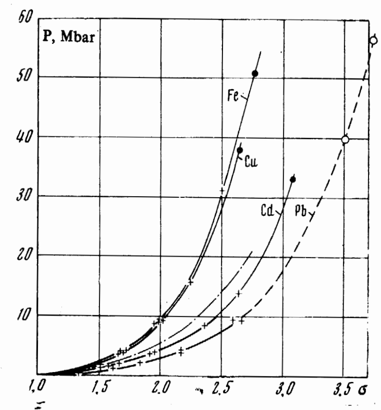

FIG. 3

FIG. 2. D–U diagrams of the metals. ×–data from [3-7], ●–present results, ○–initial parameters in lead. The thick and thin lines represent the absolute and relative measurements, respectively; the dashed line is an interpolated curve for lead.

FIG. 3. Pressure versus relative compression. ×–data from [3,5-7], ●–present results, ○–initial parameters in lead. The dot-dash line is the P_c ("cold") curve for iron.

constants C_0' and λ given in Table I.

In Fig. 2 the experimental parameters of shock waves in the test metals are shown in D – U coordinates. The maximum registered velocity was D ≈ 32.00 km/sec for iron. The curves shown here are smooth and monotonic. Their slopes, which are initially $\Delta D/\Delta U \approx 1.4$ (Pb)–1.75 (Fe, Cu) are reduced to 1.2–1.3 in the region of maximum shock wave amplitudes, i.e., they approach close to their limits. It is also characteristic that, beginning at certain wave velocities (D > 10 km/sec), the D – U curve for each metal is practically a straight line. Table I gives the parameters of the linear D – U relations and their limits of applicability. The P – σ measurements are represented in Fig. 3. The highest pressures were obtained in the iron samples; the maximum degree of compression was registered in cadmium. For comparison, the figure also shows the "cold" compression curve (the T = 0°K isotherm) of iron, which was obtained by extrapolating data published in[3]. At the highest degrees of comparison the "cold" component comprises ≈40% of the total pressure $P_{H,Fe}$; similarly, P_c comprises ≈40 and 45% for cadmium and copper. These components play a considerably smaller role in the total energy balance of shock compression. Thus, for iron E_C/E_{tot} ≈10%; the ratio is 18 and 13% for copper and cadmium, respectively. In turn, the thermal components of pressure and energy are determined mainly by the electronic

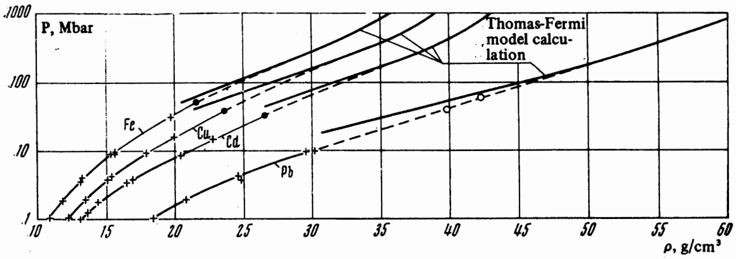

FIG. 4. Comparison of the calculated (Thomas-Fermi) and experimental shock wave parameters for the investigated metals. X—data from [3, 5-7], ●—present results, O—initial parameters for lead.

Table II

Metal	ρ_0, g/cm³	P, Mbar								
		40	60	80	100	150	200	300	400	500
Pb	11.34	37.15	40.65	43.15	45.05	48.45	50.80	53.75	55.70	57.10
Fe	7.85	19.55	21.55	23.20	24.45	26.75	28.30	30.40	31.80	32.80
Cu	8.93	21.65	23.90	25.65	27.10	29.65	31.50	34.00	35.65	36.80
Cd	8.64	26.05	28.60	30.40	31.85	34.35	36.10	38.25	39.70	40.70

components. In the case of iron, for example, $\Delta P_{th\text{-}el}/\Delta P_{th} \approx 80\%$ ($\sigma_{Fe} = 2.76$).

In Fig. 4 the experimental parameters of the shock adiabats are compared with calculated shock adiabats (see Table II) based on a model where electrons are described by the Thomas-Fermi theory and nuclei are considered to comprise an ideal monatomic gas. The locations of the experimental points confirm for the given metals the validity of the customary smooth interpolation between the experimental and calculated shock adiabats, in which the interpolated curve "merges" with the calculated curve where their slopes coincide. This coincidence occurs for $P \sim 150$–200 Mbar and thus determines the lower limit for the Thomas-Fermi calculations. Characteristically, the interpolated curve "merges" with the calculated curve from below, i.e., at the lower pressure end. We emphasize once more that our conclusions are based on the interpolated compression curve of the heavy metal (lead), whose properties are described most reliably by the quantum statistical theory.

We now, in conclusion, discuss the accuracy of the experimental measurements. In addition to the errors of the wave velocities we must consider the inaccuracy of interpolating the standard material, lead. The wave velocities were determined quite reliably, with at most ±1.0% error; for the accuracy of interpolating the lead adiabat we assume $\Delta\sigma_{st} \le \pm 0.1$. Then, from [6],

$$\frac{\Delta\rho}{\rho} = \pm(\sigma - 1)\left\{\left[\frac{\Delta\sigma_{st}}{\sigma_{st}(\sigma_{st} - 1)}\right]^2 + \left(\frac{\Delta D}{D}\right)_{st}^2 + \left(\frac{\Delta D}{D}\right)^2\right\}^{1/2}$$

At the maximum measured degrees of compression the accuracy of all the metal densities is given by $\Delta\rho/\rho \approx \pm 0.03$. We can assume on this basis that our experimental maximum pressures are close to the limits for the given experimental procedure. At higher pressures the error $\Delta\rho/\rho$ would grow, while the accuracy of the calculated values would become increasingly greater. For this reason we consider that it would not be advisable to extend the pressure scale for the investigated metals.

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