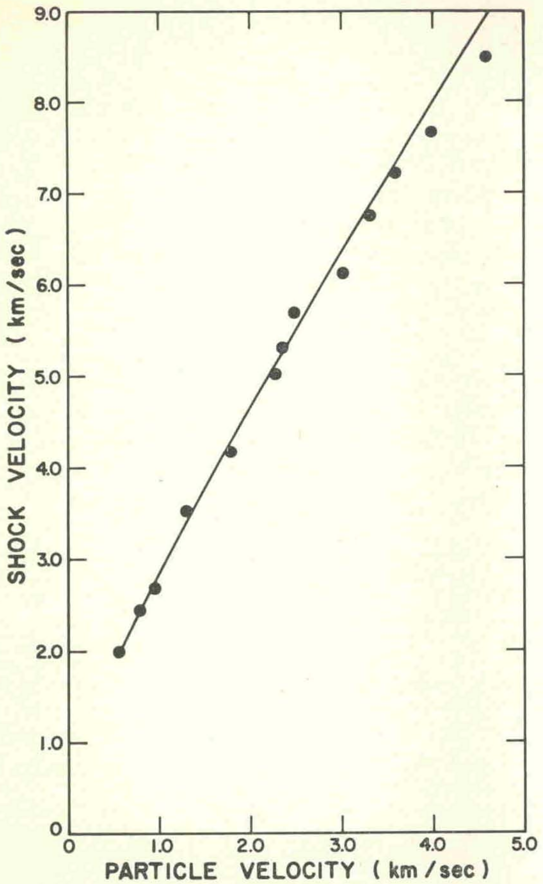

FIG. 2. Shock velocity versus particle velocity plot for solid argon showing the experimental Hugoniot data (solid circles) and the calculated Hugoniot curve (solid curve) from an exp-6 potential.

and in the 2024 aluminum standard, the pressure (P), volume (V), and particle velocity are determined from the impedance match method[10] and the Rankine–Hugoniot relations

$$P=\rho_0 U_s U_p, \qquad V=V_0(1-U_p/U_s), \quad \text{and} \quad V_0=1/\rho_0, \tag{1}$$

where ρ_0 is the initial density and U_s and U_p have been defined previously. It was necessary to adjust the 2024 aluminum Hugoniot[11] (measured at an initial temperature of 300°K) to the initial experimental temperature of 75°K. The U_s–U_p relation of the standard at this temperature is

$$U_s=5.387+1.335U_p. \tag{2}$$

A density of 2.820 g/cc at 75°K and a Gruneisen ratio of 2.0 for the standard were also utilized in the analysis. The errors given for the shock velocities are single standard deviations determined from a least-squares fit to the time–distance data. The least-squares fit is corrected also for a slight amount of tilt of the plane of the pressure wave with respect to the plane of the aluminum plate.

The U_s–U_p data of Table I are depicted in Fig. 2. The data can be interpreted as two straight line segments. A least-squares fit to the data in the interval $2.00\leq U_s\leq 5.79$ km/sec results in the equation

$$U_s=(1.04\pm0.11)+(1.79\pm0.06)U_p \tag{3}$$

and in the interval $5.79\leq U_s\leq 8.50$ km/sec,

$$U_s=(2.14\pm0.30)+(1.38\pm0.07)U_p. \tag{4}$$

The intersection occurs at $U_s=5.79$ km/sec and $U_p=2.65$ km/sec, which corresponds to a pressure of 253 kbar.

The above interpretation, however, is not unique. An equally good fit can be made for all shock velocities by

$$U_s=(0.87\pm0.12)+(2.08\pm0.11)U_p-(0.09\pm0.02)U_p^2. \tag{5}$$

It is noted that both interpretations result in an intercept ($U_p=0$) which agrees, within the errors, with the bulk sound speed (1.05 km/sec) calculated from adiabatic compressibility data.[12]

The Hugoniot of argon has been calculated for the exp-6, LJD (6–12), and the modified Morse potential. In the computation[13] the cell model of Lennard-Jones and Devonshire[14] was used and the pair potentials were assumed to be additive. The computation was performed utilizing a computer program developed by Fickett.[15]

The best fit to the experimental data occurred with the exp-6 form of the interatomic potential,

$$\Phi(r)=[kT_0/(\alpha-6)]\{6\exp[\alpha(1-r/r_0)]-(r/r_0)^{-6}\}, \tag{6}$$

where α is the family parameter representing the steepness of the repulsive part of the potential. The potential minimum is at r_0 with a potential well depth of kT_0. The relevant parameters were determined to be $T_0=118$°K, $r_0=3.70$ Å, and $\alpha=14.5$. These values are consistent with previous shock data,[2] molecular-beam data,[16] and various calculations.[13,17–19] The calculated U_s–U_p relation and the experimental data are illustrated in Fig. 2. They agree up to $U_s=6$ km/sec. The resultant Hugoniot is illustrated in Fig. 3 for comparison with the earlier liquid[2] and gas[3] studies.

IV. CONCLUSIONS

The Hugoniot of solid argon has been determined from 18 to 645 kbar, and the data have been fit with an exp-6 interatomic potential with good agreement up to 300 kbar. For this pressure range the assumption of pair additivity and the choice of the potential form is reasonable. The departure of the calculated Hugoniot from the experimental data occurs at higher pressures and temperatures. Apparently, the cell model needs to be modified to account for phenomena such as populating the conduction band, narrowing the band gap, ionization, and liquefaction. Under these conditions the potential form may also require modification.

The U_s–U_p data can be interpreted two different ways. The two-line segment interpretation, Eqs. (3) and (4), implies a phase transformation at 253 kbar. Since solid argon has a close-packed crystal structure, a polymorphic phase change is not expected and the transformation would likely be melting. In the pressure–volume plane a melting curve[2] calculated by the Monte Carlo method intersects the solid argon Hugoniot at about 250 kbar, agreeing well with the pressure associated with the discontinuous slope change in the U_s–U_p relation. The temperature calculated from the exp-6 potential at the transition pressure is about 5900°K.

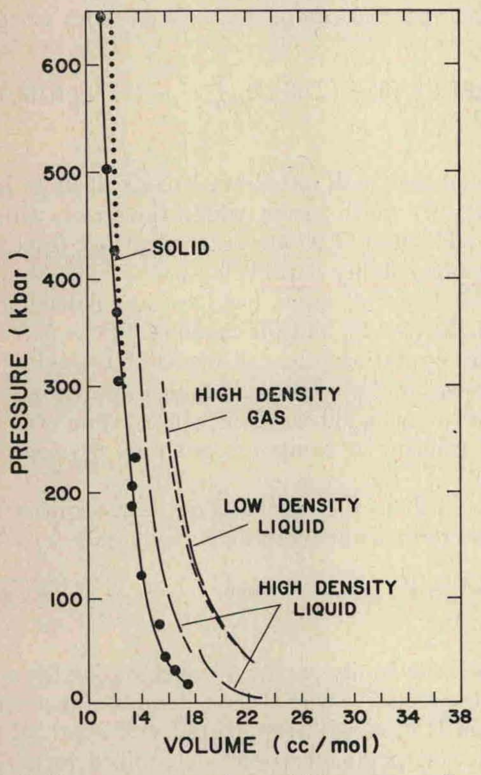

FIG. 3. Pressure versus volume plot for argon. —●—, experimental solid argon Hugoniot (V_0=24.21 cc/mol); – –, high- (V_0=28.43 cc/mol) and low- (V_0=43.46 cc/mol) density liquid argon Hugoniot data from Ref. 2; - - -, high- (V_0=40.93 cc/mol) density argon gas Hugoniot data from Ref. 3; •••, solid argon Hugoniot calculated from an exp-6 potential.

An alternate interpretation is that the data are represented by a single quadratic curve, Eq. (5). This would indicate that no transition occurs over the investigated pressure range. Some support for this interpretation arises from the slight curvature present in the theoretical U_s–U_p relation.

ACKNOWLEDGMENTS

We wish to thank C. D. Reese and T. E. Gould for their invaluable aid in carrying out the experimental program. We are indebted to Wildon Fickett and Stan Landeen for useful discussions throughout this investigation.

* Work performed under the auspices of the U.S. Atomic Energy Commission.

† Experimental investigation started while employed at the Los Alamos Scientific Laboratory.

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