the usual statistical theories of the equation of state. On the experimental side, the high compressions required can be reached by means of shock waves generated by condensed explosives. Pressure and volume can be obtained from measurements of shock and particle velocity,[4] or by x-ray densitometry.[5] Since the compression takes place along a Hugoniot curve, however, a considerable rise in temperature is unavoidable.

Liquid argon would appear to be the material of choice. The pair potential is spherically symmetric, and its repulsive portion has been experimentally determined in the appopriate range of distances.[2] Monte Carlo equation-of-state calculations[3] have been done for a form of the pair potential and a range of reduced temperatures and volumes which are appropriate, and some points on the shock Hugoniot have been measured.[5]

Accordingly, the calculations presented here are for the shock Hugoniot of liquid argon. They are based on the experimentally determined repulsive portion of the pair potential and the Monte Carlo calculation of the equation of state. Since the Monte Carlo calculations are expensive in computer time, and were done with a somewhat different pair potential, the Lennard-Jones-Devonshire (LJD) cell model equation-of-state[6] is used as a substitute for the Monte Carlo method in order to calculate the Hugoniot with the experimental pair potential. The Hugoniots calculated from the LJD and Monte Carlo equations of state with the same pair potential agree surprisingly well, and thus afford some confidence in this procedure.

2. COMPARISON OF MONTE CARLO AND LENNARD-JONES-DEVONSHIRE EQUATIONS OF STATE

The model used is a system of argon atoms in the ground state. As discussed above, the additivity of pair forces is assumed throughout.

The shock Hugoniot curve is the solution of the equation[7]

$$E - E_0 - \tfrac{1}{2}P(V_0 - V) = 0 \qquad (2.1a)$$

$$E = \tfrac{3}{2}R(T - T_0) + E', \qquad (2.1b)$$

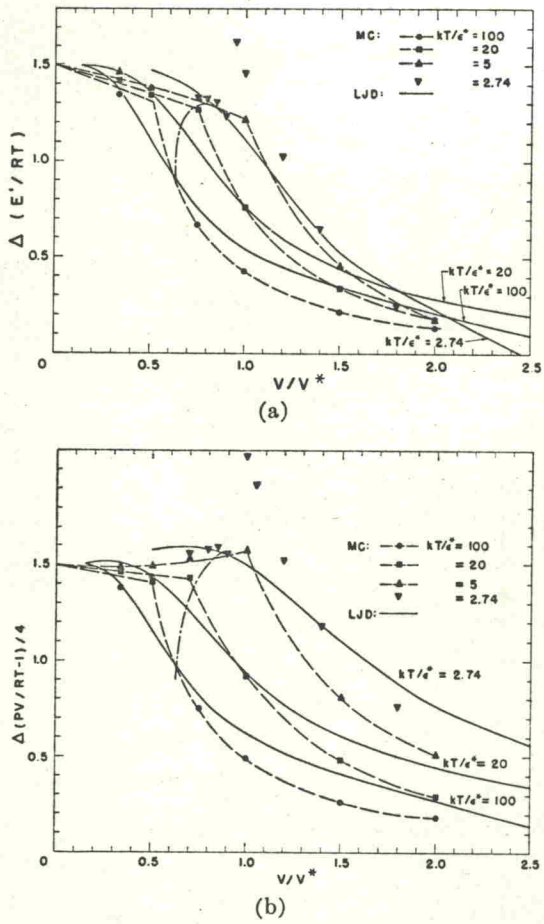

FIG. 1. Isotherms for the Monte Carlo (points and dashed curves) and LJD (solid curves) equations of state. Excess quantities over those for the regular (face-centered cubic) lattice configuration are shown (see text). The chain curves show the approximate position of the shock Hugoniot.

where P, V, and E are the pressure, molar volume, and molar internal energy, respectively, and the subscript $_0$ denotes the initial state, which is taken to be liquid argon at its boiling point:[8] $P_0 = 1$ atm; $V_0 = 28.7$ cm^3/mole; $T_0 = 87.29$ °K; and $E_0/RT_0 = -7.982$, where the reference state for the energy is gaseous argon in the ideal gas state at T_0. (We have taken $E_0/RT_0 = \Delta H_v/RT_0 - 1$, with ΔH_v the experimental enthalpy of vaporization at T_0.) The imperfection energy E' is calculated from the LJD cell theory or the Monte Carlo method.

The Monte Carlo technique has been used to generate points on four isotherms,[3] using the Lennard-Jones 6–12 form for the pair potential;

$$u(r) = \epsilon^*[(r/r^*)^{-12} - 2(r/r^*)^{-6}], \qquad (2.2)$$

where r^* and ϵ^* are the radius and well depth of the

[4] M. H. Rice, R. G. McQueen, and J. M. Walsh, *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1958), Vol. 6.

[5] J. Dapoigny, J. Kieffer, and B. Vodar, J. Phys. radium 8, 733 (1955).

[6] L. E. Lennard-Jones and A. F. Devonshire, Proc. Roy. Soc. (London) A163, 53 (1937).

[7] See, for example, R. Cournat and K. O. Friedrichs, *Supersonic Flow and Shock Waves* (Interscience Publishers, Inc., New York, 1948). p. 121 ff.

[8] F. Din, *Thermodynamic Functions of Gases* (Butterworths Scientific Publications Ltd., London, 1956), Vol. 2, p. 181.