

at the head-on collision of two plane shocks; (v) the initial shock conditions for liquid argon in contact with the explosive 60/40 RDX/TNT; (vi) shock conditions in precompressed liquids.

Since we began this work, Fickett and Wood (1960) have published the results of some LJD calculations of shock properties in liquid argon. Their method was rather more empirical than ours because it made use of the experimental density and energy of unperturbed argon. They employed the LJD theory at high pressures where they believed it right and the experimental data at low pressures where it appeared to be wrong.† For their particular purpose this was a justifiable procedure, but here we have preferred to be consistent and use the theoretical LJD equation throughout.

## II. DEFINITIONS OF SYMBOLS USED

Most of the following symbols have been defined more fully in earlier papers (Hamann 1960*b*; David and Hamann 1961).

The subscript zero denotes properties characteristic of the molecules. Asterisks indicate quantities expressed in molecular units.

- N, Avogadro's number,
- k, Boltzmann's constant,
- h, Planck's constant,
- $\epsilon_0$ , depth of the energy well in the Lennard-Jones 12 : 6 intermolecular potential,
- $r_0$ , radius of the energy well,
- $m$ , molecular mass,
- $M$ , molar mass ( $=Nm$ ),
- $\Lambda^*$ , de Boer's (1948) quantal parameter ( $=2^{1/6}h/r_0(m\epsilon_0)^{1/2}$ ),
- $C_V$ , specific heat per mole at constant volume,
- $C_V^*$ ,  $C_V/Nk$ ,
- $E$ , internal energy per mole,
- $\hat{E}$ , internal energy per unit mass,
- $E^*$ ,  $E/N\epsilon_0$ ,
- $P$ , pressure,
- $P_0$ ,  $2^{1/2}\epsilon_0/r_0^3$ ,
- $P^*$ ,  $P/P_0$ ,
- $S$ , entropy per mole,
- $S^*$ ,  $S/Nk$ ,
- $T$ , absolute temperature,
- $T_0$ ,  $\epsilon_0/k$ ,
- $T^*$ ,  $T/T_0$ ,
- $u$ , velocity of sound,
- $u_0$ ,  $(\epsilon_0/m)^{1/2}=(N\epsilon_0/M)^{1/2}$ ,
- $u^*$ ,  $u/u_0$ ,

† During the course of our calculations it has become increasingly apparent that the LJD theory is really more appropriate to the solid state than to the liquid. Barker's (1960, 1961*a*) "tunnel" model is a much better one for liquids, and we hope to apply it later in some shock calculations.

- $U$ , shock velocity,  
 $U^*$ ,  $U/u_0$ ,  
 $V$ , volume per mole,  
 $\hat{V}$ , volume per unit mass,  
 $V_0$ ,  $Nr_0^3/2^{\frac{1}{2}}$ ,  
 $V^*$ ,  $V/V_0$ ,  
 $w$ , flow velocity,  
 $w^*$ ,  $w/u_0$ .

The following subscripts are applied to shock properties :

- no subscript, indicates the initial conditions ahead of a shock wave,  
 subscript 1, denotes the conditions behind a single shock,  
 subscript 2, denotes the conditions after the interaction of one shock with another, or with a rarefaction wave.

### III. DETAILS OF THE CALCULATIONS

#### (a) General

A shock wave is a steep-fronted compression wave which causes very abrupt changes in the pressure, density, and temperature of the material through which it passes. The existence of extreme gradients in these properties through the shock front means that the compression is thermodynamically irreversible and non-adiabatic. Nevertheless there exist some rigorous relations between the conditions ahead of and behind the shock front. They are based on the principles of conservation of mass, momentum, and energy, and they are usually known as the Rankine-Hugoniot relations† (Rankine 1870; Hugoniot 1887, 1889). If the fluid ahead of the shock wave is stationary, the relations are

$$U_1 = \hat{V}[(P_1 - P)/(\hat{V} - \hat{V}_1)]^{\frac{1}{2}}, \quad (1)$$

$$w_1 = [(P_1 - P)(\hat{V} - \hat{V}_1)]^{\frac{1}{2}}, \quad (2)$$

$$\hat{E}_1 - \hat{E} = \frac{1}{2}(P_1 + P)(\hat{V} - \hat{V}_1), \quad (3)$$

where  $P$ ,  $\hat{V}$ , and  $\hat{E}$  are the pressure, volume per unit mass, and internal energy per unit mass in the initial state, and  $P_1$ ,  $\hat{V}_1$ ,  $\hat{E}_1$  are the corresponding properties of the shocked fluid.  $U_1$  denotes the velocity of the shock front and  $w_1$  the velocity of flow of the material behind the front. In the limit of low amplitude shock waves  $P_1 - P$ ,  $\hat{V} - \hat{V}_1$ ,  $w_1$ , and  $\hat{E}_1 - \hat{E}$  all approach zero and  $U_1$  approaches the normal velocity of sound,  $u = \hat{V}(-\partial P/\partial \hat{V})^{\frac{1}{2}}$ .

For a Lennard-Jones and Devonshire liquid the Rankine-Hugoniot relations can be rewritten in molecular units (defined in Section II) thus

$$U_1^* = V^*[(P_1^* - P^*)/(V^* - V_1^*)]^{\frac{1}{2}}, \quad (4)$$

$$w_1^* = [(P_1^* - P^*)(V^* - V_1^*)]^{\frac{1}{2}}, \quad (5)$$

$$E_1^* - E^* = \frac{1}{2}(P_1^* + P^*)(V^* - V_1^*). \quad (6)$$

† This title is misleading: formulae equivalent to (1) and (2) were first derived by Stokes (1848).