6.2 *Calculation of Hugoniots*

The most accurate information on solids at high pressure is available from shock wave experiments. The relevant equations are well known [59]

$$u_s = V_0\sqrt{\frac{P_1 - P_0}{V_0 - V_1}} \tag{11}$$

$$u_p = \sqrt{(P_1 - P_0)(V_0 - V_1)} \tag{12}$$

and

$$E_1 - E_0 = \tfrac{1}{2}(P_1 + P_0)(V_0 - V_1) \tag{13}$$

where u_s is the shock velocity, u_p is the particle velocity, and the subscripts 0 and 1 refer to the initial and final states, respectively.

At a given volume, equation (13) was solved numerically using tabulated values of $P(T)$ and $E(T)$ from (5) and (6). The calculated pressure was then inserted into (11) and (12) giving the theoretical Hugoniot curve in the shock-particle velocity plane. These theoretical curves are plotted along with the experimental data from Refs. [60–64] for LiBr, LiI, NaF, NaCl, NaBr and NaI in Figs. 3–8. In most cases, Hugoniots corresponding to zero and two percent porosity are plotted. Data of

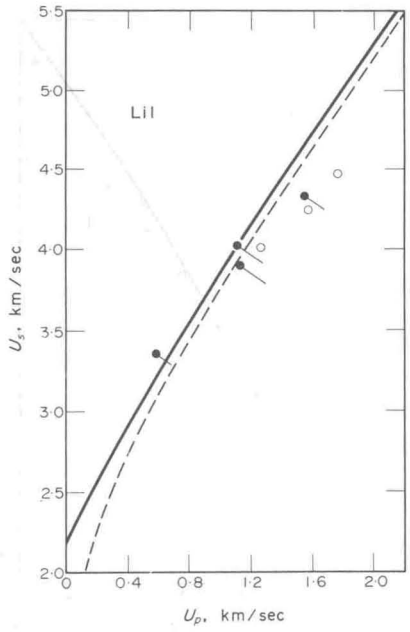

Fig. 4. Hugoniot of LiI. ——— lattice model calculation. --- model calculation for 24 porous sample. ○ Single crystal experiment [61], ● Pressed sample [62], corrected to single crystal Hugoniot.

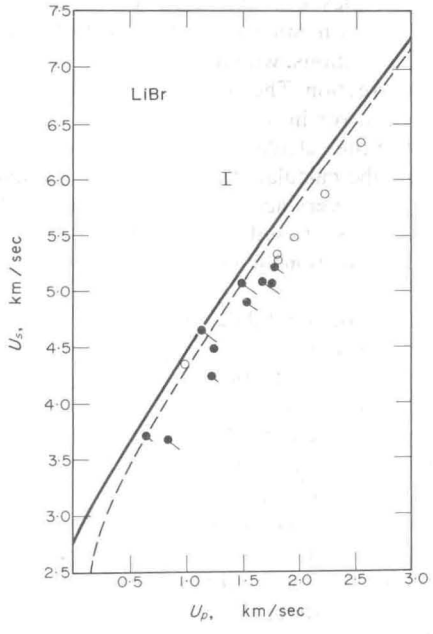

Fig. 3. Hugoniot of LiBr. ——— lattice model calculation. --- model calculation for 2 per cent porous sample. ○ Single Crystal Experiment [60]; ● Pressed Sample [61], corrected to single crystal Hugoniot.

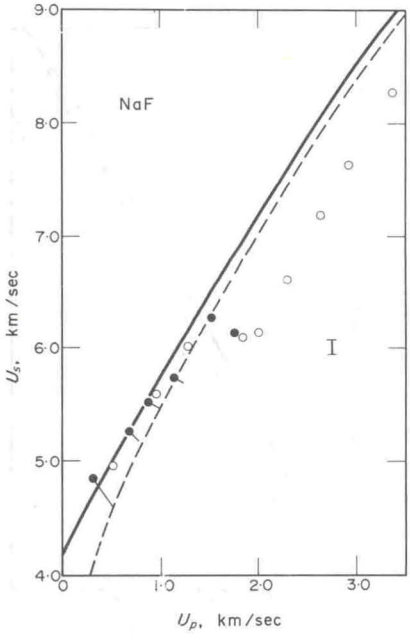

Fig. 5. Hugoniot of NaF. ——— lattice model calculation. --- model calculation for 2 per cent porous sample. ○ Single crystal experiment [60]. ● Pressed sample [61], corrected to single crystal Hugoniot.

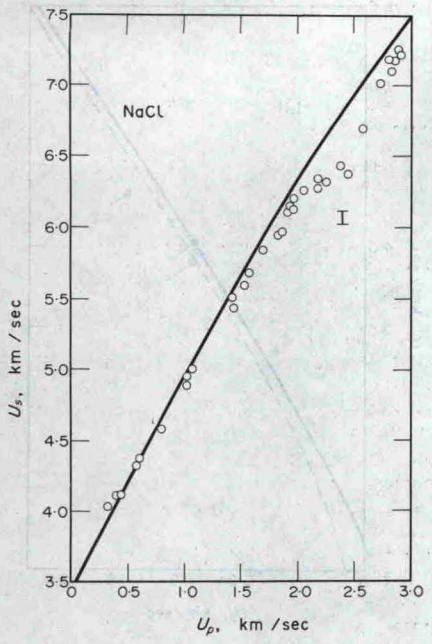

Fig. 6. Hugoniot of NaCl. ——— lattice model calculation. ○ Single crystal data [63].

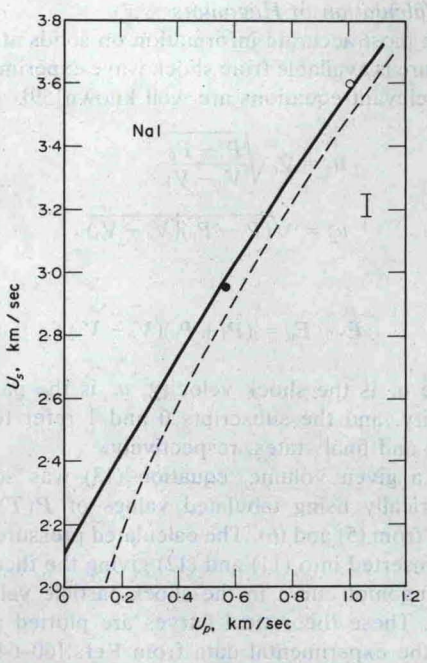

Fig. 8. Hugoniot of NaI. ——— lattice model calculation. ● Single crystal data [61]. ○ single crystal data [64].

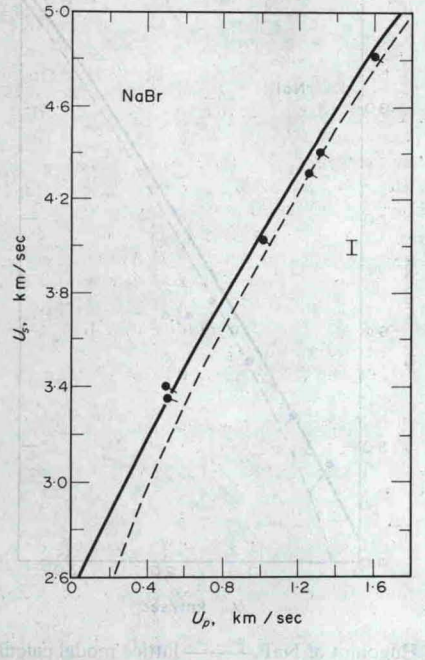

Fig. 7. Hugoniot of NaBr. ——— lattice model calculation. – – – model calculation for 2 per cent porous sample. ● experimental data from pressed sample [61], corrected to zero porosity.

porous samples was corrected to a zero porosity Hugoniot in a manner consistant with the present model calculations, with a line on the graph indicating the correction. The error bars refer to a nominal 1 per cent error in u_s.

Because the calculated γ at room temperature is too large, the calculated Hugoniot of LiBr and LiI should not be very accurate. The experimental data is sparse and scattered, and does not contradict the present calculation at compressions of less than $\Delta V/V_0 = 0{\cdot}25$.

The new Hugoniot data for NaF (Fig. 5) shows a phase change initiating at a pressure somewhere between 210 and 270 kbar on the Hugoniot. The possibility of a phase change at this point was recently suggested by Ahrens and Thomsen [27] on the basis of Christian's [61] single data point falling within the transition region. Just prior to the transition, the Hugoniot prediction of the present lattice model calculation is slightly more accurate than the prediction of Ahrens and Thomsen based on finite strain theory [27].

In NaCl (Fig. 6), the predictions of lattice theory and finite strain theory [27] are both fairly accurate up to the phase transition, which occurs at a compression of about 0·35.

The predicted Hugoniots in NaBr and NaI are in