excellent agreement with experiment, more so than the finite strain theory predictions. The calculated instabilities prevented comparison with experiment at compressions higher than those plotted ($\Delta V/V_0 = 0{\cdot}33$ and $0{\cdot}28$ respectively).

7. CONCLUSIONS

The present quasi-harmonic lattice model calculations provide a self-consistent framework for the calculation of macroscopic physical properties of crystals at arbitrary pressure and temperature. The calculated Grüneisen γ, $\partial \ln \gamma / \partial \ln V$, and δ_s are in reasonable agreement with experiment for most alkali halides. The inclusion of higher order anharmonic terms would improve the situation. The variation of γ with volume is initially dominated by coulomb effects. At very modest compressions this effect suddenly diminishes and $\gamma(V)$ is controlled mainly by the short range portion of the interatomic potential. Although simple analytic functions can adequately describe $\gamma(V)$, the presence of coulomb effects at zero pressure makes it difficult to extrapolate smoothly through this region of sudden change using low pressure experimental data.

The model calculations are in good agreement with experimental Hugoniots in cases for which the quasiharmonic theory was adequate at room temperature (NaCl, NaBr and NaI). The agreement is worse in cases for which anharmonic effects are important at room temperature (LiBr, LiI and NaF). In all cases the present theory compares favorably with recent finite strain theory calculations.

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