

NON LINEAR PROPERTIES OF ROCKSALT STRUCTURE SOLIDS

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Abstract

An effort has been made for obtaining the non linear properties of rocksalt structure solids starting from primary physical parameters viz. nearest-neighbor distance and hardness parameter assuming long- and short-range potentials at elevated temperatures. The elastic energy density for a deformed crystal can be expanded as power series of strains for obtaining coefficients of quadratic, cubic and quartic terms which are known as the second-, third- and fourth-order elastic constants, respectively. When the values of the higher order elastic constants are known for a crystal, many of the anharmonic properties of the crystal can be treated within the limit of the continuum approximation in a quantitative manner. In this study, higher-order elastic constants are computed up to their melting temperature for rocksalt structure solids, which are alkali cyanides, sodium and potassium halides. The first order pressure derivatives of second- and third-order elastic constants, the second-order pressure derivatives of second-order elastic constants and partial contractions are also evaluated at different temperatures for these substances. The results thus obtained are compared with experimental data and found in well agreement with present values.

Method for presentation: ORAL

Requirement: LCD and Sound System