INVESTIGATION OF COHESIVE, THERMAL AND ELASTIC PROPERTIES OF ALKALI SUPEROXIDES

Preeti Singh Bahadur

Amity University, Greater Noida, India

ABSTRACT

We have applied an Extended Three Body Force Shell Model (ETSM) for investigating the cohesive, thermal and elastic properties such as cohesive energy (ϕ), molecular force constant(f), compressibility (β), Restrahlen frequency (υ_0), Debye temperature (θ_D), Gruneisen parameter (γ), second Gruneisen parameter (q), Moelwyn Hughes constants (F1), and ratio of volume expansion coefficient (α_v) to volume specific heat (c_v) of alkai superoxide. We have also reported the Third order elastic constant's (TOECs), pressure and temperature derivatives of Second order elastic constant's (SOECs). Elastic constant variation and Specific heat curve of alkali superoxide are also reported on the paper. And, we could compare our result of specific heat curve with the experimental data. Our computed specific heat results follow the same trends of variation with corresponding experimental data. The values of specific heats also increase with temperature. Our calculated results on specific heat are in closer agreement with the experimental data. Here, we could compare our result of cohesive, thermal and elastic properties with other available experimental data at room temperature.

Keywords: Cohesive, Thermal, Elastic, Specific Heat