Pramana – J. Phys. (2022) 96:97
https://doi.org/10.1007/s12043-022-02318-x

Study of elastic, mechanical, thermophysical and ultrasonic properties of divalent metal fluorides XF_2 (X = Ca, Sr, Cd and Ba)

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MS received 20 February 2021; revised 26 October 2021; accepted 30 November 2021

Abstract. This paper described the behaviours of four divalent metal fluorides (CaF_2, SrF_2, CdF_2 and BaF_2) in terms of their superior elastic, mechanical and thermophysical properties. Initially, higher-order elastic constants of the chosen divalent metal fluorides have been calculated using the Coulomb and Born–Mayer interaction potential in the temperature regime 100–300 K. With the help of these constants, other elastic moduli, such as Young's modulus (Y), bulk modulus (B), shear modulus (G), Poisson's ratio (σ) and Pugh's ratio (B/G) have been computed using Voigt–Reuss–Hill approximation. The Born stability criteria and Vicker's hardness parameter (H_v) have been used for analysing the nature and strength of the materials. Later on, ultrasonic velocities including Debye average velocities were evaluated using calculated values of second-order elastic constants and density in the same physical conditions. Thermal properties such as the lattice thermal conductivity, thermal relaxation time, thermal energy density and acoustic coupling constant have also been computed at the same physical conditions and along ⟨100⟩. The temperature-dependent ultrasonic properties have been correlated with other thermophysical properties to extract important information about the microstructural quality and the nature of the materials. The obtained results have been analysed to explore the inherent properties of the chosen divalent metal fluorides, which are useful for numerous industrial applications.

Keywords. Divalent metal fluorides; elastic constants; mechanical property; thermophysical property; ultrasonic attenuation.

PACS Nos 43.35.Cg; 62.20.dc; 63.20.kr

1. Introduction

Divalent metal fluorides XF_2 (X = Ca, Sr, Cd and Ba) fascinate material scientists and researchers due to their intrinsic low phonon energies and high physical and chemical stability [1–4]. The divalent metal fluorides exhibit extensive optical, electrical, thermal, superconducting, semiconducting, thermo-optical and wide transmission band properties [3–6]. The potential applications of the divalent metal fluorides are raw materials for manufacturing optical elements for average and high power lasers, elementary particle and γ-ray detectors, sensors, high-temperature batteries, chemical filters, etc. [7–10]. In recent years, several studies have been conducted on the optical, thermal and electronic properties of divalent metal fluorides. In particular, optical anisotropy parameters and Euler angles of crystallographic axis orientation of CaF_2, SrF_2 and BaF_2 cubic crystals were measured by Snetkov *et al* [3]. The structural phase stability of the alkaline-earth divalent metal fluorides had been studied by Kanchana *et al* [4]. Band structures of divalent metal fluorides were reported by Ching *et al* [5]. A detailed study considering the effect of pressure in the electronic and optical properties of BaF_2, by applying the equation of state has been done by Jiang *et al* [6]. Heise *et al* [7] investigated pressure dependency of the elastic constants of CaF_2 using phase comparison and Cook's method. The thermodynamic and phonon transport properties of FCC structured divalent metal fluorides at high temperature

Published online: 17 May 2022