Metals and Materials International
https://doi.org/10.1007/s12540-020-00633-9

Mechanical, Thermophysical, and Ultrasonic Properties of Thermoelectric HfX_2 (X = S, Se) Compounds

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Received: 20 October 2019 / Accepted: 28 January 2020

Abstract
In the present study, ultrasonic and thermophysical behaviour of thermoelectric hexagonal structured HfX_2 (X = S, Se) compounds have been analysed by the theoretical evaluation of second and third order elastic constants (SOECs and TOECs) using many body interaction potential model. The computed SOECs have been used to determine the temperature dependent specific heat, thermal energy density, elastic coupling constants, Grüneisen parameters, ultrasonic velocities, Debye average velocity, ultrasonic attenuation, and thermal relaxation time. We have observed that the temperature dependent ultrasonic attenuation and thermal relaxation time for HfX_2 are mainly affected by thermal conductivity. The elastic properties of the material are compared with existing data in literature for the validation of the work. The obtained values of elastic stiffness are found very large in comparison to that of other material from transition metal dichalcogenides of group IVB indicating better mechanical properties than the same group materials. Calculated elastic, thermal, and ultrasonic properties are correlated for better characterization of the materials which are useful for thermoelectric and energy transport applications.

Keywords Elastic constant · Phonon–phonon interaction · Thermal relaxation time · Ultrasonic attenuation · Ultrasonic velocity

1 Introduction

Ultrasonic characterization of materials is the main theme of interest for engineers and material scientists for a long time because ultrasonics is a non-destructive and useful technique having wide variety of applications in every field of life [1–3]. Non-destructive ultrasonic techniques can be used to study the physical properties of the materials by measuring the ultrasonic attenuation [4–6]. The interaction of ultrasonic wave with material is very inventive tool for determination of higher order elastic constants as well as several physical properties of materials. Important thermophysical properties of the materials such as thermal conductivity, Grüneisen parameters, Debye temperature, and specific heat can be determined using SOECs and TOECs. We can find the information about the structural behaviour of the materials on the basis of these properties [7–9].

The compelling demand of higher performance devices gives inspiration to material scientist and engineers for the development of high efficient materials [10]. Since the discovery of exotic properties of graphene, two dimensional materials (2DMs) have revolutionized the nanoscience and nanotechnology [11]. The discovery of graphene paved the way for rediscovery of many other 2DMs, such as metal chalcogenides, transition metal oxides, transition metal dichalcogenides (TMDs), etc. [10, 11]. Among these semiconducting transition metals, dichalcogenides from group IVB have attracted great interest due to their distinct mechanical, electric, optical, and thermal properties [12]. In recent years, the thermoelectric response of nanomaterials has become a hot topic in the science community [13–16]. In the race of high thermoelectric performance, two-dimensional monolayer materials have attracted great interest due to their novel thermophysical properties [14–17]. It has been proposed that low-dimensional materials could have better thermoelectric performance than their bulk due to the diverse scattering mechanism for phonons [18]. The efficiency of thermoelectric devices, which can directly convert waste of heat into electricity, is characterized by the dimensionless figure of merit (*ZT*) and given by

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Published online: 12 February 2020