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Ultrasonic wave propagation in thermoelectric ZrX_2 (X = S, Se) compounds

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Abstract. In the present work, we have calculated temperature-dependent second- and third-order elastic constants (SOECs and TOECs) of thermoelectric zirconium disulphide (ZrS_2) and zirconium diselenide ($ZrSe_2$) using a simple interaction potential model. SOECs have been used for the calculation of ultrasonic velocity along different orientations of propagation. Thermal relaxation time and ultrasonic attenuation have been determined with the help of SOECs and thermal conductivity. Temperature-dependent specific heat, thermal energy density, elastic coupling constants and Grüneisen parameters are also calculated using SOECs and other parameters. The dominating cause behind ultrasonic attenuation, in the temperature range of 300–900 K, is the interaction of acoustical phonon and lattice phonon. In the present study, we observed that the thermal conductivity and energy density play significant roles in ultrasonic attenuation. Ultrasonic velocity and attenuation are correlated with other thermophysical properties extracting important information about the quality and nature of the materials which are useful for industrial applications.

Keywords. Elastic constant; ultrasonic attenuation; phonon–phonon interaction; thermal conductivity; Grüneisen parameter.

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1. Introduction

Nowadays, most of the energy waste is in the form of heat. The thermoelectric (TE) technology may be an alternative and environment-friendly technology for energy conversion which directly converts this heat into electrical energy [1,2]. The efficiency of TE materials is defined as the dimensionless figure of merit (ZT) which is a symbol of TE performance. The figure of merit (ZT) is given by the formula $\mathrm{ZT} = S^2\sigma T/k$, where S, σ, T and k stand for the Seebeck coefficient, electrical conductivity, temperature and thermal conductivity, respectively. The main challenging task for the research community is the lower efficiency of these devices because of low figure of merit (ZT). Conceptually, to obtain a better figure of merit, materials must have a high value of Seebeck coefficient with good electrical conduction property and low thermal conductivity [1–7].

Acoustics is a powerful tool to study the properties of different types of materials. Ultrasonics is a non-destructive and useful technique for determining the structural integrity of materials [8,9]. The ultrasonic technique can be used for detecting discontinuities, measuring thickness, studying metallurgy, detecting damage in composites and determining elastic properties along with other thermophysical properties of materials. Non-linear elastic properties (second- and third-order elastic constants (SOEC and TOEC)) can be utilised to determine ultrasonic scientific parameters like attenuation and to provide information about the microstructural features of materials [10,11].

In the race for high-performance TE materials, semiconducting transition metal dichalcogenides (TMDCs) from group IVB have attracted great interest due to their small thermal conductivity. In our present evaluation, we have studied ZrS_2 and $ZrSe_2$ which have a hexagonal close-packed (HCP) structure with lattice