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On the scaling factor in Debye–Grüneisen model: A case study of the Mg–Zn binary system

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ABSTRACT

The utility of the Debye–Grüneisen has been investigated with respect to a finite-temperature fitting parameter known as the scaling factor. This scaling factor is studied using bcc, fcc, hcp systems and the Mg–Zn binary system. Predicted Debye temperatures, using a calculated scaling factor, show good agreement with experiments and improvements over the scaling factor derived by Moruzzi et al. Finite-temperature thermodynamic properties of Mg, Zn, Mg_4Zn_7, $MgZn_2$, and Mg_2Zn_{11} are investigated to show the efficiency and improved accuracy of the calculated scaling factor. For the intermetallic compounds except Mg_2Zn_{11}, Θ_D predictions are improved upon greatly by implementing a calculated scaling factor. Along the same line, heat capacity is also predicted, showing good agreement with experimental values for these compounds. For Mg_2Zn_{11}, the Debye–Grüneisen model cannot account for anomalous lattice dynamics at low temperatures.

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1. Introduction

Within the fields of applied physics, materials modeling and thermodynamics property predictions, the Debye–Grüneisen model is used extensively due to its simplicity and accuracy in the low temperature regime for crystalline systems, simple and complex. Such an advantage becomes better seen with more complex crystal systems that significantly amplify computation times [1]. However, when the Debye–Grüneisen model is applied in many cases, the predicted Debye temperatures (Θ_D) do not match with experimental values, a consequence of simplifying the speeds of sounds with respect to the bulk modulus (B) and density (ρ), or $v = \sqrt{B/\rho}$. In such instances, the model requires a semi-empirical multiplicative scaling factor which will help yield the correct Θ_D [1–4]. While previous studies have utilized empirical scaling factors successfully for various crystal systems, the agreements with experiments are somewhat coincidental due to the fact that most materials have a Poisson ratio of approximately 1/3 [2]. It is thus desirable to develop an approach to predict the scaling factor.

Typically, the Debye model is described with just a single speed of sound accounted for all acoustic and optical modes, i.e. a linear phonon dispersion that has no directional dependence and is identical for transverse and longitudinal waves. Crystal speed of sound anisotropy is also ignored as Debye acoustic modes are isotropic and non-directional [5]. However, even for an isotropic medium, the assumption of a single speed of sound for transverse and longitudinal waves is incorrect [2], as shown schematically in Fig. 1. Thus, one actually uses an *effective speed of sound* that incorporates the transverse and longitudinal speeds in the Debye model. As discussed by Anderson [6], for an isotropic solid, this effective speed of sound can be expressed as:

$$v = \left[\frac{1}{3}\left(\frac{2}{v_t^3} + \frac{1}{v_l^3}\right)\right]^{-1/3} \tag{1}$$

where v is the effective speed of sound, $v_t = \sqrt{S/\rho}$ the transverse speed, $v_l = \sqrt{L/\rho}$ the longitudinal speed, ρ the density, S the shear modulus, and L the longitudinal modulus. If instead of calculating the effective speed of sound from Eq. (1), one calculates v by the formula for the speed of sound in a medium ($v = \sqrt{B/\rho}$) and obtains the Debye temperature as follows

$$(\Theta_D)_0 = \frac{\hbar v}{k_B}\left(\frac{6\pi^2 N}{V}\right)^{1/3} \tag{2}$$

where $\hbar$ is the reduced Planck constant, v the constant velocity of sound, k_B the Boltzmann constant, N the number of particles, and V the volume [5]. However, thus calculated Debye temperature is significantly different from the ones evaluated from experimental data. Often, this discrepancy is mended by the introduction of a scaling factor s that scales the predicted $(\Theta_D)_0$ to an experimental

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one, as shown below, which was implemented by Moruzzi et al. [2] and modified by Shang et al. [4]:

$$\Theta_D = sAV_0^{1/6}\left(\frac{B_0}{M}\right)^{1/2}\left(\frac{V_0}{V}\right)^{\gamma} \tag{3}$$

In this equation, s is the Debye temperature scaling factor, γ the Grüneisen parameter, A a constant equal to $(6\pi^2)^{\frac{1}{3}}\hbar/k_B$ with the equilibrium volume V_0 given in Å^3, the bulk modulus at 0 K represented by B_0 in GPa, and the atomic mass M in grams [4]. The averaged atomic mass of an intermetallic compound is taken as the geometric mass to account for large differences in the masses of the pure elements. As shown in previous studies, the logarithmic average of mass can also be used [7]. If the scaling factor is fit from experimental results, then the Debye temperature is not strictly calculated from "first-principles". Note that the Grüneisen parameter γ scales $(\Theta_D)_0$ with the following equation:

$$\Theta_D = (\Theta_D)_0\left(\frac{V_0}{V}\right)^{\gamma} \tag{4}$$

where V_0 and V are the volumes of the rigid-lattice equilibrium (separation distance) and the evaluation volume, respectively. There are three commonly used models for the Grüneisen parameter γ to account for vibrational anharmonicity: Slater (S) [8], Dugdale–MacDonald (DM) [9], and Vaschenko–Zubarev (VZ) [10]. By expressing the parameter as $\gamma = (1 + B'_0)/2 - x$ and choosing $x = 2/3$, $x = 0$, or $x = 1$, one arrives at the Slater, VZ and DM limits [11]. This formulation captures the linearity of the parameter with respect to the derivative of the bulk modulus [10] and can represent the high and low temperature assumptions of Grüneisen parameter, respectively [1,2,4]. Tests must be conducted to select the models for γ. In this work, as per recommended by Shang et al. [4], the Slater and Dugdale–MacDonald approximations will be evaluated.

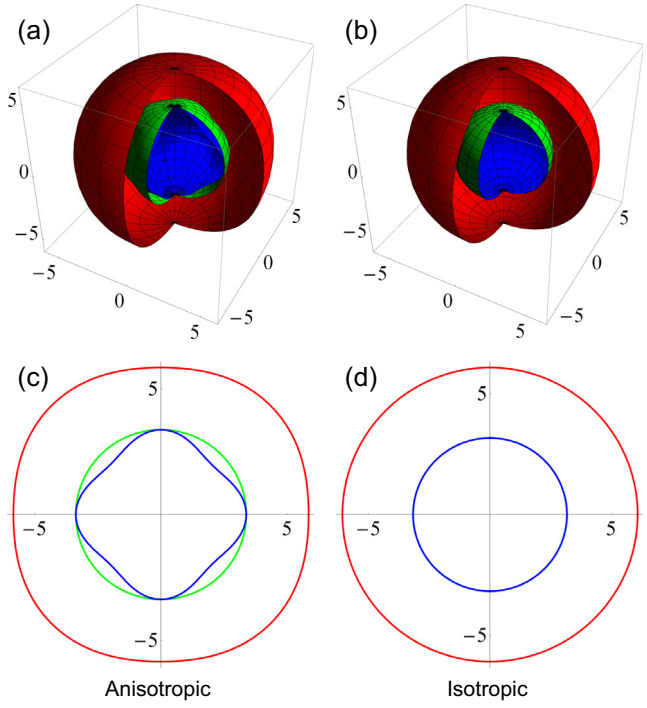

Fig. 1. Shown in (a and b) are spherical plots of the speeds of sound in units of km/s for the anisotropic and isotropic cases, respectively. Plots (b and d) represent the (0 0 1)-plane cross-sections of (a and b). Red (dot dashed), green (solid) and blue (dashed) represent the longitudinal, transverse 1 and transverse 2 speeds of sound. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Moruzzi et al. [2] and Herper et al. [3] studied the contributions of such a scaling factor in terms of magnetic and non-magnetic cubic elements. It was demonstrated that by fitting the longitudinal and shear moduli with respect to B, roughly constant scaling factors can be derived for many cubic transition metals with a few exceptions. The fitted scaling factors are 0.617 and 0.7638 for non-magnetic and magnetic transition metals, respectively. Chen & Sundman [1] and Lu et al. [7,12] have also studied the scaling contributions for transition metals, cubic carbides, and nitrides.

In this work, we will validate the findings of Lu et al. and extend the method to perform a case study on the Mg–Zn binary system. While Chen and Sundman [1] and Lu et al. [7,12] have studied various classes of crystals, a systematic study of the scaling factor for one binary system has not be accomplished. The Mg–Zn system is chosen as a case study because it contains a multitude of stoichiometric intermetallics that have been studied extensively using experiments [13–19]. Mg–Zn intermetallics also have very different crystallography including monoclinic, hexagonal Laves, and cubic phases. The data availability, complexities and crystallographic differences make the Mg–Zn a suitable case study.

2. Methodology

The Debye model describes the vibrational properties of an isotropic material. Eq. (1) shows that the effective speed of sound in a material can be averaged by the transverse and longitudinal speeds of sound v_t and v_l. Both moduli can be represented by the Poisson ratio, υ, and bulk modulus, B:

$$L = \frac{3B(1-\upsilon)}{1+\upsilon} \quad \text{and} \quad S = \frac{3B(1-2\upsilon)}{2(1+\upsilon)} \tag{5}$$

Substituting Eq. (5) into Eq. (1) yields an equation for the scaling factor as a function of the Poisson ratio, which is also shown in Fig. 2 and in agreement with previous findings [1,7]:

$$s(\upsilon) = 3^{5/6}\left[4\sqrt{2}\left(\frac{1+\upsilon}{1-2\upsilon}\right)^{3/2} + \left(\frac{1+\upsilon}{1-\upsilon}\right)^{3/2}\right]^{-1/3} \tag{6}$$

The validation of this equation can be done with experimental values obtained by Moruzzi et al. [2] and Herper et al. [3]. Moruzzi determined, by fitting cubic non-magnetic metals, that L and S can be represented by $1.42B$ and $0.30B$, respectively. When these values are put into Eq. (6), the predicted value of the scaling factor is 0.617 ($\upsilon = 0.3661$), as found by Moruzzi. The same analysis can be applied to L and S determined for cubic magnetic metals by

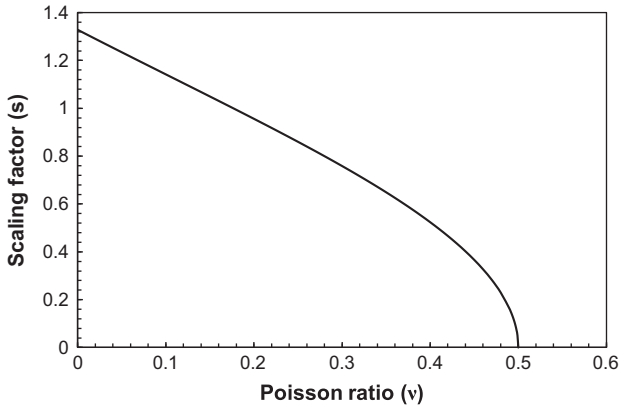

Fig. 2. Scaling factor, s, as a function of the isotropic Poisson ratio, ν. Please note that a $\nu = 0$ does not denote a s of 1, but rather 1.327.

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