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Shear sound velocity of hexagonal close packed iron at extreme pressure

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The present paper proposes the expression to predict the values of shear sound velocity. The present expression has been developed by using the reciprocal form of Grüneisen parameter (γ). The formulation thus developed has been used to calculate shear sound velocity for hexagonal close packed (hcp) iron at high pressures. It is found that the shear sound velocity increases with the increase in compression or pressure in a non-linear manner. Volume dependence of shear sound velocity shows linearity with Debye temperature and Grüneisen parameter. Shear sound velocity increases with the increase in Debye temperature whereas decreases with the increase in Grüneisen parameter. The calculations for the Grüneisen parameter, Debye temperature and shear sound velocity are also found to be in good agreement with the experimental data.

Keywords: Metals, Thermodynamic properties, Hexagonal colosed packed iron

1 Introduction

A significant phenomenon in high pressure elasticity is that the behavior of the shear elastic constants does not follow the simple rules found in the equation of state (EoS), which are restricted to relationships of the bulk modulus in *P*, *V* and *T* space[1]. The behavior of EoS is not very structure dependent. On the other hand, the shear constants under pressure are very dependent on structure even to the extent of being different from point group to point group in the same crystal class. It can be shown from a number of different approaches (continuum elasticity, lattice dynamics, and atomic physics) that the shear sound velocity associated with the shear elastic constants[1]. For a single crystals, as pressure increases, the shear sound velocity increases. In the quasi-harmonic approximation, the Debye temperature (θ_D) can be defined in terms of sound velocity as[1]:

$$\theta_D = 251.2 V^{-1/3} v_m \qquad \text{… (1)}$$

where v_m is the mean sound velocity. The value of v_m is heavily weighted by shear sound velocity (v_s). Anderson[2] gave the following relationships:

$$v_m = 1.1 v_s \qquad \text{… (2)}$$

And

$$v_s = \frac{\theta_D V^{1/3}}{276.3} \qquad \text{… (3)}$$

where V is the volume and θ_D is the Debye temperature which is the characteristic temperature of a solid defined within the framework of the Debye model for the specific heat of solids and related to the Debye cut -off frequency ω_D such as:

$$\theta_D = \frac{\hbar\omega_D}{k_B} \qquad \text{… (4)}$$

where $\hbar$ is the reduced Planck's constant which is equivalent to $h/2\pi$, h and k_B are, respectively, the Planck's constant and Boltzmann's constant.

From the Debye model, the relation between the vibrational Grüneisen parameter (γ) and Debye temperature (θ_D) as:

$$\gamma = -\left(\frac{d\ln\theta_D}{d\ln V}\right)_T \qquad \text{… (5)}$$

It is commonly known that the key ingredient of the Earth's core is hexagonal close packed (hcp) iron, which is also known as ε-phase[3-5]. It is a matter of

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interest to study the physics of Earth's deep interior which requires information on the properties of hcp iron at extreme pressure (P) and temperature[6] (T), hcp iron probably appears in the phase diagram of iron at the triple point near pressure of 55 GPa and temperature[3,7] of 2800 K. Some researchers[8-12] have suggested the existence of an intermediate phase (beta phase) which complicates the phase diagram between 30 GPa and 60 GPa, however, there is no consensus regarding the existence of this phase or its structure. Furthermore, analysis has shown that even if a separate beta phase exists, its physical properties are essentially indistinguishable from those of hcp iron[13].

2 Formulation for Shear Sound Velocity

Srivastava *et al.*[14] proposed the following reciprocal form of Grüneisen parameter (γ) as:

$$\frac{1}{\gamma}=\frac{1}{\gamma_\infty}+\left(\frac{1}{\gamma_0}-\frac{1}{\gamma_\infty}\right)\left(\frac{V}{V_0}\right)^c \qquad \dots (6)$$

where c is a constant and γ_0, γ_∞ are, respectively, the value of γ at $P\to 0$ or $V\to V_0$ and $P\to\infty$ or $V\to 0$.

Using Eqs (5) and (6) one can get the following result:

$$\frac{\theta_D}{\theta_{D_0}}=\left(\frac{\gamma}{\gamma_0}\right)^{-\gamma_\infty/\lambda_\infty}\times\left(\frac{V}{V_0}\right)^{-\gamma_\infty} \qquad \dots (7)$$

Or

$$\frac{\theta_D}{\theta_{D_0}}=\left(\frac{1}{\gamma_0\left[\frac{1}{\gamma_\infty}+\left(\frac{1}{\gamma_0}-\frac{1}{\gamma_\infty}\right)\left(\frac{V}{V_0}\right)^c\right]}\right)^{-\gamma_\infty/\lambda_\infty}\times\left(\frac{V}{V_0}\right)^{-\gamma_\infty} \qquad \dots (8)$$

At $P\to 0$ or $V\to V_0$ Eq. (3) becomes:

$$v_{s_0}=\frac{\theta_{D_0}V_0^{1/3}}{276.3} \qquad \dots (9)$$

Using Eqs (3) and (9) one can get:

$$\frac{v_s}{v_{s_0}}=\left(\frac{\theta_D}{\theta_{D_0}}\right)\times\left(\frac{V}{V_0}\right)^{1/3} \qquad \dots (10)$$

Inserting Eq. (8) in Eq. (10) we get:

$$\frac{v_s}{v_{s_0}}=\left(\frac{1}{\gamma_0\left[\frac{1}{\gamma_\infty}+\left(\frac{1}{\gamma_0}-\frac{1}{\gamma_\infty}\right)\left(\frac{V}{V_0}\right)^c\right]}\right)^{-\gamma_\infty/\lambda_\infty}\times\left(\frac{V}{V_0}\right)^{1/3-\gamma_\infty} \qquad \dots (11)$$

where all symbols are having their usual meanings.

3 Results and Discussion

In the present study, we have established a new relationship for the volume dependence of shear sound velocity. Thus, it is clear from Eqs (8) and (11) that Grüneisen parameter (γ) is a fundamental parameter of central importance for investigating thermoelastic properties for solids at high temperatures and high pressures. On differentiating Eq. (6), we get the following relationship:

$$-\frac{q}{\gamma}=c\left[\frac{1}{\gamma}-\frac{1}{\gamma_\infty}\right] \qquad \dots (12)$$

where q is the second-order Grüneisen parameter which is defined as:

$$q=\left(\frac{d\ln\gamma}{d\ln V}\right)_T \qquad \dots (13)$$

At $P\to 0$ or $V\to V_0$ Eq. (12) gives:

$$c=\frac{q_0\gamma_\infty}{(\gamma_0-\gamma_\infty)} \qquad \dots (14)$$

At $P\to\infty$ or $V\to 0$, Eq. (12) results $q_\infty\to 0$. Now on differentiating Eq. (12) we get:

$$\frac{q}{\gamma^2}\left(\frac{d\gamma}{dV}\right)-\frac{1}{\gamma}\left(\frac{dq}{dV}\right)=-\frac{c}{\gamma^2}\left(\frac{d\gamma}{dV}\right). \qquad \dots (15)$$

which yields:

$$\lambda - q = c \quad \ldots (16)$$

where λ is the third order Grüneisen parameter which is defined as:

$$\lambda = \left(\frac{d \ln q}{d \ln V}\right)_T \quad \ldots (17)$$

At $P \to \infty$ or $V \to 0$, Eq. (16) gives:

$$\lambda_\infty = c \quad \ldots (18)$$

As c is positive and finite which is apparent from Eq. (14) so here λ_∞, the value of λ at infinite pressure is positive and finite which is given by following expression:

$$\lambda_\infty = \frac{K_\infty^{'2}}{K_0^{'}} \quad \ldots (19)$$

where $K_0^{'}$ and $K_\infty^{'}$ are respectively the values of first order pressure derivative of isothermal bulk modulus (K_T) at $P \to 0$ or $V \to V_0$ and at $P \to \infty$ or $V \to 0$.

To evaluate the value of $K_\infty^{'}$ in Eq. (13) one can use the following expression[17]:

$$\gamma_\infty = \frac{K_\infty^{'}}{2} - \frac{1}{6} \quad \ldots (20)$$

Or

$$K_\infty^{'} = 2\left(\gamma_\infty + \frac{1}{6}\right) \quad \ldots (21)$$

To make a judgment of the theoretical formulation developed here, we make use of two sets of input parameters for γ_0, γ_∞, $K_0^{'}$ (first pressure derivative of isothermal bulk modulus (K_T) at zero pressure), $K_\infty^{'}$ (first pressure derivative of isothermal bulk modulus (K_T) at infinite pressure) and λ_∞ (third order Gruneisen parameter (λ) at infinite pressure). To find the values of Grüneisen parameter (γ), Debye temperature (θ_D) and shear sound velocity (v_s), we should have to choose the value of γ_∞ in Eqs (6), (8) and (11). Some researchers[14,15] have assumed $\gamma_\infty = 2/3$, however, Stacey and Davis[16] used $\gamma_\infty = 1.33$. Putting the value of $\gamma_\infty = 2/3$ in the above Eq. (15) which yields $K_\infty^{'} = 5/3$, is consistent with that value used by many researchers[17-23] following the Thomas-Fermi theory, is a valid result. However, in case of $\gamma_\infty = 1.33$, $K_\infty^{'} = 3.0$. The values of $K_0^{'} = 5.5$[7], and $K_\infty^{'} = 5/3$ give $\lambda_\infty = 0.51 = c$ through Eq. (13), and $K_0^{'} = 5.0$[16], $K_\infty^{'} = 3.0$[16] and $\lambda_\infty = 3.061$[16]. The values of input parameters $\gamma_0 = 1.71$, $\theta_{D_0} = 422$ and $v_{s_0} = 2.89$ have been taken from Anderson *et al.*[24]. We have calculated the values of Grüneisen parameter (γ), Debye temperature (θ_D) and shear sound velocity (v_s) through Eqs (6), (8) and (11) using these input parameters and are to be discussed as:

The calculated values of γ through Eq. (6) are compared with experimental data[24] and those values calculations made on Stacey and Davis in put parameters[16] in Fig. 1. The results are consistent with experiment[24] in the wide range of pressure. It is evident from Fig. 1 that γ decreases with the increase in pressure or compression. We have used the expression (Eq. (6)) due to Srivastava *et al.*[14] for volume dependence of γ. Equation (6) satisfies the thermodynamic constraints for solids at $P \to \infty$ or $V \to 0$. These constraints disclose that $\gamma_0 \rangle \gamma_\infty \rangle 0$, $q_\infty = 0$ and $\lambda_0 \rangle \lambda_\infty \rangle 0$. Stacey and Davis[16] preferred the reciprocal form of thermoelastic properties. Thus, it supports our approach to study volume dependence of γ and other thermodynamic properties.

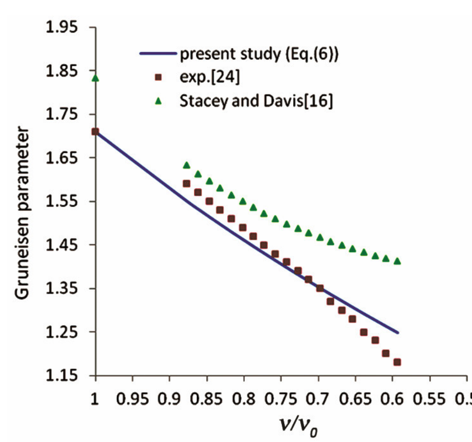

Fig. 1 – Volume dependence of Grüneisen parameter (γ) for hcp iron

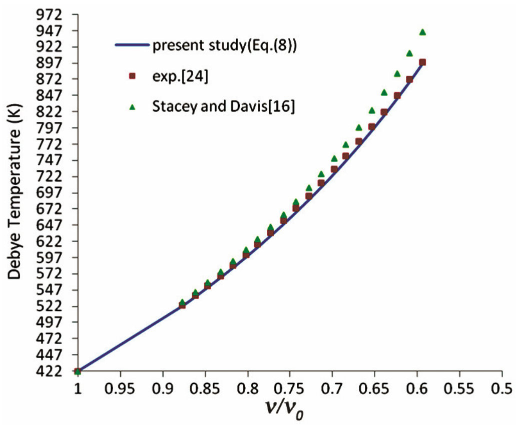

Fig. 2 – Volume dependence of Debye temperature (θ_D) for hcp iron

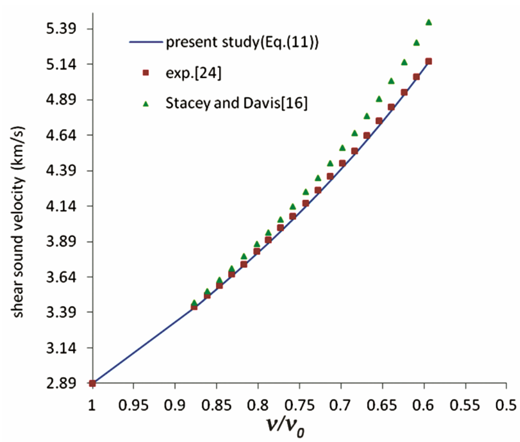

Fig. 3 – Volume dependence of shear sound velocity (v_s) for hcp iron

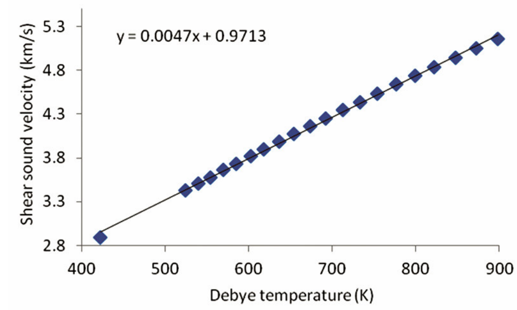

Fig. 4 – Graph between Shear sound velocity and Debye temperature for hcp iron

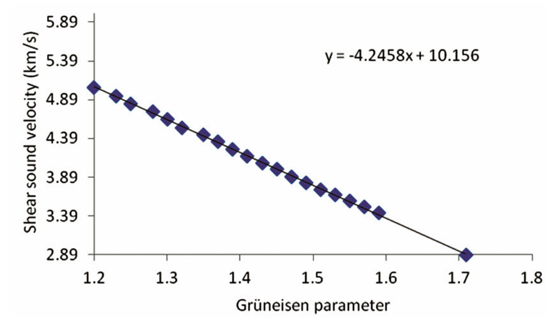

Fig. 5 – Graph between Shear sound velocity and Grüneisen parameter for hcp iron

(i) We have calculated the value of $q_0 = 0.798$ at T = 300 K and $P = 0$ or $V = V_0$, which is consistent with those values obtained by many researchers, such as, $q_0 = 0.82$[23], $q_0 = 0.56$[25], $q_0 = 0.70$[26] and $q_0 = 0.60$[27] .This analysis also validates our relationship (Eq.(6)).

(ii) Figure 2 shows the volume dependence of Debye temperature (θ_D). Figure 2 explores that θ_D increases with the increase in compression or pressure. Consistency of calculated values through Eq. (8) with experimental data[24] reveals the validity of present model, however, the results obtained through Stacey and Davis[16] input parameters are not fairly consistent above $V/V_0 = 0.75$.

(iii) The extracted values of shear sound velocity (v_s) through Eq. (11) along with experimental data[24] and based on Stacey and Davis input parametrs[16] are plotted in Fig. 3. An excellent agreement between calculated values through Eq. (11) and experimental data[24] explores the validity of present approach. However, the results obtained through Stacey and Davis[16] input parameters are not consistent above $V/V_0 = 0.75$.

(iv) As it is evident from Fig. 3 that v_s increases with the increase in compression or pressure. This is mainly due to increment in θ_D with the increase in compression or pressure. We should have to draw the graphs for v_s vs θ_D and v_s vs γ to discuss the nature of v_s. v_s vs θ_D and v_s vs γ are shown in Figs 4 and 5. Figure 4 reflects that v_s increases with the increase in θ_D. However, v_s increases with the decrease in γ which is noticeable from Fig. 5. It is interesting to note that volume dependence of v_s shows linearity with θ_D and γ.

4 Conclusions

In the present paper it has been concluded that the relationships for θ_D and v_s as a function of volume has been determined using the reciprocal expression for the volume dependence of Grüneisen parameter (γ)[14]. Grüneisen parameter decreases with increase in pressure or compression however, Debye temperature increases with increase in pressure or compression. The present formulation (Eq. (11)) illustrates effectively some important features of shear sound velocity, such as (i) v_s increases with the increase in compression or pressure, (ii) $v_s = v_{s_0}$ at $P = 0$, (iii) v_s becomes infinitely large at extreme pressure, i.e., $P \to \infty$ or $V \to 0$, (iv) volume dependence of shear sound velocity shows linearity with Debye temperature and Grüneisen parameter and (v) v_s increases with the increase in Debye temperature whereas decreases in the increase of Grüneisen parameter. Results are all found in good agreement with the experimental values[24], however, are not in good agreement with those results based on Stacey and Davis input parameters[16]. Lastly, it should be mentioned that the results for v_s at different compressions obtained from Eq. (11) depend sensitively on the values of γ_∞ and λ_∞.

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