Elastic Constants and Pressure Derivatives of Iron-Platinum Alloy

Vinu T P

Department of Physics, NSS Hindu College, Changanassery, Kerala-686102, India

Abstract: *The complete set of second-and third-order elastic constants of cubic $Fe_{72}Pt_{28}$ have been obtained using the strain energy density derived from interactions up to three nearest neighbours of each atom in its unit cell. The finite strain elasticity theory has been used to get the strain energy density of $Fe_{72}Pt_{28}$. The strain energy density is compared with the strain dependent lattice energy density obtained from the continuum model approximation and the expressions for the second-and third-order elastic constants of $Fe_{72}Pt_{28}$ are derived. The second-order potential parameter is deduced from the measured second-order elastic constants of $Fe_{72}Pt_{28}$ and the third-order potential parameter is estimated from the Lennard-Jones inter atomic potential for $Fe_{72}Pt_{28}$. The inter lattice displacements; the three independent second-order elastic constants and the six independent third-order elastic constants of $Fe_{72}Pt_{28}$ are also determined. The second-order elastic constants are compared with the experimental elastic constants of $Fe_{72}Pt_{28}$. The third-order elastic constants are found to exhibit anisotropy in certain directions of the elastic wave propagation in the crystal. We also study the effect of pressure on the second-order elastic constants of $Fe_{72}Pt_{28}$.*

Keywords: Elastic constants, Pressure derivatives, Strain energy

1. Introduction

Large capacity and high-speed information storage systems are in growing demands. Although many new candidates such as near field optical recording. A millipede storage system of antiferromagnetic tips array, and MRAM are available, a high density magnetic recording system of HDD is still the main target in the development of information society [1]. [2], [3]. At room temperatures the ordered $Fe_{72}Pt_{28}$ has a face-centered cubic structure. $Fe_{72}Pt_{28}$ is isostructural, which shows strong invar effects including negative thermal expansion.

Higher order elastic constants and the pressure derivatives of the second-order elastic constants provide insight in to the nature of binding forces between atoms in the crystal. [7]. The response of a material to an applied stress is determined by the elastic constants and the pressure derivatives of the elastic constants. Here we study the vibrational anharmonicity of long wavelength acoustic modes of elastic waves in terms of the second-and third-order elastic constants using the finite strain elasticity theory [8]. Using the second-and third order potential parameters expressions have been derived for the second-and third-order elastic constants for $Fe_{72}Pt_{28}$.

2. Theory

A. Elastic Constants

The method of homogenous deformation [8] is applied for the determination of the strain energy density for $Fe_{72}Pt_{28}$. During homogenous deformation, the lattice vector is deformed as

$$R_i' \begin{pmatrix} L & L^{'} \\ \mu & \mu' \end{pmatrix} = R_i \begin{pmatrix} L & L^{'} \\ \mu & \mu' \end{pmatrix} + \sum_j \varepsilon_{ij} R_j \begin{pmatrix} L & L^{'} \\ \mu & \mu' \end{pmatrix} + W_i (1 - \delta_{\mu\mu'}) \tag{1}$$

where $R_i \begin{pmatrix} L & L^{'} \\ \mu & \mu' \end{pmatrix}$ is the vector distance in the unstrained state between the particle μ in the cell L and atom μ' in the cell $L^{'}$ in the undeformed state. $R_i' \begin{pmatrix} L & L^{'} \\ \mu & \mu' \end{pmatrix}$ refers to the corresponding vector distance after the deformation. Here i and j are the component indices and δ is the Kroneker delta. The ε_{ij} are the deformation parameters related to the macroscopic Lagrangian strains η_{ij} defined as

$$\eta_{ij} = \frac{1}{2} \left(\varepsilon_{ij} + \varepsilon_{ji} + \sum_k \varepsilon_{ik} \varepsilon_{jk} \right) \tag{2}$$

W_i are the components of the internal displacements of the sub lattice $\eta = 2$ relative to the sub lattice $\eta = 1$. Here $\sum_k \varepsilon_{ik} \varepsilon_{jk}$ represents geometric nonlinearity in the Lagrangian strain.

The absolute internal displacement components W_i are related to the relative internal displacements $\overline{W_i}$ using the relation

$$\overline{W_i}(\mu\mu') = W_i(\mu\mu') + \sum_j \varepsilon_{ji} W_j(\mu\mu') \tag{3}$$

The internal energy of an infinite crystal in its lowest electronic state is expressed as a function θ, which contains the individual atomic co ordinates as variables. The elastic properties are expressed by means of the derivatives of θ with respect to atomic displacements when the lattice is deformed. The equations of motion are expressed in terms of the derivatives of θ. The development involves both translational symmetry of the lattice and the conditions of atomic equilibrium. The first -order equations give the relative internal displacements of the various atoms in the

unit cell, which occur when the crystal is strained uniformly. Expressions for the elastic constants are obtained in terms of

parameters of the generalized theory [9] .The potential θ of the lattice can be expanded in Taylor series as

$$\theta = \theta_0 + O'\theta\left[\sum_1 \Delta R^2(l)\right] + \frac{1}{2}O''\theta\left\{\sum_1 \left[\Delta R^2(l)\right]^2\right\} + \frac{1}{6}O'''\theta\left\{\sum_1 \left[\Delta R^2(l)\right]^3\right\} + ----\quad (4)$$

where l refers to the nearest neighbors. $O'\theta, O''\theta, O'''\theta$ are the first, second and third-order co ordinate derivatives of the potential function θ and

$$\left[\Delta R^2(l)\right]^2 = \left[R'\begin{pmatrix}L & L'\\ \mu & \mu'\end{pmatrix}\cdot R'\begin{pmatrix}L & L''\\ \mu & \mu''\end{pmatrix} - R\begin{pmatrix}L & L'\\ \mu & \mu'\end{pmatrix}\cdot R\begin{pmatrix}L & L''\\ \mu & \mu''\end{pmatrix}\right]^2 \text{ and}$$

$$\left[\Delta R^2(l)\right]^3 = \left[R'\begin{pmatrix}L & L'\\ \mu & \mu'\end{pmatrix}\cdot R'\begin{pmatrix}L & L''\\ \mu & \mu''\end{pmatrix} - R\begin{pmatrix}L & L'\\ \mu & \mu'\end{pmatrix}\cdot R\begin{pmatrix}L & L''\\ \mu & \mu''\end{pmatrix}\right]^3 \quad (5)$$

The above expressions are invariant towards rigid rotations and translations of the lattice since the potential energy expressions involve only changes in scalar products of interatomic vectors. If the atoms suffer displacement

because of the deformation of the lattice, the potential due to two-body interactions arising from three nearest neighbors can be written as

$$\theta' = \theta + \frac{1}{2}\sum_{N=1}^{3}\sum_{\mu=1}^{4}\left\{\frac{1}{2}k_2\left[R'\begin{pmatrix}L & L+N\\ \mu & \mu'\end{pmatrix}\cdot R'\begin{pmatrix}L & L+N\\ \mu & \mu'\end{pmatrix} - R\begin{pmatrix}L & L+N\\ \mu & \mu'\end{pmatrix}\cdot R\begin{pmatrix}L & L+N\\ \mu & \mu'\end{pmatrix}\right]^2 + \right.$$

$$\left.\frac{1}{6}k_3\left[R'\begin{pmatrix}L & L+N\\ \mu & \mu'\end{pmatrix}\cdot R'\begin{pmatrix}L & L+N\\ \mu & \mu'\end{pmatrix} - R\begin{pmatrix}L & L+N\\ \mu & \mu'\end{pmatrix}\cdot R\begin{pmatrix}L & L+N\\ \mu & \mu'\end{pmatrix}\right]^3\right\} \quad (6)$$

where k_2 and k_3 are the second-and the third-order potential parameters respectively. Substituting equation. (2), (3) in equation (1) and evaluating the scalar product

$$R'\begin{pmatrix}L & L'\\ \mu & \mu'\end{pmatrix}\cdot R'\begin{pmatrix}L & L''\\ \mu & \mu''\end{pmatrix} \text{ and substituting in equation (6)}$$

$$\theta' - \theta = k_2\left\{\sum_{N=1}^{3}\left[4\sum_{ijkl}\eta_{ij}\eta_{kl}R_i(N)R_j(N)R_k(N) + 4\sum_{ij}\overline{W_i}\,\overline{W_j}R_i(N)R_j(N) + \right.\right.$$

$$\left.4\sum_{ijkl}\eta_{ij}\overline{W_k}\,\overline{W_l}R_i(N)R_j(N) + 8\sum_{ijk}\eta_{ij}\overline{W_k}R_i(N)R_j(N)R_k(N) + 4\sum_{ijk}\overline{W_i}\,\overline{W_j}\,\overline{W_k}\right]\right\}$$

$$+ k_3\left\{\sum_{N=1}^{34}\left[8\sum_{ijklmn}\eta_{ij}\eta_{kl}\eta_{mn}R_i(N)R_j(N)R_k(N)R_l(N)R_m(N)R_n(N)\right.\right. \quad (7)$$

$$\left.+ 24\sum_{ijkl}\eta_{ij}\overline{W_k}\,\overline{W_l}R_i(N)R_j(N)R_k(N)R_l(N)\right.$$

$$\left.\left.+ 24\sum_{ijklm}\eta_{ij}\eta_{kl}\overline{W_m}R_i(N)R_j(N)R_k(N)R_l(N)R_m(N) + 8\sum_{ijk}\overline{W_i}\,\overline{W_j}\,\overline{W_k}R_i(N)R_j(N)R_k(N)\right]\right\}$$

where N refers to the number of atoms in the unit cell. To obtain the second-and third- order elastic constants one has to know the relative internal strains $\overline{W_i}$ only to the first-order in the Lagrangian strains η_{ij}. By minimizing the strain energy from equation (7) with respect to internal displacements $\overline{W_i}$ and retaining only the linear terms in $\overline{W_i}$ and η_{ij}, we get

$$\overline{W_j}(N) = -4k_2\sum_{klm}\eta_{km}D_{ijk}M_{jl}^{-1} \quad (8)$$

where

$$M_{jl} = \sum_N 4k_2 R_j(N)R_l(N) \quad (9) \text{ and}$$

$$D_{lkj} = \sum_N R_k(N)R_l(N) \quad (10)$$

M_{jl}^{-1} is the inverse of the matrix M_{jl}.

Substituting for the inter atomic vectors of three nearest neighbors of each atom in the unit cell of $Fe_{72}Pt_{28}$ in the matrix M_{jl} and D_{lkj}, we obtain the internal strain components as

$$\overline{W_x}(1) = \overline{W_y}(1) = \overline{Wz}(1) = 0$$
$$\overline{W_x}(2) = \overline{W_y}(2) = \overline{Wz}(2) = 0$$
$$\overline{W_x}(3) = \overline{W_y}(3) = \overline{Wz}(3) = 0 \qquad (11)$$
$$\overline{W_x}(4) = \overline{W_y}(4) = \overline{Wz}(4) = 0$$

Substituting for $\overline{W_x}(N), \overline{W_y}(N)$ and $\overline{W_z}(N)$ from equation (11) in to equation (7), and taking the lattice sums using the position co ordinates of the nearest neighbors of the atoms in the unit cell of $Fe_{72}Pt_{28}$ and dividing the resulting expression by the volume of the unit cell V_Z, we get the strain energy density in the undeformed state. This is compared with the strain dependant lattice energy density expression from the continuum model approximation [9],

$$U = \frac{1}{2}\sum_{ijkl} C_{ijkl}\eta_{ij}\eta_{kl} + \frac{1}{6}\sum_{ijklmn} C_{ij,kl,mn}\eta_{ij}\eta_{kl}\eta_{mn} + ----$$
$$(12)$$

Equating coefficients of similar terms in $\eta_{ij}\eta_{kl}$, we get the expressions (13) for the second order elastic constants of $Fe_{72}Pt_{28}$ and equating the coefficients of similar terms in $\eta_{ij}\eta_{kl}\eta_{mn}$, we get the expressions (14) for second-order elastic constants of $Fe_{72}Pt_{28}$.

$$C_{11} = 276k_2'$$
$$C_{12} = 114k_2' \qquad (13)$$
$$C_{44} = 114k_2'$$

$$\text{where } k_2' = \frac{k_2 a^4}{V_z} \qquad (14)$$

and V_z is the volume of unit cell of $Fe_{72}Pt_{28}$.

The potential parameter k_2 has been obtained from the measured value of C_{11} calculated by Saunders [6]. The values of the second-order elastic constants of $Fe_{72}Pt_{28}$ are evaluated from equation (13) and are given in table [I] along with other reported values. The expressions for the third-order elastic constants are

$$C_{111} = 1494k_3'$$
$$C_{144} = 252k_3'$$
$$C_{112} = 387k_3'$$
$$C_{123} = 252k_3'$$
$$C_{456} = 387k_3'$$
$$C_{155} = 252k_3' \qquad (15)$$

$$\text{where } k_3' = \frac{-k_3 a^6}{V_z}$$

k_3, the third order potential parameter evaluated by assuming a Lennard -Jones type of inter atomic potential for $Fe_{72}Pt_{28}$ where

$$\theta(r) = \frac{B}{R^n} - \frac{A}{R^m} \qquad (16)$$

where m =12 and n = 6

$$\text{Thus, } k_3 = \left[\frac{1}{6}\left(\frac{d^2\theta}{dx^2}\right)\right]_{r=a} = \frac{-4k_2}{a^2} \qquad (17)$$

Using the values of k_2 and k_3 all the six third order elastic constants of $Fe_{72}Pt_{28}$ are evaluated and given in Table [II].

B. Pressure derivative of the elastic constants.

Let a_i be the coordinate of any atom in the natural state and X_i the coordinate of the same atom after applying the pressure P. An infinitesimal stress is superimposed on the deformed state and the final coordinate of the atom X_i is given by

$$x_i = X_i + \sum_j \beta_{ij} X_j \qquad (18)$$

where β_{ij} are the infinitesimal strain parameters. The Langrangian Strain parameters η_{ij} in the final state are given by

$$\eta_{ij} = \frac{1}{2}\sum_{p=1}^{3}\left(\frac{\partial x_p}{\partial a_i}\frac{\partial x_p}{\partial a_j} - \delta_{ij}\right) \qquad (19)$$

where δ is the Kroneker delta.
The stress tensor is given by

$$\eta_{ij} = \frac{\rho}{\rho_0}\sum_{pq}\frac{\partial x_i}{\partial a_p}\frac{\partial U}{\partial \eta_{pq}}\frac{\partial x_j}{\partial a_q} \qquad (20)$$

where ρ_0 is the density in the natural state and ρ is that in the deformed state and U is the internal energy of the crystal. The effective second-order elastic constants $C_{ij,kl}'$ can be obtained by comparing (20) with

$$\eta_{ij} = -P\delta_{ij} + \sum_{kl} C_{ij,kl}'\beta_{kl} \qquad (21)$$

The first derivatives of the effective $C_{ij,kl}'$ with respect to p are

$$\frac{dC_{11}}{dP} = \frac{-1}{C_{11}+2C_{12}}\left[C_{111} + 2C_{112} + 3C_{11} + 4C_{12}\right]$$

$$\frac{dC_{12}}{dP} = \frac{-1}{C_{11}+2C_{12}}\left[2C_{112} + C_{123} + C_{12}\right]$$

$$\frac{dC_{44}}{dP} = \frac{-1}{C_{11}+2C_{12}}\left[C_{144} + 2C_{155} + C_{44} + C_{11} + 2C_{12}\right]$$
$$(22)$$

Substituting the values the of second-and third-order elastic constants of $Fe_{72}Pt_{28}$ from Tables [I] and [II] respectively in equation (22) we get the pressure derivatives of the second-order elastic constants of $Fe_{72}Pt_{28}$ and are collected in Table [III] along with the other reported values.

3. Results and Discussions

The Second-Order Elastic Constants [SOECs] of $Fe_{72}Pt_{28}$ are given in table [I]. C_{11} and C_{12} are 143.9 Gpa and 59.4 Gpa respectively. while the corresponding values obtained by Saunders [11]are 143.9 Gpa and 107 Gpa. The percentage of deviation for C_{12} is 44.4 while C_{44} deviates by 25.8%

The Bulk Modulus is calculated as 87.7 Gpa, where B is defined as $(C_{11}+2C_{12})/3$. The corresponding value of B obtained by Saunders [6] is 119.3 Gpa. The percentage deviation is 26.5. The anisotropy factor A, defined as A= $2C_{44}/(C_{11}-C_{12})$, is calculated as 1.41 with the present values, while the corresponding values of A obtained by Saunders is 4.4. The Poisson's ratio $\zeta = C_{12}/(C_{12}+C_{11})$, ζ = 0.3, Saunders has calculated the value of ζ as 0.43. The percentage of deviation is 30. The value should satisfy the relation $o < \zeta < 1/2$.

Martin's criteria have been used for testing the numerical validity of the SOEC's. According to Martin [10], the elastic constants satisfy the relation

$$A = (7/6)\ 2C_{44}(C_{11}+ (2/7)\ C_{12})/((C_{11}+2C_{12})(C_{11}-C_{12})) = 1$$

With the present results, we get A = 1.005, while Saunders calculated the value of A as 2.5. This deviates much from the present results.

The complete sets of third-order elastic constants of $Fe_{72}Pt_{28}$ are given in table [II]. C_{111} is the largest in magnitude compared to the magnitudes of C_{123}, C_{144}, and C_{456}. C_{111} is largest in the case of diamonds, also showing some similar anisotropy.

Table [III] gives the calculated values of pressure derivatives of $Fe_{72}Pt_{28}$ along with values by other workers. It is seen that all the pressure derivatives of C_{11}, C_{12} and C_{44} are positive, which shows that these elastic constants are increasing with pressure. The present value of the pressure derivatives of C_{11} is 15.4 Saunders has calculated the value of dC_{11}/dp as -19.2. The pressure derivatives for C_{12} and C_{44} are 7.9 and 6.9 respectively. The corresponding values by Saunders are 26 and 0.6 respectively. A remeasurement of the pressure variation of elastic constants is recommended for $Fe_{72}Pt_{28}$.

Table [I].
Second order elastic constants of $Fe_{72}Pt_{28}$ in units of Gpa

	C_{11}	C_{12}	C_{44}
Present work	94.2	38.9	38.9
Saunders[11]	94.2	35.8	84.7

Table [II].
Third order elastic constants of $Fe_{72}Pt_{28}$ in units of Gpa

	C_{111}	C_{112}	C_{155}	C_{123}	C_{144}	C_{456}
Present Work	-3115.7	-807.1	-807.1	-450.5	-450.5	-450.5

Table [III].
The pressure derivative of the second-order elastic constants of $Fe_{72}Pt_{28}$ in the unit of Gpa

	$\dfrac{dC_{11}}{dP}$	$\dfrac{dC_{12}}{dP}$	$\dfrac{dC_{44}}{dP}$
Present work	15.4	7.6	6.6
Saunders	-19.2	-26	0.6

References

[1] Kazunhiro Ouchi, IEEE Transations on magnetics, Vol 37, No 4 (2001).

[2] E.N Abarra et al., Digest Intermag 2000, Toronto, Apr..

[3] M. Madison et al., Digest Intermag 2000, Toronto, Apr..

[4] P. W Bellary and J. Crangle, J. Appl. Phys, Vol. 39. No. 2, (1968).

[5] J. Kastner, W. Petry, S. M Shapiro et. Al, Eur. Phys. J. B **10**, 641-648,(199).

[6] Hideaki Takano, Naohisa Oba, Shigeyuki Murayama, Kensuke Hoshi et. al, J. Alloys and Compounds, 287, 256-263, (1999).

[7] E. Kren, G. Kadar, L. Pal, J. Solyom, Phys.Rev, Vol.171, 2 (1968).

[8] G.A Saunders, M. Cankurtaran, P. Ray, Phys.Rev. B, Vol. 48, No. 5 (1993).

[9] W. Wasserbach, Phys. Stat. Sol (B), 159, 689 (1990).

[10] F. D Murnaghan, Finite Deformation of an Elastic Solid. Wiely, New York. 1951.

[11] M. Born, k. Huang, Dynamical Theory of Crystal Lattice. Oxford, London. 1954.

[12] M.R Martin, Phys. Rev, B1, 4005 (1997).