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LATTICE THERMAL EXPANSION OF IRON-PLATINUM ALLOY

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Abstract

A simple procedure is described to calculate the generalized Gruneisen parameter for cubic crystals from third-order elastic constants data. The anisotropy of low-temperature thermal expansion of the $Fe_{72}Pt_{22}$ is analyzed theoretically. The generalized Gruneisen parameters (GPs) of elastic waves propagating in different directions are calculated using the measured values of second-order elastic constants. For this, we have used the measured values of the second-order elastic constants. The six third-order elastic constants of $Fe_{72}Pt_{22}$ are calculated from the expressions of effective second-order elastic constants. All the third order elastic constants are negative. Some values of generalized Gruneisen parameters are negative.

Key words-Thermal expansion, Gruneisen parameters, third-order elastic constants

1. INTRODUCTION

The anisotropic thermal expansion of Invar alloys has received a great deal of attention in recent years. Demands on large capacity and high-speed information storage are recently growing in accordance with rapidly increasing markets of mobile phones and wearable PC's. Although many new candidate storage systems such as near field optical recording, a millipede storage system of antiferromagnetic tips array, and MRAM are proposed, a high density magnetic recording system of HDD is still main target of developments to answer the demands in information society [1]. However, a conventional longitudinal recording medium is facing on fatal thermal instability even though anew media construction of Antiferromagnetic under layer medium has been recently proposed as the countermeasure [2], [3]. The $Fe_{72}Pt_{22}$ alloy has been much studied because of its first ordered phase transition between two ordered antiferromagnetic phases [4]. At room temperature the ordered $Fe_{72}Pt_{22}$ phases are stable in the 16-29 % Pt. Concentration range[5]. $Fe_{72}Pt_{22}$ has the cubic Cu_3aAu ordered structure. The compound $Fe_{72}Pt_{22}$ is isostructural material, which shows strong Invar effects including negative thermal expansion. The Gruneisen parameter is commonly used to describe anharmonic properties of solids. It can be approximated by means of continuum model from elastic data. The scalar Gruneisen parameter is expressed in terms of second-and third-order elastic coefficients for arbitrary crystal symmetry and the relation are specified for isotropic, cubic and rhombohedral materials [6].

2. THEORY

2.1 Second-and Third-order Elastic Constants of $Fe_{72}Pt_{22}$.

Second-and-Third order elastic constants determine the anharmonic properties of solids such as thermal expansion, thermal expansion, temperature and pressure dependence of elastic constants, and interaction of acoustic and thermal phonons. The second-and third-order elastic constants can be determined using the

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finite strain elasticity theory of Murnaghan [7], where elastic stress is nonlinear with elastic strain. If the higher order constants are known, on the basis of continuum approximation, it is possible to calculate the scattering of phonons with the aid of nonlinear elasticity theory. The expressions for the effective second-order elastic constants and its pressure derivatives for the strained crystal in cubic system are given by Ramji Rao and Padmaja [8] and Jayachandran and Menon [9]. The pressure derivatives of the second-order elastic constants are in terms of higher order elastic constants up to third order. We have calculated the complete set of three independent second-order elastic constants and six third-order elastic constants and they are presented in Table [I] and in Table [II] respectively. The third-order elastic constants bear their thermodynamic definitions introduced by Brugger [10].

2.2 Low temperature thermal expansion of $Fe_{72}Pt_{22}$.

Thermal expansion is a direct consequence of the anharmonicity of the lattice and is calculated from the anharmonic terms in the power series expansion of the crystal potential energy. In cubic crystal, a measure of this anharmonicity is the Gruneisen gamma, and is defined by

$$\bar{\gamma}(T) = \frac{\beta V}{\chi C_v} = \frac{\sum_i \gamma_i C_{vi}}{\sum_i C_{vi}} \tag{1}$$

where β is the volume coefficient of expansion, V the molar volume, χ the isothermal compressibility and C_v the specific heat at constant volume and γ_i the generalized Gruneisen parameters (GPs) associated with the i^{th} normal mode frequency ω_i of the lattice and is defined by

$$\gamma_i = -\frac{d\log\omega_i}{d\log V} \tag{2}$$

At low temperature, the number of normal modes exited in the j^{th} acoustic branch is proportional to wave velocity v_j^{-3}. So the Gruneisen gamma, at low temperatures, is again a constant designated as and is given by

$$\gamma_L = \frac{\int \gamma_i(\theta,\varphi) V_i^{-3}(\theta,\varphi) d\Omega}{\sum_{i=3}^{3} V_i^{-3}(\theta,\varphi) d\Omega} \tag{3}$$

where Ω is the solid angle. Here GPs are calculated for the elastic waves propagating in cubic crystals from the knowledge of third-order elastic constants.

Thurston and Brugger [10] give the equation for elastic wave propagation in homogeneously deformed crystal.

$$\rho_0 \omega^2 U_i = 4\pi^2 \sum_{kjl} U_j Y_l Y_k \left[C_{ik,jl} + \sum_{mn} \varepsilon_{mn} \left(C_{ik,jl,mn} + C_{ik,nl}\delta_{mj} + C_{nk,jl}\delta_{mi} + C_{kl,mn}\delta ij \right) \right] \tag{4}$$

where Y_i's are the component of the arbitrary direction in which the wave is propagating, U_j's the components of displacements and ε_{mn} are the deformation parameters. When a cubic crystal subjected to a

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hydrostatic pressure, it will experience a uniform volume strain ε and we have for ε_{mn} in the equation (4)

$$\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} = \left(\frac{-\varepsilon}{3}\right)$$

$$\varepsilon_{ij} = 0$$

when $i \neq j$

From the elements of the secular determinant formed by the coefficients of U_i's, the expression for the effective second-order elastic constants in terms of the strain component is obtained as

$$C'_{11} = C_{11} - \left[(C_{111} + 2C_{112} + 3C_{11} + 2C_{12}) \frac{\varepsilon'}{3} \right]$$

$$C'_{12} = C_{12} - \left[(2C_{112} + C_{123} - C_{11}) \frac{\varepsilon'}{3} \right] \qquad (5)$$

$$C'_{44} = C_{44} - \left[(2C_{155} + C_{144} + 2C_{12} + C_{11} + 2C_{44}) \frac{\varepsilon'}{3} \right]$$

The general expressions for GPa from the equation (24) are

$$\gamma_i = \frac{-1}{2X_j} \left\{ \frac{\left[X_j \frac{\partial}{\partial \varepsilon'} (A + B) \right] - \left[\frac{\partial}{\partial \varepsilon'} (AB - C^2) \right]}{[2X_j - (A + B)]} \right\} \qquad (6)$$

where

$$A = C'_{11} \sin^2\theta + C'_{44} \cos^2\theta,$$

$$B = C'_{44} \sin^2\theta + C'_{11} \cos^2\theta,$$

$$C = \sin\theta \cos\theta (C'_{12} + C'_{44})$$

and

$$X_j = \rho_0 V_j^2(\theta).$$

The evaluated second-and third-order elastic constants of $Fe_{72}Pt_{22}$ are used to obtain the Gruneisen functions γ_i to the acoustic modes using equation (6). The results of wave velocity obtained from equation (4) and the Gruneisen parameters for the corresponding elastic wave velocities at different angles of θ are plotted in fig.(1).

3. RESULTS AND DISCUSSIONS

The Gruneisen constant is important in application involving thermo elastic and dielectric properties of

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solids. The Gruneisen constant gives us an insight in to the nature of these properties, which provide information regarding the shift of lattice vibrational energies with compression. To a large extent the Invar properties of an alloy are determined by the anharmonicity of its vibrational states. The theory of the low temperature thermal expansion has been applied to determine the mode gamma and low temperature thermal expansion of $Fe_{72}Pt_{22}$. The Gruneisen Parameter of the acoustic modes in different wave propagation direction has been calculated, which shows anisotropy in all the acoustic wave propagation directions. Fig [1] gives the variation of generalized GPs with propagation theta for different acoustic wave propagation in $Mn_{78}Pt_{22}$. The results obtained are in agreement with the results obtained by Saunders [11].

Table [I].

Second order elastic constants of Fe72Pt22 in units of Gpa

	C_{11}	C_{12}	C_{44}
Present work	94.2	38.9	38.9

Table [II].

Third order elastic constants of $Fe_{72}Pt_{22}$ in units of Gpa

	C_{111}	C_{112}	C_{144}	C_{155}	C_{123}	C_{456}
Present Work	-2039.6	-528.3	-344	-528.3	-344	-344

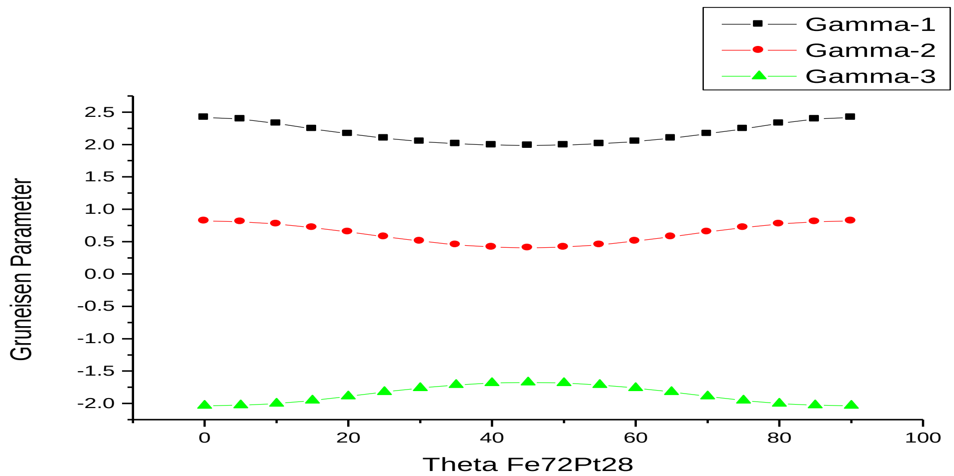

FIG.1 Variation of generalized GPs with θ for different acoustic waves in$Fe_{72}Pt_{22}$.

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