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# Fourth-order elastic constants of nonideal hcp crystal Mg and Er

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The expressions for the 19 fourth-order elastic constants of an hcp crystal with nonideal axial ratio have been derived with interactions extending up to second neighbors and using sublattice displacements to the second degree in strains. These formulas have been used to evaluate the fourth-order elastic constants of magnesium and erbium. The results reveal higher-order elastic anisotropy in erbium. The second pressure derivatives of the effective second-order elastic constants of magnesium and erbium have been obtained using their fourth-order elastic constants and are positive. The magnitudes of the second pressure derivatives of  $C_{12}^I$ ,  $C_{33}^I$ , and  $C_{11}^I$  in magnesium and that of  $C_{12}^I$  in erbium are extremely large, lending support to the phase changes that occur in these metals when subjected to hydrostatic pressure.

## I. INTRODUCTION

Higher-order elastic constants provide insight into the anharmonic nature of the solid. The anharmonic parameters of the crystal potential can be evaluated from a knowledge of third- and fourth-order elastic constants (TOEC and FOEC) of the crystal. The first pressure derivatives of the effective second-order elastic constants (SOEC) of a crystal are expressible in terms of its natural SOEC and TOEC. The second pressure derivatives of a solid can be obtained from a knowledge of its natural SOEC, TOEC, and FOEC. In the hexagonal system, the classes 622, 6mm,  $\bar{6}m2$ , and 622/mmm have 19 independent FOEC. In this paper, the expressions for the 19 FOEC of a hexagonal crystal with nonideal axial ratio have been derived using the method of homogeneous deformation. These expressions have been used to obtain the FOEC of hexagonal metals Mg and Er. Using the finite strain theory of Murnaghan,<sup>1</sup> expressions for the second pressure derivatives of the effective SOEC of a hexagonal solid had been derived by Ramji Rao and Padmaja<sup>2</sup> in terms of its natural SOEC, TOEC, and FOEC. These expressions have been utilized in this paper to obtain the second pressure derivatives of Mg and Er.

## II. FOEC OF A NONIDEAL HEXAGONAL CRYSTAL

Interactions up to second neighbors are considered in the present work. The potential energy per unit cell is

$$\Phi = \sum_{I=1}^6 \Phi[R(I)] + \sum_{J=1}^6 \Phi[R(J)]. \quad (1)$$

Here  $I$  atoms are the six nearest neighbors of the same type in the basal plane, and the  $J$  atoms are the six nonequivalent atoms which are the out of plane neighbors. In a homogeneously deformed lattice, the components of the interatomic vectors are given by

$$R_i(I) = R_i(I) + \sum_j \epsilon_{ij} R_j(I), \quad (2)$$

$$R_i(J) = R_i(J) + \sum_j \epsilon_{ij} R_j(J) + W_i. \quad (3)$$

Here  $\epsilon_{ij}$  are the deformation parameters. In the case of  $J$  atoms,  $W_i$  refers to the components of the internal displacement of the lattice of particles of type  $J$  relative to the lattice

of particles of type  $I$ . The potential energy is expanded in powers of the changes in the squares of the vector distances  $\bar{R}(I)$  and  $\bar{R}(J)$  [i.e.,  $\Delta R^2(K)$ , where  $K = I, J$ ]:

$$\begin{aligned} \Phi = & \Phi_0 + k_2 \left( \sum_I [\Delta R^2(I)]^2 + \sum_J [\Delta R^2(J)]^2 \right) \\ & + k_3 \left( \sum_I [\Delta R^2(I)]^3 + \sum_J [\Delta R^2(J)]^3 \right) \\ & + k_4 \left( \sum_I [\Delta R^2(I)]^4 + \sum_J [\Delta R^2(J)]^4 \right). \quad (4) \end{aligned}$$

Here  $k_2$  is the harmonic parameter, and  $k_3$  and  $k_4$  are the third- and fourth-order anharmonic parameters, respectively:

$$k_2 = \frac{1}{2} \left( \frac{\partial^2 \Phi(r)}{\partial (r^2)^2} \right)_{\text{equilibrium}}, \quad (5)$$

$$k_3 = \frac{1}{6} \left( \frac{\partial^3 \Phi(r)}{\partial (r^2)^3} \right)_{\text{equilibrium}}, \quad (6)$$

$$k_4 = \frac{1}{24} \left( \frac{\partial^4 \Phi(R)}{\partial (r^2)^4} \right)_{\text{equilibrium}}. \quad (7)$$

The term  $[\partial \Phi(r) \partial (r^2)]_{\text{equilibrium}}$  is zero as the derivatives are taken in the equilibrium configuration.

A central potential of the type

$$\Phi = -\frac{a}{r^m} + \frac{b}{r^n} \quad (8)$$

is used. The values of  $k_2$ ,  $k_3$ , and  $k_4$  with this potential are given by

$$k_2 = \frac{1}{4} \frac{\eta M}{D^2}, \quad (9)$$

$$k_3 = -\frac{k_2}{6D^2} (m+n+6), \quad (10)$$

$$k_4 = \frac{k_2}{48D^4} [(m+n)(m+n+12) - mn + 44], \quad (11)$$

$$\eta = \frac{nb(n-m)}{2MD^{n+2}}. \quad (12)$$

$M$  is the mass of the atom, and  $D$  is the nearest-neighbor distance in the basal plane.

Using Eqs. (2) and (3), one obtains

$$\Delta R^2(K) = 2\sum_{ij}\eta_{ij}R_i(K)R_j(K) + 2\sum_i R_i(K)\bar{W}_i + \sum_i \bar{W}_i^2 - 2\sum_{ij}\bar{W}_i\bar{W}_j\eta_{ij}. \quad (13)$$

$\eta_{ij}$  is the Lagrangian strain given by

$$\eta_{ij} = \frac{1}{2}\left(\epsilon_{ij} + \epsilon_{ji} + \sum_k \epsilon_{ki}\epsilon_{kj}\right) \quad (14)$$

and

$$\bar{W}_i = W_i + \sum_j \epsilon_{ij}W_j. \quad (15)$$

For  $K = I$ ,  $\bar{W}$  is equal to zero. The powers of  $\Delta R^2(K)$  are obtained from Eq. (13) and are substituted into Eq. (4). Retaining only terms up to fourth degree in the strain, one obtains expressions for the strain energy per unit volume of the unstrained lattice.

Ramanand, Murthy, and Rao<sup>3</sup> had shown that, in order to evaluate the FOEC of an hcp lattice, it is enough to obtain sublattice displacement up to second degree in strain. The internal displacement  $\bar{W}_i$  can be obtained in terms of the Lagrangian strains by minimizing the strain energy with respect to  $\bar{W}_i$ . One gets the following expressions for  $\bar{W}_i$ :

$$\bar{W}_x = \frac{-D}{2\sqrt{3}}(\eta_{yy} - \eta_{xx}) + \frac{D}{2\sqrt{3}}(\eta_{yy}^2 - \eta_{xx}^2) + \frac{\sqrt{3}p^2D}{4}\eta_{zz}(\eta_{yy} - \eta_{xx}), \quad (16)$$

$$\bar{W}_y = -\frac{D}{\sqrt{3}}\eta_{xy} + \frac{D}{\sqrt{3}}\eta_{xy}(\eta_{yy} + \eta_{xx}) + \frac{\sqrt{3}}{2}p^2D\eta_{xy}\eta_{zz}, \quad (17)$$

$$\bar{W}_z = 0. \quad (18)$$

Substituting for  $\bar{W}_i$  in the expression for the strain energy per unit volume of the underformed state and comparing the resulting expression with that for the elastic energy density,

$$U = \frac{1}{2}\sum_{ijkl}C_{ijkl}\eta_{ij}\eta_{kl} + \frac{1}{6}\sum_{ijklmn}C_{ijklmn}\eta_{ij}\eta_{kl}\eta_{mn} + \frac{1}{24}\sum_{ijklmnop}C_{ijklmnop}\eta_{ij}\eta_{kl}\eta_{mn}\eta_{op} + \dots \quad (19)$$

One gets the following expressions for the FOEC of the nonideal hcp lattice:

$$C_{1111} = 8780A + 8B - (143/3)C, \quad (20)$$

$$C_{1112} = 2948A + (23/3)C, \quad (21)$$

$$C_{1113} = 48p^2A + 6p^2B - 24p^2C, \quad (22)$$

$$C_{1122} = 1004A - (8/3)B + 11C, \quad (23)$$

$$C_{1123} = 48p^2A - 2p^2B + 12p^2C, \quad (24)$$

$$C_{1133} = 72p^4A + 3p^4B - 6p^4C, \quad (25)$$

$$C_{1144} = 48p^2A - 2p^2B, \quad (26)$$

$$C_{1155} = 48p^2A + 6p^2B, \quad (27)$$

$$C_{1166} = 2922A + (4/3)B + (25/9)C, \quad (28)$$

$$C_{1233} = 72p^4A - 3p^4B + 6p^4C, \quad (29)$$

$$C_{1244} = 48p^2A - 2p^2B, \quad (30)$$

$$C_{1255} = 48p^2A - 2p^2B, \quad (31)$$

$$C_{1333} = 108p^6A, \quad (32)$$

$$C_{1344} = 72p^4A - 3p^4B, \quad (33)$$

$$C_{1355} = 72p^4A + 3p^4B, \quad (34)$$

$$C_{2223} = 48p^2A + 6p^2B - 12p^2C, \quad (35)$$

$$C_{3333} = 162p^8A, \quad (36)$$

$$C_{3344} = 108p^6A, \quad (37)$$

$$C_{4444} = 108p^4A. \quad (38)$$

The expressions for TOEC and SOEC derived with the present potential are also given here:

$$C_{111} = (494/3)B + 4C, \quad (39)$$

$$C_{112} = (170/3)B - (4/3)C, \quad (40)$$

$$C_{113} = 4p^2B + 2p^2C, \quad (41)$$

$$C_{123} = 4p^2B - 2p^2C, \quad (42)$$

$$C_{133} = C_{344} = 6p^4B, \quad (43)$$

$$C_{144} = C_{155} = 4p^2B, \quad (44)$$

$$C_{222} = (602/3)B + 4C, \quad (45)$$

$$C_{333} = 9p^6B, \quad (46)$$

$$C_{11} = (116/3)C, \quad (47)$$

$$C_{12} = (44/3)C, \quad (48)$$

$$C_{13} = C_{44} = 4p^2C, \quad (49)$$

$$C_{33} = 6p^4C, \quad (50)$$

$$C_{66} = 12C, \quad (51)$$

$$A = \frac{k_4D^5}{9\sqrt{3}p}, \quad B = \frac{k_3D^3}{\sqrt{3}p}, \quad C = \frac{k_2D}{\sqrt{3}p}. \quad (52)$$

### III. RESULTS AND DISCUSSION

The value of  $k_2$  is necessary to calculate the FOEC of the crystal. The experimental SOEC  $C_{11}$  and  $C_{33}$  have been used to obtain an average value of  $k_2$  in both Mg<sup>4</sup> and Er.<sup>5</sup> The  $m$  and  $n$  values have been so chosen to give a satisfactory agreement to the experimental TOEC of Mg measured by Naimon,<sup>6</sup> and these are  $m = 4$  and  $n = 7$ . The first pressure derivatives of Er were measured by Fisher, Manghnani, and Kikuta.<sup>5</sup> Jiles and Palmer<sup>7</sup> also determined the TOEC and first pressure derivatives of Er. However, there is large discrepancy between the values of Fisher and co-workers<sup>5</sup> and those of Jiles and Palmer.<sup>7</sup> The reference to the theoretical TOEC given in the paper of Jiles and Palmer<sup>7</sup> is incorrect. The theoretical values quoted in Ref. 7 are those obtained by Ramji Rao<sup>8</sup> for Er using central force model for an ideal hcp crystal. In particular, the experimental values of  $C_{222}$ ,  $C_{333}$ , and  $C_{123}$  seem to be defective. Based on Keating's approach,<sup>9</sup> Ramji Rao and Menon<sup>10</sup> obtained the TOEC of Er using the pressure derivatives of Fisher and co-workers,<sup>5</sup> and these are used in the present work. The values of the 19 FOEC of Mg and Er are presented in Table I.  $C_{1111}$  and  $C_{3333}$  have the

TABLE I. FOEC in  $10^{10}$  Nt/M<sup>2</sup>.

Serial No.	$C_{ijkl}$	Mg ( $m = 4, n = 7$ )	Er ( $m = 3, n = 4$ )
(1)	$C_{1111}$	816.5	750.0
(2)	$C_{1112}$	278.9	255.0
(3)	$C_{1113}$	-4.4	-10.5
(4)	$C_{1122}$	97.4	91.3
(5)	$C_{1123}$	19.0	19.6
(6)	$C_{1133}$	32.0	21.0
(7)	$C_{1144}$	14.2	12.8
(8)	$C_{1155}$	5.2	3.0
(9)	$C_{1166}$	275.1	254.5
(10)	$C_{1253}$	62.4	55.8
(11)	$C_{1244}$	14.2	12.8
(12)	$C_{1255}$	14.2	12.8
(13)	$C_{1333}$	186.6	142.5
(14)	$C_{1344}$	50.3	47.4
(15)	$C_{1355}$	38.3	29.3
(16)	$C_{2223}$	0.4	-3.7
(17)	$C_{3333}$	738.3	529.0
(18)	$C_{3344}$	186.6	142.5
(19)	$C_{4444}$	70.8	57.6

TABLE II. Second pressure derivatives of the effective  $C_{ij}^1$  in  $10^{-10}$  M<sup>2</sup>/Nt.

Serial No.	$\frac{\partial^2 C_{ij}^1}{\partial p^2}$	Mg	Er
(1)	$\frac{\partial^2 C_{11}^1}{\partial p^2}$	9.0	3.7
(2)	$\frac{\partial^2 C_{12}^1}{\partial p^2}$	12.1	6.3
(3)	$\frac{\partial^2 C_{13}^1}{\partial p^2}$	3.4	1.6
(4)	$\frac{\partial^2 C_{33}^1}{\partial p^2}$	10.6	3.6
(5)	$\frac{\partial^2 C_{44}^1}{\partial p^2}$	1.9	0.5

largest magnitudes in both these metals. The large difference in the magnitudes of  $C_{1111}$  and  $C_{3333}$  of Er indicate higher-order elastic anisotropy.

Ramji Rao and Padmaja<sup>2</sup> have derived expressions for the second pressure derivatives of effective SOEC of a hexagonal crystal using the finite strain theory.<sup>1</sup> These expressions have been used to obtain the second pressure derivatives of Mg and Er, and are presented in Table II. All the second pressure derivatives for both Mg and Er are positive. The magnitudes of the second pressure derivatives of  $C_{12}^1$ ,  $C_{33}^1$ , and  $C_{11}^1$  are extremely large in Mg, and that of  $C_{12}^1$  is quite large in Er, indicating that phase changes would occur in these metals when subjected to hydrostatic pressure. This is confirmed by experimental evidence. The occurrence of phase change, from hcp to bcc in Mg at 50 GPa was reported by Olijnyk and Holzapfel.<sup>11</sup> Drickamer, Clendenen, and Perez-Albuern<sup>12</sup> measured the changes in the lattice constants of Er with pressure until 200 kbars and found that distinct changes in the pressure derivatives of the  $c$  and  $a$  lattice constants occur at approximately 90 kbars. The diffraction data indicated that the high-pressure phase in Er has the double hcp symmetry.

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