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Electrostatic contributions to the second- and third-order inner elastic constants of HCP metals for a range of axial ratios

C S G Cousins

Physics Department, University of Exeter, Stocker Road, Exeter EX4 4QL, UK

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Abstract. The electrostatic contributions to the inner elastic constants of HCP metals have been calculated for axial ratios in the range 1.56–1.90, using the Ewald–Fuchs method.

1. Introduction

The electrostatic contribution to the energy is of fundamental importance in any model of a metal. Some time ago we published the contributions of this interaction to the first-, second- and third-order elastic constants of HCP metals over a range of axial ratios (Cousins 1972a). Many elastic constants of certain non-primitive crystals can be expressed as the sum of two parts, one dependent on inner displacement and the other, called the partial elastic constant, independent of it. A full description of the formalism and a consistent notation for inner elastic constants was set out in our recent paper (Cousins 1978a). Strictly speaking our former calculations were of partial elastic constants, and in the present paper we complete the task by supplying the electrostatic contributions to the inner elastic constants for the same range of axial ratios as before.

One previous calculation along these lines has been given by Fuller and Naimon (1972, referred to as FN) who presented results for the HCP structure at the ideal ratio only. Our corresponding calculation agrees with theirs when due account has been taken of certain differences of crystal orientation and scaling factors.

2. Formal expressions

For each order up to the third we write, in general,

$$C_I = C_I^O + C_I^A$$

$$C_{IJ} = C_{IJ}^O + C_{IJ}^A$$

and

$$C_{IJK} = C_{IJK}^O + C_{IJK}^A$$

where C_I^0 etc are the partial elastic constants and the dependent parts are given by

$$\begin{aligned}
 C_I^A &= A_{iI} D_i \\
 C_{IJ}^A &= A_{iI} (D_{iJ} + E_{ij} A_{jJ}) + A_{iJ} (D_{iI} + E_{ij} A_{jI}) - A_{iI} A_{jJ} E_{ij} \\
 C_{IJK}^A &= (A_{iI} D_{iJK} + A_{iJ} D_{iIK} + A_{iK} D_{iIJ}) + (A_{iI} A_{jJ} E_{ijk} + A_{iI} A_{jK} E_{ijJ} + A_{iJ} A_{jK} E_{ijI}) \\
 &\quad + A_{iI} A_{jJ} A_{kK} F_{ijk}.
 \end{aligned} \tag{1}$$

The subscripts i, j and k run from 1 to 3 and I, J and K run from 1 to 6. Terms are summed over repeated indices. The tensors $D_i, D_{iJ}, D_{iJK}, E_{ij}, E_{ijK}$ and F_{ijk} are the six species of inner elastic constant that arise in describing the elasticity through third order and represent the variation of the energy per unit initial volume with respect to at least one component of inner displacement (lower case subscripts) and possibly to components of finite strain (upper case subscripts). The net contribution of inner displacement depends on the internal strain tensor A_{iJ} whose components are in turn determined by the overall equilibrium of the crystal.

For the HCP metals an analysis of the symmetry of inner elastic constants (Cousins 1978b) shows that $D_i \equiv 0$ and yields the non-zero components of the remainder and all relations of dependence between them. These are listed in the appendix. Substituting the various non-zero components in equations (1) reveals the second- and third-order elastic constants that are affected by inner displacement. They are as follows:

$$\begin{aligned}
 C_{11}^A &= -C_{12}^A = C_{66}^A = 2D_{16}A + E_{11}A^2 \\
 C_{111}^A &= 3D_{211}A + 3E_{112}A^2 - F_{112}A^3 \\
 C_{112}^A &= C_{266}^A = -(2D_{211} + D_{222})A + (E_{111} - 2E_{112})A^2 + F_{112}A^3 \\
 C_{122}^A &= -C_{166}^A = (D_{211} + 2D_{222})A - (2E_{111} - E_{112})A^2 - F_{112}A^3 \\
 C_{222}^A &= -3D_{222}A + 3E_{111}A^2 + F_{112}A^3 \\
 C_{113}^A &= C_{223}^A = -C_{123}^A = C_{366}^A = 2D_{136}A + E_{113}A^2 \\
 C_{144}^A &= -C_{155}^A = -C_{244}^A = C_{255}^A = -C_{456}^A = -D_{145}A
 \end{aligned} \tag{2}$$

where $A (= A_{16} = A_{21} = -A_{22})$ is the single parameter needed to describe the internal strain. Only when all contributions to the energy have been considered can A be determined. It is then given by

$$A = -(D_{16})_{\text{TOTAL}}(E_{11})_{\text{TOTAL}}.$$

3. Geometry and strain

3.1. Crystal geometry

The geometry behind the calculation of tensor components in the HCP structure needs to be made explicit because different authors use different unit cells and confusion can occur (see Cousins 1972b). We use a Cartesian set of axes with Ox_1 perpendicular to a mirror plane. The basic vectors of the hexagonal Bravais lattice are then given by

$$a_1 = a[1, 0, 0], \quad a_2 = a[-\frac{1}{2}, \sqrt{3}/2, 0], \quad a_3 = a[0, 0, \gamma]$$

where a is the basal-plane parameter and γ is the axial ratio c/a . The two atomic sites in the unit cell are the origin and the point $\rho_0 = \frac{1}{2}a[1, 1/\sqrt{3}, \gamma]$. The volume per atom is $\Omega_0 = \sqrt{3}\gamma a^3/4$.

The basic vectors of the reciprocal lattice are

$$\mathbf{b}_1 = a^{-1}[1, 1/\sqrt{3}, 0], \quad \mathbf{b}_2 = a^{-1}[0, 2/\sqrt{3}, 0], \quad \mathbf{b}_3 = a^{-1}[0, 0, 1/\gamma].$$

Because there are two atoms per unit cell each vector \mathbf{h}_m of the reciprocal lattice has an associated amplitude structure factor given by

$$S(\mathbf{h}_m, \boldsymbol{\rho}_0) = \cos(\pi \mathbf{h}_m \cdot \boldsymbol{\rho}_0) \exp(i\pi \mathbf{h}_m \cdot \boldsymbol{\rho}_0)$$

3.2. Finite strain and inner displacement

A homogeneous deformation can be described by a matrix \mathbf{J} . If the HCP structure is thought of as two interpenetrating sublattices, the vectors between points in one sublattice transform as

$$\mathbf{r} = \mathbf{J}\mathbf{x}$$

whereas vectors between the sublattices transform as

$$\mathbf{r} = \mathbf{J}\mathbf{x} + \mathbf{J}^{-1}\boldsymbol{\zeta}$$

where \mathbf{r} and $\mathbf{x} \equiv (x_1, x_2, x_3)$ are the deformed and undeformed vectors and $\boldsymbol{\zeta}$ is the inner displacement. The finite strain $\boldsymbol{\eta}$ is defined by

$$\boldsymbol{\eta} = \frac{1}{2}(\mathbf{J}\mathbf{J} - \mathbf{I})$$

so that the square of the magnitude of an interlattice vector transforms as

$$r^2 = \tilde{x}_i M_{ij} x_j + 2\tilde{x}_i \zeta_i + \tilde{\zeta}_i M_{ij}^{-1} \zeta_j \quad (3)$$

where \mathbf{M} denotes $\mathbf{I} + 2\boldsymbol{\eta}$.

In reciprocal space the corresponding deformed and undeformed vectors \mathbf{h} and $\mathbf{y} \equiv (y_1, y_2, y_3)$ are related by

$$\mathbf{h} = \mathbf{J}^{-1}\mathbf{y}$$

so that

$$h^2 = \tilde{y}_i M_{ij}^{-1} y_j. \quad (4)$$

The scalar product that occurs as the argument of the structure factor transforms as

$$\mathbf{h} \cdot \boldsymbol{\rho} = \mathbf{y} \cdot \boldsymbol{\rho}_0 + \tilde{y}_i M_{ij}^{-1} \zeta_j \quad (5)$$

since $\boldsymbol{\rho}_0$ is an interlattice vector.

Finally the atomic volume changes in a manner given by

$$\Omega = \Omega_0 (\det \mathbf{M})^{1/2}. \quad (6)$$

4. Calculations and results

The electrostatic energy per unit initial volume for a homogeneously deformed HCP crystal is given by

$$\begin{aligned} \rho_0 F(\boldsymbol{\eta}, \boldsymbol{\zeta}) = & \left(\frac{Z^2 e^2}{8\pi\epsilon_0 \Omega_0} \right) \left[\sum_{\mathbf{r}_1 \neq 0} \frac{1 - \operatorname{erf}(\epsilon |\mathbf{r}_1|)}{|\mathbf{r}_1|} + \sum_{\mathbf{r}_1} \frac{1 - \operatorname{erf}(\epsilon |\mathbf{r}_1 + \boldsymbol{\rho}|)}{|\mathbf{r}_1 + \boldsymbol{\rho}|} + \frac{2\epsilon}{\sqrt{\pi}} \right. \\ & \left. + \frac{1}{\pi\Omega} \sum_{\mathbf{h}_m \neq 0} S^*(\mathbf{h}_m \cdot \boldsymbol{\rho}) S(\mathbf{h}_m \cdot \boldsymbol{\rho}) \frac{\exp(-\pi^2 \mathbf{h}_m^2 / \epsilon^2)}{\mathbf{h}_m^2} - \frac{\pi}{\Omega \epsilon^2} \right] \end{aligned}$$

where the symbols have their usual meanings. Only the second and fourth terms in the square bracket contribute to the inner elastic constants and in these the parameters depend on η and ξ through equations (3), (4), (5) and (6).

A full description of the calculation is given in FN. We now note slight differences between their approach and ours. Firstly, they work with Ox_1 parallel to a mirror plane, secondly, they use inner displacement vectors scaled to $\sqrt{3}a/2$ where a is the basal-plane parameter whereas here the scaling is to a , and thirdly, they give their results in units of Z^2e^2/a^4 whereas ours are in units of $Z^2/\Omega_0^{4/3}$. When due allowance for these differences has been made our calculations at the ideal ratio are in perfect agreement (to 10 significant places). All the present calculations were checked at two values of the convergence parameter and gave identical results, again to 10 significant places. The results, quoted to somewhat fewer figures, are given in tables 1 and 2.

Table 1. Electrostatic contributions to the second-order inner elastic constants of HCP metals. Entries to be multiplied by $Z^2/\Omega_0^{4/3}$, where Z is the valence and Ω_0 the atomic volume in 10^{-30} m^3 , to give the constants in units of 10^{10} Nm^{-2} .

| c/a | D_{16} | E_{11} | E_{33} |
|---------------------|----------|----------|----------|
| 1.56 | 44.012 | 53.062 | 835.340 |
| 1.5689 ^a | 42.910 | 51.530 | 834.840 |
| 1.58 | 41.572 | 49.679 | 834.145 |
| 1.60 | 39.258 | 46.503 | 832.700 |
| 1.62 | 37.067 | 43.524 | 831.024 |
| 1.6220 ^b | 36.854 | 43.236 | 830.845 |
| 1.6330 ^c | 35.706 | 41.687 | 829.820 |
| 1.64 | 34.991 | 40.728 | 829.135 |
| 1.66 | 33.026 | 38.107 | 827.050 |
| 1.75 | 25.407 | 28.199 | 815.624 |
| 1.80 | 21.932 | 23.829 | 808.140 |
| 1.8280 ^d | 20.190 | 21.679 | 803.680 |
| 1.85 | 18.915 | 20.123 | 800.063 |
| 1.8616 ^e | 18.274 | 19.347 | 798.120 |
| 1.90 | 16.298 | 16.982 | 791.536 |

^a Beryllium; ^b magnesium; ^c ideal ratio; ^d zinc; ^e cadmium.

Appendix

Non-zero inner elastic constants of HCP crystals

D_i : None

D_{ij} : D_{16} $D_{21} = -D_{22} = D_{16}$

E_{ij} : E_{11} $E_{22} = E_{11}$
 E_{33}

D_{ijk} : D_{136} $D_{116} = -\frac{1}{4}(D_{211} + 3D_{222})$, $D_{ijk} = D_{ikj}$
 D_{145} $D_{126} = \frac{1}{4}(3D_{211} + D_{222})$
 D_{211} $D_{212} = D_{266} = -\frac{1}{2}(D_{211} + D_{222})$
 D_{222} $D_{213} = -D_{233} = D_{136}$
 D_{314} $D_{244} = -D_{255} = -D_{145}$
 $D_{324} = -D_{356} = -D_{314}$

Table 2. Electrostatic contributions to the third-order inner elastic constants of HCP metals. Units as in table 1.

| c/a | D_{136} D_{145} D_{314} | D_{211} | D_{222} | E_{111} | E_{112} | E_{113} | E_{315} E_{135} | E_{331} | E_{333} | F_{112} |
|---------------------|-------------------------------------|-----------|-----------|-----------|-----------|-----------|------------------------|-----------|-----------|-----------|
| 1.56 | -210.179 | -7.412 | 12.353 | -8.022 | 32.701 | -289.988 | -1125.328 | -1072.266 | -2032.168 | -345.428 |
| 1.5689 ^a | -206.305 | -6.184 | 10.306 | -6.418 | 32.214 | -283.445 | -1118.285 | -1066.755 | -2040.691 | -335.227 |
| 1.58 | -201.548 | -4.732 | 7.887 | -4.541 | 31.605 | -275.458 | -1109.602 | -1059.924 | -2050.875 | -322.915 |
| 1.60 | -193.188 | -2.328 | 3.880 | -1.479 | 30.509 | -261.546 | -1094.246 | -1047.743 | -2068.013 | -301.834 |
| 1.62 | -185.097 | -0.179 | 0.298 | 1.203 | 29.417 | -248.237 | -1079.262 | -1035.738 | -2083.645 | -282.099 |
| 1.6220 ^b | -184.303 | 0.023 | -0.039 | 1.451 | 29.308 | -246.939 | -1077.784 | -1034.548 | -2085.128 | -280.196 |
| 1.6330 ^c | -179.984 | 1.091 | -1.819 | 2.758 | 28.711 | -239.906 | -1069.727 | -1028.039 | -2093.024 | -269.960 |
| 1.64 | -177.273 | 1.737 | -2.895 | 3.540 | 28.332 | -235.514 | -1064.650 | -1023.921 | -2097.835 | -263.627 |
| 1.66 | -169.712 | 3.436 | -5.727 | 5.564 | 27.260 | -223.359 | -1050.409 | -1012.302 | -2110.645 | -246.340 |
| 1.75 | -138.845 | 8.855 | -14.759 | 11.567 | 22.655 | -175.218 | -990.843 | -962.643 | -2152.835 | -181.344 |
| 1.80 | -123.818 | 10.618 | -17.696 | 13.242 | 20.300 | -152.690 | -960.830 | -937.000 | -2166.699 | -152.859 |
| 1.8280 ^d | -116.024 | 11.306 | -18.843 | 13.806 | 19.054 | -141.254 | -944.933 | -923.255 | -2171.890 | -138.883 |
| 1.85 | -110.199 | 11.719 | -19.532 | 14.095 | 18.113 | -132.823 | -932.885 | -912.763 | -2174.789 | -128.792 |
| 1.8616 ^e | -107.231 | 11.896 | -19.826 | 14.199 | 17.631 | -128.565 | -926.685 | -907.338 | -2175.923 | -123.766 |
| 1.90 | -97.896 | 12.303 | -20.506 | 14.340 | 16.101 | -115.353 | -906.889 | -889.907 | -2177.868 | -108.472 |

^{a, b, c, d, e} As in table 1.

$$\begin{array}{lll}
 E_{ijk}: & E_{111} & E_{222} = E_{111}, \quad E_{ijk} = E_{jik} \\
 & E_{112} & E_{221} = E_{112} \\
 & E_{113} & E_{223} = E_{113} \\
 & E_{135} & E_{126} = E_{216} = \frac{1}{2}(E_{111} - E_{112}) \\
 & E_{315} & E_{234} = E_{135} \\
 & E_{331} & E_{324} = E_{315} \\
 & E_{333} & E_{332} = E_{331} \\
 F_{ijk}: & F_{112} & F_{121} = F_{211} = -F_{222} = F_{112}
 \end{array}$$

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