Electrostatic energy and its contribution to elastic coefficients for body-centered-tetragonal metallic lattices*

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(Received 14 April 1975)

General expressions for the electrostatic energy and its contribution to the first- and second-order elastic coefficients are presented which can be used to evaluate the change in these quantities with arbitrary homogeneous deformations. Results are given for a bcc lattice under finite uniaxial deformation, i.e., the bct lattice. All the quantities calculated are shown to satisfy the internal check that the bct lattice with $c/a = (2)^{1/2}$ is identical to the fcc lattice.

I. INTRODUCTION

An important part of the calculation of the elastic constants of metallic solids is the evaluation of the electrostatic energy of the jellium model (i.e., a lattice of positive ions embedded in a uniform sea of electrons). General expressions for the electrostatic energy and its contribution to the first- and second-order elastic coefficients are presented which can be used to evaluate the change in these quantities with arbitrary homogeneous deformations. Results are given for a bcc lattice under finite uniaxial deformation. Similar general expressions have appeared elsewhere[1,2] but they are not directly applicable to the calculations presented here.

Fuchs[3,4] was the first to use the Ewald transformation of the electrostatic energy in an evaluation of the second-order elastic constants of metallic solids. In the Fuchs calculations the derivatives of the transformed electrostatic energy expression are taken with respect to pure shear and pure dilatational strain parameters. Following the Fuchs method Cousins obtained the third-order shear constants for bcc and fcc metallic structures,[5] and the elastic constants through third order for hexagonal metal structures[6,7] with various c/a ratios. Suzuki *et al.*[8] calculated the elastic constants to third order for bcc structures by first taking derivatives of the untransformed electrostatic energy with respect to general Lagrangian strain parameters. The resulting expressions were then transformed to facilitate rapid convergence of the lattice sums.

Using a general method MacDonald *et al.*[1] (referred to as I) obtained elastic constants to third order for bcc and fcc metallic structures. The transformed electrostatic energy expression is first simplified by choosing the Ewald convergence parameter so that the reciprocal-lattice terms can be omitted. The remaining parameters of the transformed electrostatic energy are then expressed in terms of Green's deformation tensor and derivatives taken with respect to Green's deformation tensor.

By a similar general method Fuller and Naimon[2] calculated the electrostatic energy contribution to the elastic constants to third order for six metallic and five ionic structures. Here again the parameters of the transformed electrostatic energy are expressed in terms of Green's deformation tensor but the derivatives are taken with respect to the Lagrangian strain parameter. The elastic coefficient expressions of Fuller and Naimon are applicable to nonmetallic lattices and in that respect are more general than those of I.

In one respect the expressions of I are advantageous in that the elastic coefficients are defined for a homogeneously deformed state, whereas in Fuller and Naimon's[2] paper they are defined just at the equilibrium state. Thus, only the expressions in I are applicable to the evaluation of the change in the elastic coefficients under finite homogeneous deformations. This paper illustrates the usefulness of the approach used in I and serves to clarify the interpretation of the expressions given there for the elastic coefficients.

General expressions for the complete transformed electrostatic energy and its contribution to the elastic coefficients to second order are given in Sec. II. The results for the body-centered-tetragonal metallic lattice for c/a from 0.5 to 2.0 are given in Sec. III.

II. ELASTIC-COEFFICIENT EXPRESSIONS

Using the Ewald-Fuchs method the electrostatic energy per atom of a homogeneously deformed lattice of positive ions embedded in a uniform electron gas can be written[3]

$$E'_{\mathrm{ES}} = \frac{Z^2e^2}{2}\left(\frac{\pi}{\Omega}\sum_m{}' \frac{\exp(-K'^2_m/E^2)}{K'^2_m} + \sum_n{}' \frac{\operatorname{erfc} E|\vec{R}'_n|}{|\vec{R}'_n|} - \frac{2E}{\sqrt{\pi}} - \frac{\pi}{E^2\Omega}\right) , \quad (1)$$

where the summation signs indicate triple sums over the lattice sites and the prime on the lattice sums indicates that the origin lattice site is omitted. $\vec{R}'_n$ and $\vec{K}'_m$ are the homogeneously deformed direct and reciprocal-lattice vectors, respectively; Ω is the deformed atomic sphere volume; e is the electron charge; and Z is the ion valence. The abbreviation erfc denotes the complementary error function and E is the Ewald convergence parameter.

For calculations of the variation of the electrostatic energy under finite homogeneous deformation, it is convenient to write the variables $\vec{R}'_n$, $\vec{K}'_m$, and Ω in terms of the Green's deformation tensors, C_{st} and C^{-1}_{st}, referred to coordinates of the undeformed lattice configuration[1]:

$$|\vec{R}'_n| = \tfrac{1}{2}\, a(n_s n_t C_{st})^{1/2}\,, \tag{2}$$

$$K'^2_m = (\pi/a)^2 m_s m_t C^{-1}_{st}\,, \tag{3}$$

$$\Omega = \Omega_0 I_3^{1/2}\,, \quad I_3 = \det|C_{st}|\,. \tag{4}$$

In the above, a is the lattice constant, Ω_0 is the undeformed atomic sphere volume, and I_3 is the third principal invariant of C_{st}.

By writing the convergence parameter as $E = \eta/a$ and the undeformed atomic sphere volume as $\Omega_0 = a^3/2\mu$, the explicit volume dependence of the electrostatic energy can be factored out. Here μ is a parameter that depends on how many atoms there are per unit cell (e.g., $\mu = 1$ for bcc and $\mu = 2$ for fcc). The resulting expression for the electrostatic energy in terms of the Green's deformation tensor is then

$$E'_{ES} = \frac{Z^2e^2}{a}\left(\frac{\mu I_3^{-1/2}}{\pi}\sum_m{}' \frac{\exp(-\pi^2 m_a m_b C^{-1}_{ab}/\eta^2)}{m_a m_b C^{-1}_{ab}} + \sum_n{}' \frac{\operatorname{erfc}[\frac{1}{2}\eta(n_a n_b C_{ab})^{1/2}]}{(n_a n_b C_{ab})^{1/2}} - \frac{\eta}{\sqrt{\pi}} - \frac{\mu\pi}{\eta^2} I_3^{-1/2}\right). \tag{5}$$

The electrostatic energy contribution to the total strain energy density is found by dividing Eq. (5) by the initial volume, i.e., $\Sigma_{ES} = E'_{ES}/\Omega_0$. The elastic coefficients are defined here as derivatives of the strain energy density with respect to the Green's deformation measure evaluated at a homogeneously deformed state. The electrostatic energy contribution to the first-order elastic coefficient is then

$$T^{ES}_{ij}(C) = 2\left(\frac{\partial \Sigma_{ES}}{\partial C_{ij}}\right)_{C\neq I} = \frac{Z^2e^2}{a\Omega_0}\left\{\frac{\mu I_3^{-1/2}}{\pi}\sum_m{}' \frac{\exp(-\pi^2 m_a m_b C^{-1}_{ab}/\eta^2)}{m_a m_b C^{-1}_{ab}} \times\left[-C^{-1}_{ij} + m_a m_b(C^{-1}_{ai}C^{-1}_{bj} + C^{-1}_{aj}C^{-1}_{bi})\left(\frac{\pi^2}{\eta^2} + \frac{1}{m_a m_b C^{-1}_{ab}}\right)\right] - \sum_n{}' \frac{n_i n_j}{n_a n_b C_{ab}} \times\left(\frac{\eta}{\sqrt{\pi}}\exp[-\tfrac{1}{4}\eta^2(n_a n_b C_{ab})] + \frac{\operatorname{erfc}[\frac{1}{2}\eta(n_a n_b C_{ab})^{1/2}]}{(n_a n_b C_{ab})^{1/2}}\right) + \frac{\mu\pi C^{-1}_{ij} I_3^{-1/2}}{\eta^2}\right\}. \tag{6}$$

The electrostatic energy contribution to the second-order elastic coefficient is then

$$C^{ES}_{ijkl}(C) = 2\left(\frac{\partial T^{ES}_{ij}}{\partial C_{kl}}\right)_{C\neq I} = \frac{Z^2e^2}{a\Omega}\left(\frac{\mu I_3^{-1/2}}{\pi}\sum_m{}' \frac{\exp(-\pi m_a m_b C^{-1}_{ab}/\eta^2)}{m_a m_b C^{-1}_{ab}}\left\{\left[-C^{-1}_{ij} + m_a m_b \times(C^{-1}_{ai}C^{-1}_{bj} + C^{-1}_{aj}C^{-1}_{bi})\left(\frac{\pi^2}{\eta^2} + \frac{1}{(m_a m_b C^{-1}_{ab})}\right)\right]\left[-C^{-1}_{kl} + m_e m_f(C^{-1}_{ek}C^{-1}_{fl} + C^{-1}_{el}C^{-1}_{fk})\left(\frac{\pi^2}{\eta^2} + \frac{1}{m_a m_b C^{-1}_{ab}}\right)\right] + (C^{-1}_{ik}C^{-1}_{jl} + C^{-1}_{jk}C^{-1}_{il}) - m_a m_b\left(\frac{\pi^2}{\eta^2} + \frac{1}{m_a m_b C^{-1}_{ab}}\right)[C^{-1}_{ai}(C^{-1}_{bk}C^{-1}_{jl} + C^{-1}_{jk}C^{-1}_{bl}) + C^{-1}_{bj}(C^{-1}_{ak}C^{-1}_{il} + C^{-1}_{ik}C^{-1}_{al}) + C^{-1}_{aj}(C^{-1}_{bk}C^{-1}_{il} + C^{-1}_{ik}C^{-1}_{bl}) + C^{-1}_{bi}(C^{-1}_{ak}C^{-1}_{jl} + C^{-1}_{jk}C^{-1}_{al})] + \frac{m_a m_b(C^{-1}_{ai}C^{-1}_{bj} + C^{-1}_{aj}C^{-1}_{bi})\, m_e m_f(C^{-1}_{ek}C^{-1}_{fl} + C^{-1}_{el}C^{-1}_{fk})}{(m_a m_b C^{-1}_{ab})^2}\right\} + \sum_n{}' \frac{n_i n_j n_k n_l}{(n_a n_b C_{ab})}\left[\left(\frac{\eta^3}{2\sqrt{\pi}} + \frac{3\eta}{\sqrt{\pi}(n_a n_b C_{ab})}\right)\exp[-\tfrac{1}{4}\eta^2(n_a n_b C_{ab})] + \frac{3\operatorname{erfc}[\frac{1}{2}\eta(n_a n_b C_{ab})^{1/2}]}{(n_a n_b C_{ab})^{3/2}}\right] - \frac{\mu\pi I_3^{-1/2}}{\eta^2}(C^{-1}_{ij}C^{-1}_{kl} + C^{-1}_{ik}C^{-1}_{jl} + C^{-1}_{jk}C^{-1}_{il})\right). \tag{7}$$

In the above expressions the following relations have been used[1]:

$$\frac{\partial I_3^p}{\partial C_{jk}} = pI_3^p C^{-1}_{jk}\,, \tag{8}$$

$$\frac{\partial C_{rs}}{\partial C_{jk}} = \tfrac{1}{2}(\delta_{rj}\delta_{ks} + \delta_{sj}\delta_{kr})\,, \tag{9}$$

$$\frac{\partial C^{-1}_{rs}}{\partial C_{jk}} = -\tfrac{1}{2}(C^{-1}_{rj}C^{-1}_{ks} + C^{-1}_{sj}C^{-1}_{kr})\,, \tag{10}$$

$$\frac{\partial}{\partial C_{jk}}\{\operatorname{erfc}[\tfrac{1}{2}\eta(n_a n_b C_{ab})^{1/2}]\} = \frac{-\eta}{2\sqrt{\pi}}\frac{n_i n_k \exp[-\tfrac{1}{4}\eta^2(n_a n_b C_{ab})]}{(n_a n_b C_{ab})^{1/2}}\,. \tag{11}$$

The coefficients in expressions (6) and (7) are defined relative to the undeformed state since the Green's deformation tensor is referred to the coordinates of the undeformed lattice. It should be pointed out here that in I an expression similar to Eq. (7) above [i.e., Eq. (7) of I] was incorrectly described as being the contribution to the second-order elastic coefficients relative to the deformed state. The distinction between coefficients evaluated at the deformed state but relative to either the undeformed or deformed state is significant when dealing with finite deformations.

In general, the first derivative of the strain energy density with respect to a deformation measure results in an expression for the thermodynamic tensions (or "stress") conjugate to the deformation. The particular type of "stress" depends on the deformation measure used. The T_{ij}^{ES} shown in Eq. (6) are in fact the pseudostress components introduced by Piola.[9] The actual stress components at any deformed state are obtained from the derivative of the strain energy density with respect to the strain measured from that state.[10] Thus, the actual stress components t_{ij}^{ES} and the pseudostress components of Eq. (6) can be related by

$$t_{ij}^{ES}(C) = I_3^{-1/2} \frac{\partial X_i}{\partial a_r} \frac{\partial X_j}{\partial a_s} T_{rs}^{ES}(C) , \qquad (12)$$

where a_i and X_i are the coordinates of the undeformed and deformed states, respectively. Equation (12) for the actual stress $t_{ij}^{ES}(C)$ is the general expression for the electrostatic energy contribution to the first-order elastic coefficients defined relative to any deformed state.

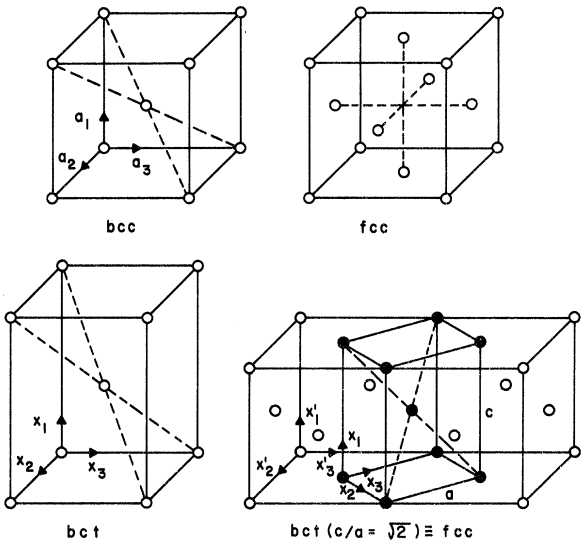

FIG. 1. Unit cells for bcc, fcc, and bct lattice structures. The relationship between the fcc and bct unit cells is illustrated for bct with $c/a = \sqrt{2}$.

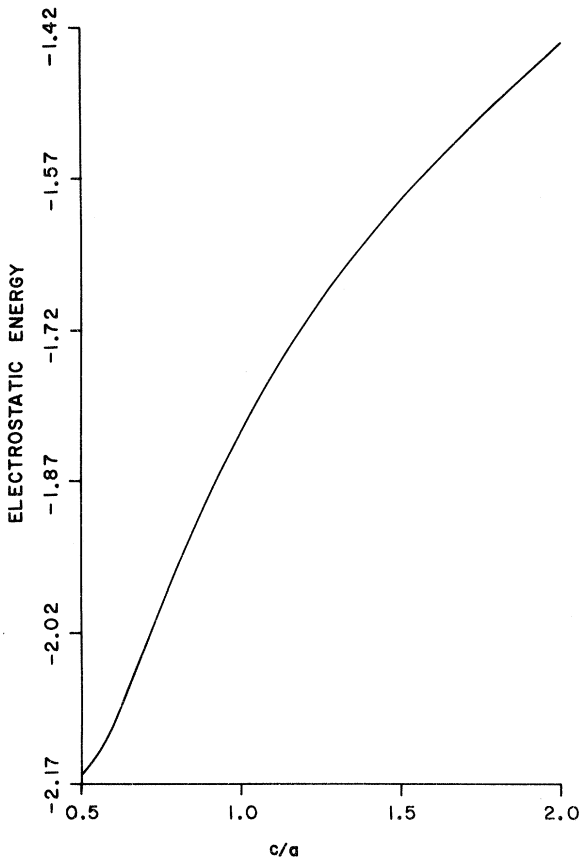

FIG. 2. Variation of the electrostatic energy in units of Z^2e^2/a as a function of the axial ratio c/a, here a is the "undeformed" bcc lattice constant.

The true general expression for the electrostatic energy contribution to the second-order elastic coefficients defined relative to any deformed state can likewise be found by substituting Eq. (7) for C_{ijkl}^{ES} into

$$c_{ijkl}^{ES}(C) = I_3^{-1/2} \frac{\partial X_i}{\partial a_p} \frac{\partial X_j}{\partial a_q} \frac{\partial X_k}{\partial a_r} \frac{\partial X_l}{\partial a_s} C_{pqrs}^{ES}(C) . \qquad (13)$$

III. RESULTS FOR bct LATTICE

To obtain results for the body-centered-tetragonal lattice, a bcc lattice was subjected to uniaxial deformation along one of the edges of the unit cell (i.e., along a_1, see Fig. 1). The transformation equations representing this uniaxial deformation are

$$X_1 = \lambda a_1 , \quad X_2 = a_2 , \quad \text{and} \quad X_3 = a_3 , \qquad (14)$$

where as before a_i and X_i are the coordinates of the undeformed and deformed states, respectively. (Note that the ratio $c/a = \lambda$.) Since the Green's deformation tensor can be defined as[9]

$$C_{ij} = \frac{\partial X^m}{\partial a_i} \frac{\partial X^m}{\partial a_j} , \tag{15}$$

the values for uniaxial deformation are given as

$$C_{11} = \lambda^2 , \quad C_{11}^{-1} = 1/\lambda^2 , \quad I_3 = \lambda^2 , \tag{16}$$

and $C_{ij} = C_{ij}^{-1} = \delta_{ij}$ for all other i and j.

The electrostatic energy for the bct lattice is obtained from Eq. (5) using Eq. (16), i.e.,

$$E'_{\rm ES} = E'_{\rm ES}(C_{11} = \lambda^2 , \ C_{11}^{-1} = 1/\lambda^2 , \ldots , \text{ etc.}) . \tag{17}$$

Using Eqs. (14) and (16) together with the general expressions (6) and (12), the relations for the electrostatic energy contribution to the first-order elastic coefficients for the bct lattice can be represented schematically by

$$\begin{aligned} t_{11}^{\rm ES} &= \lambda T_{11}^{\rm ES}(C_{11} = \lambda^2, \ C_{11}^{-1} = 1/\lambda^2 , \ldots , \text{etc.}) , \\ t_{22}^{\rm ES} &= (1/\lambda)\, T_{22}^{\rm ES}(C_{11} = \lambda^2 , \ C_{11}^{-1} = 1/\lambda^2 , \ldots , \text{etc.}) , \end{aligned} \tag{18}$$

where $t_{22}^{\rm ES} = t_{33}^{\rm ES}$, and all other $t_{ij}^{\rm ES} = 0$.

Similarly, starting with the general expressions (7) and (13), the relations for the electrostatic energy contribution to the second-order elastic coefficients for the bct lattice can be represented by

$$\begin{aligned} c_{1111}^{\rm ES} &= \lambda^3 C_{1111}^{\rm ES}(C_{11} = \lambda^2 , \ C_{11}^{-1} = 1/\lambda^2, \ldots , \text{etc.}) , \\ c_{2222}^{\rm ES} &= \lambda^{-1} C_{2222}^{\rm ES}(C_{11} = \lambda^2 , \ C_{11}^{-1} = 1/\lambda^2, \ldots , \text{etc.}) , \\ c_{1122}^{\rm ES} &= \lambda C_{1122}^{\rm ES}(C_{11} = \lambda^2 , \ C_{11}^{-1} = 1/\lambda^2, \ldots , \text{etc.}) , \\ c_{2233}^{\rm ES} &= \lambda^{-1} C_{2233}^{\rm ES}(C_{11} = \lambda^2, \ C_{11}^{-1} = 1/\lambda^2, \ldots , \text{ etc.}) , \end{aligned} \tag{19}$$

where $c_{2222}^{\rm ES} = c_{3333}^{\rm ES}$, $c_{1122}^{\rm ES} = c_{1133}^{\rm ES}$ and all other $c_{ijkl}^{\rm ES} = 0$. The relations represented by (17)–(19) were programmed on an IBM 370 computer and results obtained for the axis ratio c/a from 0.5 to 2.0.

There are several ways the values of the computed quantities can be presented. For instance, the electrostatic energy in Eq. (5) is expressed in terms of the dimensions of the "undeformed" bcc lattice constant a, i.e.,

$$E'_{\rm ES} = (Z^2 e^2/a)\, \alpha_a , \tag{20}$$

where the expression within large parentheses in Eq. (5) is written here as α_a and is known as the geometric coefficient. The plot of α_a for c/a

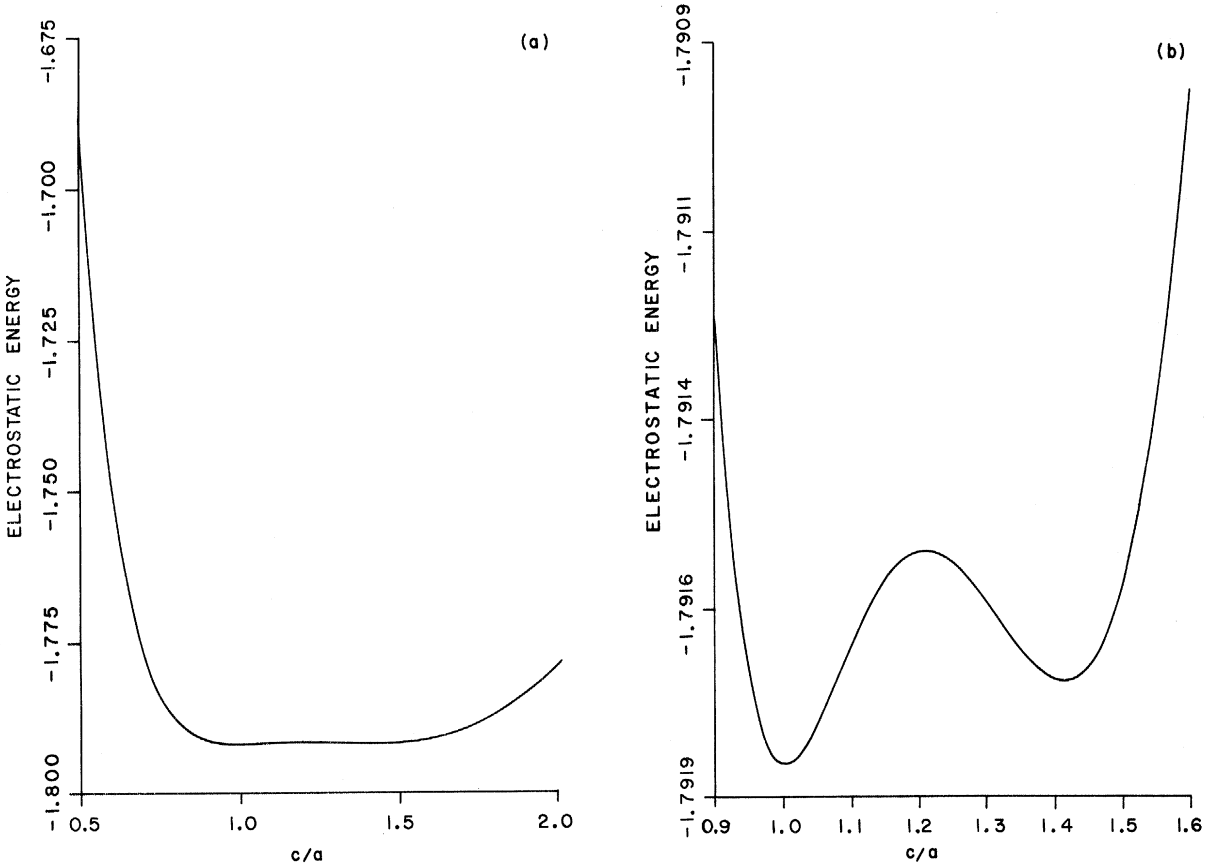

FIG. 3. Variation of the electrostatic energy in units of $Z^2e^2/2r_s$ as a function of the axial ratio c/a, where r_s is the atomic sphere radius in the deformed state. The minima in (b) at $c/a = 1$ and $c/a = \sqrt{2}$ correspond to the bcc and fcc structures, respectively.

TABLE I. Electrostatic energy and its contribution to the elastic coefficients for body-centered-tetragonal structure. Electrostatic energy entries are in units of $Z^2e^2/2r_s$ and the elastic coefficient entries are in units of $Z^2e^2/2r_s\Omega$, where r_s and Ω are the atomic sphere radius and volume, respectively, in the deformed state.

c/a	Electrostatic energy	t_1	t_2	c_{11}	c_{22}	c_{12}	c_{23}
0.5	−1.688 771 841	0.119 060 694	0.784 855 573	1.158 307 548	−1.812 381 895	−0.757 744 481	0.215 559 989
0.6	−1.750 183 044	0.343 160 770	0.703 511 137	0.223 721 988	−1.636 578 260	−0.626 602 150	0.152 646 999
0.7	−1.777 169 870	0.474 833 518	0.651 168 176	−0.422 074 576	−1.524 120 561	−0.501 212 989	0.071 829 022
0.8	−1.787 861 712	0.547 762 737	0.620 049 488	−0.866 892 503	−1.447 763 108	−0.388 197 853	−0.024 187 502
0.9	−1.791 270 047	0.583 557 958	0.603 856 045	−1.157 606 812	−1.386 999 107	−0.296 533 531	−0.128 035 495
1.0[a]	−1.791 858 511	0.597 286 170	0.597 286 170	−1.328 364 763	−1.328 364 763	−0.231 746 874	−0.231 746 874
1.1	−1.791 693 349	0.599 512 845	0.596 090 252	−1.408 721 977	−1.264 466 865	−0.194 908 279	−0.328 895 611
1.2	−1.791 571 097	0.597 404 865	0.597 083 116	−1.424 710 901	−1.192 239 909	−0.183 751 847	−0.415 257 592
1.3	−1.791 639 883	0.595 567 318	0.598 036 282	−1.398 286 443	−1.111 245 318	−0.194 207 756	−0.488 655 773
1.4	−1.791 744 588	0.596 741 574	0.597 501 507	−1.346 955 267	−1.022 385 777	−0.221 634 727	−0.548 484 016
$\sqrt{2}$[b]	−1.791 747 230	0.597 249 077	0.597 249 077	−1.338 452 706	−1.009 197 246	−0.226 647 262	−0.555 902 722
1.5	−1.791 614 797	0.602 372 350	0.594 621 224	−1.283 915 457	−0.927 075 369	−0.261 600 797	−0.595 187 505
1.6	−1.790 962 484	0.613 045 169	0.588 958 657	−1.218 569 425	−0.826 769 595	−0.310 283 042	−0.629 823 336
1.7	−1.789 528 445	0.628 807 414	0.580 360 516	−1.157 206 253	−0.722 737 162	−0.364 607 995	−0.653 736 390
1.8	−1.787 100 475	0.649 393 678	0.568 853 398	−1.103 701 637	−0.615 977 200	−0.422 239 699	−0.668 343 296
1.9	−1.783 516 663	0.674 377 421	0.554 569 621	−1.060 149 297	−0.507 215 400	−0.481 491 483	−0.675 001 979
2.0	−1.778 661 500	0.703 268 640	0.537 696 430	−1.027 387 222	−0.396 937 559	−0.541 209 349	−0.674 942 382

[a] $c/a=1$ corresponds to bcc.

[b] $c/a=\sqrt{2}$ corresponds to fcc referred to the rotated axes X_1, X_2, and X_3 of Fig. 1.

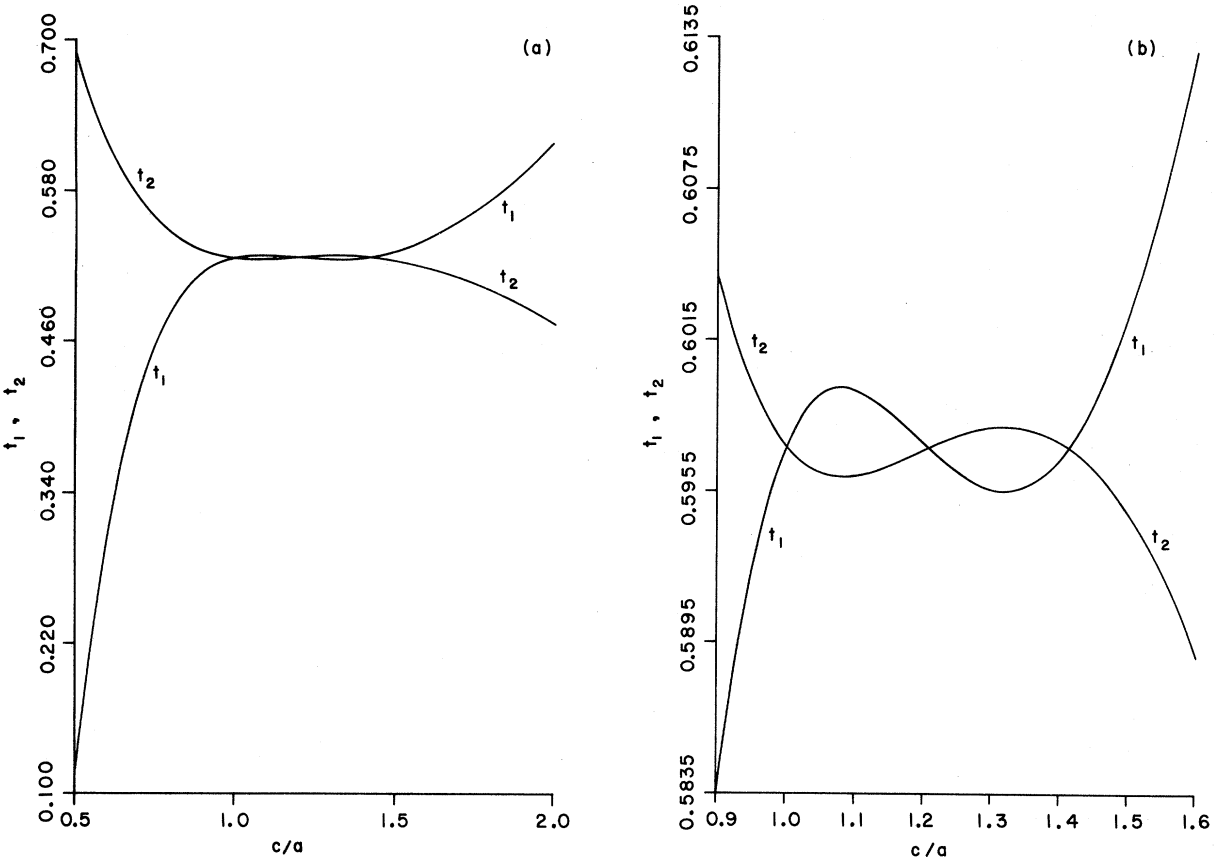

FIG. 4. Variation of the first-order elastic coefficients t_1 and t_2 in units of $Z^2e^2/2r_s\Omega$ as a function of the axial ratio c/a, where r_s and Ω are the atomic sphere radius and volume, respectively, in the deformed state. The points in (b) where $t_1=t_2$ correspond to the bcc and fcc structures as well as to the intermediate metastable structure.

from 0.5 to 2.0 is shown in Fig. 2. With this particular representation of the electrostatic energy, however, it is not apparent that for $c/a=\sqrt{2}$ the bct lattice is identical to the fcc lattice (see Fig. 1).

In order to sensibly display the variation of the electrostatic energy and its contribution to the first- and second-order elastic coefficients, the computed values are scaled to the "deformed" atomic sphere radius r_s and volume $\Omega=\frac{4}{3}\pi r_s^3$. That is, the results are presented for the particular bct lattice at equilibrium and not in terms of the "undeformed" bcc lattice dimensions.

For example, the electrostatic energy can also be written

$$E'_{\mathrm{ES}}=(Z^2e^2/2r_s)\alpha_s\,, \tag{21}$$

where α_s is the geometric coefficient relative to $2r_s$. The variation of α_s with c/a from 0.5 to 2.0 shown in Fig. 3(a) now exhibits a broad relatively flat region for α_s when the axial ratio c/a is between 0.9 and 1.6. Figure 3(b) is a greatly expanded plot of this region showing the minima corresponding to the bcc ($c/a=1$) and fcc ($c/a=\sqrt{2}$) structures.

In Table I the values of the electrostatic energy in units of $Z^2e^2/2r_s$ at these minima $c/a=1$ and $c/a=\sqrt{2}$ agree with the published values for the bcc and fcc structures, respectively.[1,2]

Also included in Table I are the values of the electrostatic energy contribution to the first- and second-order elastic coefficients listed in terms of the Voigt reduced notation and expressed in units of $Z^2e^2/2r_s\Omega$. The plots of the first-order elastic coefficients for c/a from 0.5 to 2.0 are shown in Fig. 4(a). The detail plot in Fig. 4(b) of the region $0.9\leq c/a\leq 1.6$ shows that, as required, $t_1=t_2$ for the bcc and fcc structures as well as at the intermediate metastable structure. The graphs of c_{11} and c_{22} in Fig. 5(a) and c_{12} and c_{23} in Fig. 5(b) cross at $c/a=1$ and the values there (see Table I) correspond to the proper ones for the bcc structure[8]. The match of c_{11} and c_{22} as well as c_{12} and c_{23} for the fcc structure ($c/a=\sqrt{2}$) is not apparent from Figs. 5(a) and 5(b).

In order to see that the second-order elastic coefficients satisfy the requirement that bct ($c/a=\sqrt{2}$) $\equiv$ fcc, the following coordinate transformation

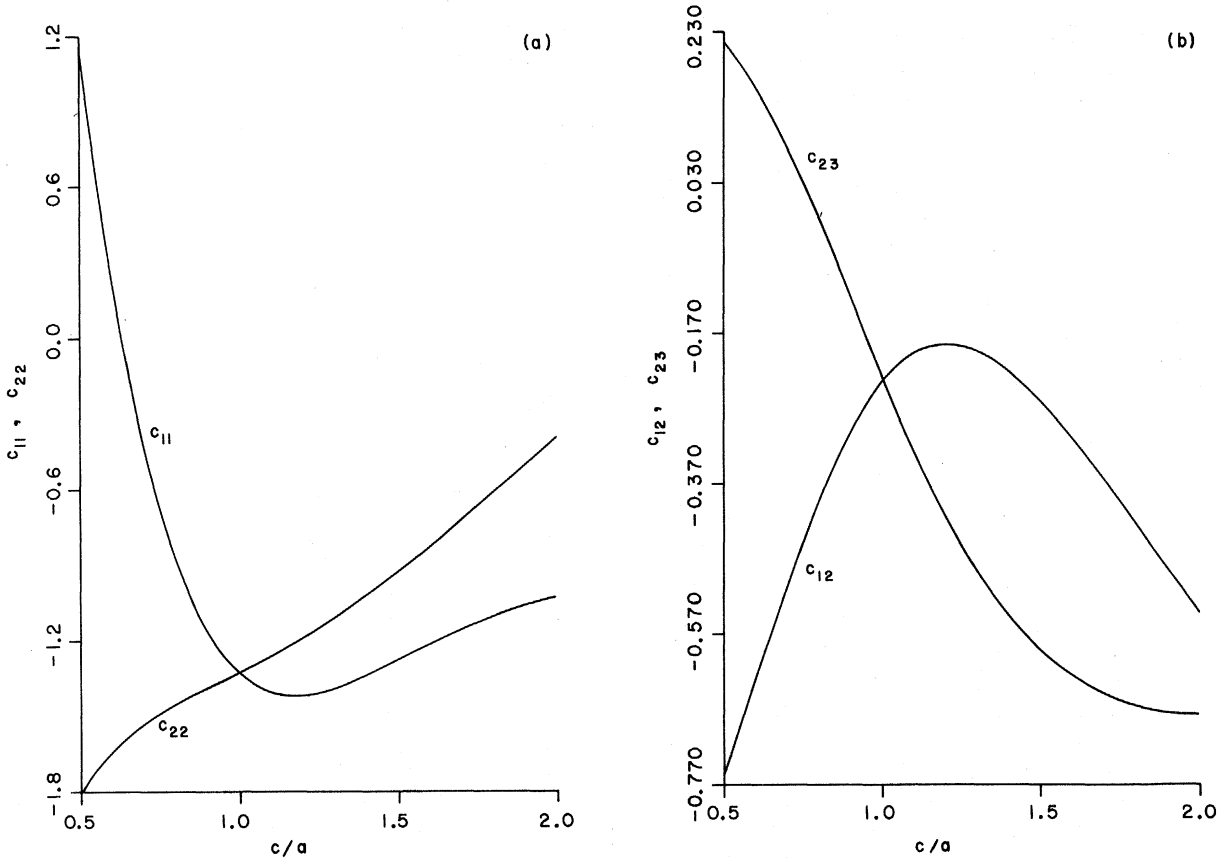

FIG. 5. Variation of the second-order elastic coefficients in units of $Z^2e^2/2r_s\Omega$ as a function of the axial ratio c/a, where r_s and Ω are the atomic sphere radius and volume, respectively, in the deformed state. (a) c_{11} and c_{22}. (b) c_{12} and c_{23}.

is needed (see Fig. 1):

$$X_1' = X_1 ,$$
$$X_2' = (1/\sqrt{2})(X_2 - X_3) , \qquad (22)$$
$$X_3' = (1/\sqrt{2})(X_2 + X_3) .$$

Using the transformation equations (12) and (13) the relations between the elastic coefficients for the bct (unprimed) and fcc (primed) coordinates are

$$t_{11}' = t_{11} , \quad t_{22}' = t_{22} , \quad c_{1111}' = c_{1111} , \quad c_{1122}' = c_{1122} ,$$
$$c_{2222}' = \tfrac{1}{2}(c_{2222} + 3c_{2233}) , \qquad (23)$$
$$c_{2233}' = \tfrac{1}{2}(c_{2222} - c_{2233}) .$$

The entries in Table I for $c/a = \sqrt{2}$ confirm that $c_{1111}' = c_{2222}'$ and that $c_{1122}' = c_{2233}'$ and that these values correspond to the fcc structure.[8] Thus, all the calculations satisfy the internal check that bct $(c/a = \sqrt{2}) \equiv$ fcc.

ACKNOWLEDGMENT

The author would like to thank H. R. Scholz for checking the expressions for the elastic coefficients and for writing programs to generate graphs.

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*Research support was provided by the National Science Foundation.

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