Nonequivalence of general tensor force and Clark, Gazis, and Wallis angular force models

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The general tensor force (GTF) model, the general scalar force (GSF) model as well as the Clark, Gazis, and Wallis (CGW) angular force model are analyzed by resolving the atomic displacements along three mutually perpendicular directions. It is shown that the GTF model that neglects three-body and mixed neighbor interactions confined to the plane of a triangle but incorporates two-body interactions perpendicular to the plane, is not equivalent to the CGW model that incorporates the former while neglecting the latter. However, the relations between the tensor force constants of the former and the scalar constants of the latter, deduced by exploiting the basic differences in their transformation properties, reveal that the GTF model is equivalent to the GSF model in the case of bcc and fcc structures, and all earlier claims regarding its equivalence with the CGW model are therefore spurious. The role played by the coordinate axes transformations, the relations between these and other force constant models, as well as the equivalence between their force constants, are discussed. [S0163-1829(98)00710-3]

I. INTRODUCTION

The general tensor force (GTF) model[1] that is used extensively in the analysis of experimental phonon frequencies of a variety of solids, is not at all invariant with respect to rigid body rotations even in the case of high symmetry cubic crystals. The distinguishing feature of this model is that the symmetry operations of the lattice determine the number of independent force constants needed to specify completely the short-range ion-ion interactions. Irrespective of the differences in their assumptions regarding the nature and the range of interatomic forces, other lattice dynamical models such as the De Launay angular force (DAF) model,[2] the axially symmetric force (AS) model,[3] the modified axially symmetric force (MAS) model[4] and the central pair potential (CPP) model[5] that are approximate forms of the GTF model, suffer from the same deficiency. The harmonic force constants of the GTF model comply with Born-Huang conditions[6] so long as the crystal is in equilibrium, but they fail to satisfy the additional conditions that reduce the change in potential energy to zero.[7] As a consequence, this model becomes elastically inconsistent and gives rise to two different expressions for C_{44} in the case of noncubic crystals.[8] Besides, the Cauchy discrepancies due to short-range interactions reduce to zero whenever this model complies with all invariance conditions.[9] On the contrary, the elastic consistency of Clark, Gazis, and Wallis (CGW) model[10] is not destroyed by the transition from cubic to tetragonal or hexagonal symmetry.[11] The characteristic feature of this model is that the angular forces that arise from the resistance to deformation of the angles formed by three atoms, incorporate a component of three-body forces confined to the plane of the triangle.[12] The Cauchy discrepancies of a solid are not disturbed because the potential energy associated with the change in CGW angles is independent of the orientation of the coordinate axes.

The equivalence between two lattice dynamical models based on either the comparison of dynamical matrix elements in the long-wavelength limit as well as at the Brillouin-zone boundary or the number of independent parameters associated with various sets of neighbors in one model being the same as those in the other model, does not seem to have any significance.[13] Further, the above mentioned differences in the nature of atomic interactions and their manifestations invariably contradict the claim of Moore and Upadhyaya[14] that the GTF model is identical to the CGW model for cubic systems. Nevertheless, according to Moore,[15] the force constants of the former are composite quantities arising from the elementary or semimicroscopic force constants of the latter. Upadhyaya *et al.*[16] have therefore equated the force constants of the GTF model to arbitrarily assorted algebraic sum of central and angular force constants of the CGW model in the case of bcc and fcc structures. In this scheme, the GTF constants associated with first, second, and third nearest neighbors in fcc structures and third nearest neighbors in bcc structures are linked with the corresponding CGW constants associated with all neighbors, while the second neighbor GTF constants in bcc structures are linked with first and second neighbor CGW constants. As a consequence, the former become invariant with respect to coordinate axes transformation. In addition, it is necessary for these authors to presume that (i) the force constants defining the additional three-body forces between first or second set of nearest neighbors in bcc structures will contribute to the forces on the ion at the origin in the same manner as the two-body forces,[12] (ii) neglect of second-order contribution in the rotation vector ω destroys the rotational invariance of the DAF and CPP models[14] and (iii) three-body noncentral forces contribute to the ion-ion interaction of the GTF model[16] in order to justify a superficial claim regarding the equivalence between the GTF and CGW models.

On the contrary, Ramamurthy and his co-workers[8,9,13,17] have established by systematically analyzing the differences in the nature of interatomic forces of several lattice dynamical models in the case of cubic, tetragonal, and hexagonal structures that the CGW model is unique as it incorporates additional contributions from (i) same neighbor three-body interactions, (ii) mixed neighbor two-body interactions as well as (iii) mixed neighbor three-body interactions, whereas

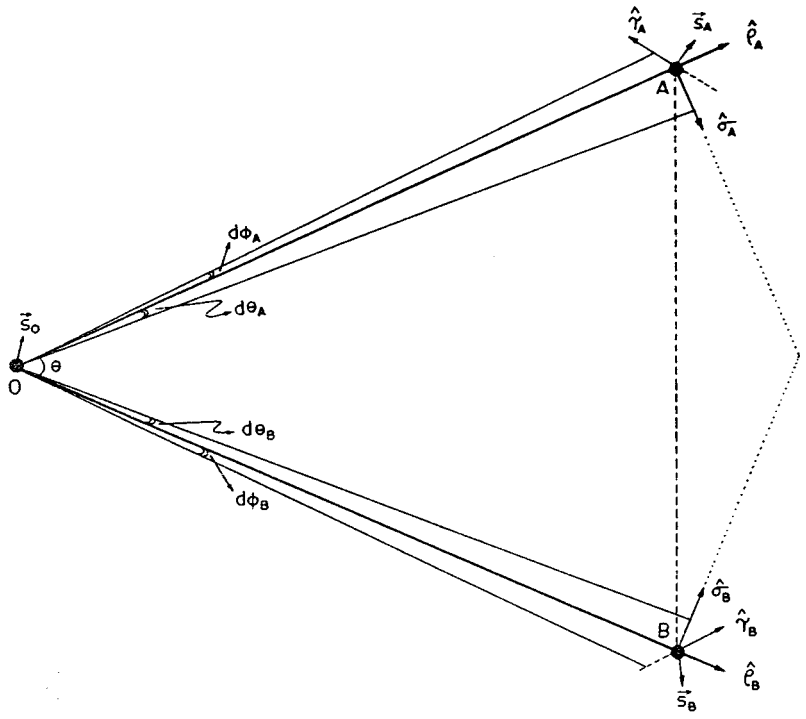

FIG. 1. Angles subtended by atomic displacements normal to the position vectors R_A and R_B at the origin. Components parallel to the plane: $d\theta_A$ and $d\theta_B$. Components perpendicular to the plane: $d\phi_A$ and $d\phi_B$.

the DAF, AS, MAS, CPP, and GTF models do not. Moreover, the force constants of the CGW model as well as those of the DAF, AS, MAS, and CPP models are invariant with respect to a coordinate axes transformation, but those of the GTF model transform as the components of a second rank tensor.[18] The present author has therefore extended the previous analysis,[13] hereinafter referred to as I, up to third nearest neighbors in the case of bcc and fcc structures to determine the degree of equivalence that exists between the CGW model and the GTF model and exploited the transformation properties of force constants to deduce the correct relations between them. It is the purpose of this paper to describe these investigations that reveal that there is no way of expressing the contributions from three-body forces in terms of two-body forces in the case of any crystal structure.

II. THEORY

To facilitate the analysis of different lattice dynamical models and the comparison of the GTF model with the CGW model, the dynamical matrix $D(q)$ is split into an ionic part D^i and an electronic part D^e representing the contributions from the short-range ion-ion interactions and the long-range electron-ion interactions, respectively. We consider three atoms O, A, and B, shown in Fig. 1, which form a triangle with angle θ at the origin. The relative displacements of the atoms A and B are resolved along three mutually perpendicular directions, denoted by unit vectors $\hat{\rho}$, $\hat{\sigma}$, and $\hat{\tau}$ that form a right-handed system, in order to express the elements of D^i in terms of central and angular forces. It was shown in I that the change in the potential energy of the atom at O due to displacements s_O, s_A, and s_B of these atoms from their equilibrium positions, in the harmonic approximation, is given by

$$dV=(\tfrac{1}{2})\beta\{[\hat{\rho}_A\cdot(s_A-s_O)]^2+[\hat{\rho}_B\cdot(s_B-s_O)]^2\}+(\tfrac{1}{2})\epsilon[(d\phi_A)^2+(d\phi_B)^2]+(\tfrac{1}{2})\gamma(d\theta)^2, \quad (1)$$

where β is the central force constant, ϵ and γ are the angular force constants, perpendicular and parallel to the plane of the triangle OAB, respectively. Further, the last term of Eq. (1) may be expanded as

$$(\tfrac{1}{2})\gamma(d\theta)^2=(\tfrac{1}{2})\gamma[(d\theta_A)^2+(d\theta_B)^2+2(d\theta_A)(d\theta_B)]. \quad (2)$$

It should be obvious from Fig. 1 that the third term of Eq. (2) involves the coordinates of all the three atoms and therefore represents the excess energy associated with three-body forces,[19] whereas the remaining terms of Eq. (1) and (2) represent the corresponding potential energies associated with two-body forces. Following the procedure adopted in I, the x components of (i) central forces F_x^c, (ii) angular forces perpendicular to the plane F_x^1, (iii) two-body angular forces parallel to the plane F_x^2 and (iv) three-body angular forces parallel to the plane F_x^3 are, respectively, given by

$$F_x^c=-\beta\{l_A[(u_O-u_A)l_A+(v_O-v_A)m_A+(w_O-w_A)n_A]+l_B[(u_O-u_B)l_B+(v_O-v_B)m_B+(w_O-w_B)n_B]\}, \quad (3)$$

$$F_x^1=-\epsilon\{(p_A[(u_O-u_A)p_A+(v_O-v_A)q_A+(w_O-w_A)r_A]/R_A^2)+(p_B[(u_O-u_B)p_B+(v_O-v_B)q_B+(w_O-w_B)r_B]/R_B^2)\}, \quad (4)$$

$$F_x^2 = -\gamma\{(\lambda_A[(u_O-u_A)\lambda_A+(v_O-v_A)\mu_A + (w_O-w_A)\nu_A]/R_A^2)+(\lambda_B[(u_O-u_B)\lambda_B + (v_O-v_B)\mu_B+(w_O-w_B)\nu_B]/R_B^2)\} \quad (5)$$

and

$$F_x^3 = -\gamma\{\lambda_A[(u_O-u_B)\lambda_B+(v_O-v_B)\mu_B+(w_O-w_B)\nu_B] + \lambda_B[(u_O-u_A)\lambda_A+(v_O-v_A)\mu_A + (w_O-w_A)\nu_A]\}/|R_A\|R_B|, \quad (6)$$

where (l,m,n), (p,q,r), and (λ,μ,ν) are the direction cosines of $\hat{\rho}$, $\hat{\tau}$, $\hat{\sigma}$.

However, a GSF model takes into account restoring forces due to all components of displacements without making any arbitrary assumptions regarding its scalar force constants, but fails to incorporate either the three-body interactions or the two-body interactions from the triangles formed by ''mixed'' neighbors.[8] The CGW model, on the other hand, includes the latter interactions at the expense of the angular forces perpendicular to the plane of the triangle. Hence, the ionic part of the dynamical matrices of these models are given by

$$[D^i]_{\mathrm{GSF}} = D^c + D^{1s} + D^{2s} \quad (7)$$

and

$$[D^i]_{\mathrm{CGW}} = D^c + D^{2s} + D^{2m} + D^{3s} + D^{3m}, \quad (8)$$

where the additional superscripts s and m denote the corresponding contributions from triangles formed by the ''same'' neighbors and ''mixed'' neighbors. Nevertheless, it is not at all clear whether D^i of the GTF model incorporates the three-body interactions or the ''mixed'' neighbor interactions, especially because the CGW model includes both using the same angular force constants. It is therefore necessary to isolate the three-body and the ''mixed'' neighbor contributions to the elements of the dynamical matrix and to ascertain the characteristic limitations of the GTF model in order to judge its equivalence with the CGW model or any other model. For this purpose, the contributions from various restoring forces to the elements of D^i are evaluated in Sec. III, with the range of ion-ion interactions extended up to third nearest neighbors in the case of bcc and fcc structures. Further the force constants of the GTF model associated with each set of nearest neighbors are represented by a 3×3 matrix. It is desirable to reduce each of these matrices to a diagonal form by making use of the principal axes. The degree of equivalence between the GTF model and the CGW model could be ascertained by comparing the diagonal elements of the former with the corresponding scalar force constants of the latter. The force constant matrices of the GTF model, referred to the crystallographic axes as well as to the principal axes, associated with the first, second, and third nearest neighbors of the bcc structure and the fcc structure are given, respectively, in Appendixes A and B.

TABLE I. CGW angles and the characteristic unit vectors associated with the first, second, and third nearest neighbors of the bcc lattice.

			Unit vectors		
Neighbor	Triangle	Angle	$\hat{\rho}$	$\hat{\sigma}$	$\hat{\tau}$
First	I_1	θ_2	[111]	[$\bar{2}$11]	[0$\bar{1}$1]
	I_2	θ_4	[111]	[2$\bar{1}$1]	[01$\bar{1}$]
Second	I_1	θ_1	[200]	[011]	[011]
	I_3	θ_6	[200]	[010]	[00$\bar{1}$]
	I_2	θ_3	[220]	[00$\bar{1}$]	[1$\bar{1}$0]
Third	I_3	θ_5	[220]	[1$\bar{1}$0]	[001]
	E_1	θ_7	[220]	[11$\bar{2}$]	[1$\bar{1}$1]

III. CALCULATIONS

A. bcc structure

An atom at the origin forms 12 isosceles triangles of S type and 24 isosceles triangles of M type, respectively, with its (i) first neighbors separated by second neighbor distance and first and second neighbors separated by first neighbor distance (I_1), (ii) first neighbors separated by third neighbor distance and first and third neighbors separated by first neighbor distance (I_2) and (iii) second neighbors separated by third neighbor distance and second and third neighbors separated by second neighbor distance (I_3) as well as 24 equilateral triangles with its third neighbors separated by third neighbor distance (E_1) when the short-range ion-ion interactions are restricted to first three nearest neighbors. The isosceles triangles of S type formed by joining the same neighbors are characterized by a nonisosceles angle denoted by an odd subscript, whereas those of M type formed by joining the mixed neighbors are characterized by an isosceles angle denoted by an even subscript, at the origin. The directions of $\hat{\rho}$, $\hat{\sigma}$, $\hat{\tau}$ associated with first, second, and third neighbor distances as well as the angles θ_k they subtend in different triangles, are given in Table I. The elements of the matrix D^i that are split in the manner described in Sec. II, obtained by summing over these four sets of triangles, are given by

$$MD_{xx}^c = (\tfrac{8}{3})\beta_1[1-C_xC_yC_z]+4\beta_2[S_x^2] + 2\beta_3[2-C_{2x}\{C_{2y}+C_{2z}\}], \quad (9)$$

$$MD_{xx}^{1s} = 8(\epsilon_1+\epsilon_2+\epsilon_3+\epsilon_4)[1-C_xC_yC_z] + 8(\epsilon_5+\epsilon_6)[S_y^2+S_z^2] + (\tfrac{16}{3})\epsilon_7[\{2-C_{2x}(C_{2y}+C_{2z})\}+\{1-C_{2y}C_{2z}\}], \quad (10)$$

$$MD_{xx}^{2s} = 8(\gamma_1+\gamma_2+\gamma_3+\gamma_4)[1-C_xC_yC_z] + 8(\gamma_5+\gamma_6)[S_y^2+S_z^2] + (\tfrac{8}{3})\gamma_7[\{2-C_{2x}(C_{2y}+C_{2z})\} + 4\{1-C_{2y}C_{2z}\}], \quad (11)$$

$$MD_{xx}^{3s}=(\tfrac{8}{3})(\gamma_3-\gamma_1)[1-C_xC_yC_z]+4\gamma_6[2S_x^2-S_y^2-S_z^2]-(\tfrac{4}{3})\gamma_7[\{2-C_{2x}(C_{2y}+C_{2z})\}+4\{1-C_{2y}C_{2z}\}], \tag{12}$$

$$MD_{xx}^{1m}=MD_{xx}^{1s}+12\epsilon_2[S_y^2+S_z^2]+3\epsilon_4[2-C_{2x}(C_{2y}+C_{2z})]+8\epsilon_6[1-C_{2y}C_{2z}], \tag{13}$$

$$MD_{xx}^{2m}=MD_{xx}^{2s}+12\gamma_2[S_y^2+S_z^2]+4\gamma_6[2-C_{2x}(C_{2y}+C_{2z})]+6\gamma_4[1-C_{2y}C_{2z}], \tag{14}$$

$$MD_{xx}^{3m}=MD_{xx}^{3s}+(\tfrac{8}{3})\{4\gamma_1[S_x^2]-(\gamma_1+3\gamma_2)[S_y^2+S_z^2]-(2\gamma_3+3\gamma_4+\gamma_7)[1-C_{2y}C_{2z}]\}+(\tfrac{4}{3})(\gamma_3-3\gamma_6+4\gamma_7)[2-C_{2x}(C_{2y}+C_{2z})], \tag{15}$$

$$MD_{xy}^{c}=(\tfrac{8}{3})\beta_1[S_xS_yC_z]+2\beta_3[S_{2x}S_{2y}]. \tag{16}$$

$$MD_{xy}^{1s}=-4(\epsilon_1+\epsilon_2+\epsilon_3+\epsilon_4)[S_xS_yC_z]-(\tfrac{16}{3})\epsilon_7[S_{2x}S_{2y}], \tag{17}$$

$$MD_{xy}^{2s}=-4(\gamma_1+\gamma_2+\gamma_3+\gamma_4)[S_xS_yC_z]-(\tfrac{8}{3})\gamma_7[S_{2x}S_{2y}], \tag{18}$$

$$MD_{xy}^{3s}=(\tfrac{4}{3})\{(\gamma_1-\gamma_3)+3(2\gamma_2+\gamma_4)\}[S_xS_yC_z]+(\tfrac{4}{3})\gamma_7[S_{2x}S_{2y}], \tag{19}$$

$$MD_{xy}^{1m}=MD_{xy}^{1s}-3\epsilon_4[S_{2x}S_{2y}], \tag{20}$$

$$MD_{xy}^{2m}=MD_{xy}^{2s}-4\gamma_6[S_{2x}S_{2y}], \tag{21}$$

and

$$MD_{xy}^{3m}=MD_{xy}^{3s}+(\tfrac{4}{3})\{\gamma_3+3(\gamma_5+\gamma_6)+5\gamma_7\}[S_{2x}S_{2y}], \tag{22}$$

where $S_x=\sin(q_xa)$, $S_{2x}=\sin(2q_xa)$, $C_x=\cos(q_xa)$ and $C_{2x}=\cos(2q_xa)$ etc., $2a$ being the lattice parameter and M is the mass of the atom. The force constants, ϵ_k and γ_k associated with the angle θ_k have been divided by a normalizing factor, square of the isosceles side of the appropriate triangle, in order to make them dimensionally equal to the central force constants β_n associated with the nth nearest-neighbor distance. Further, the diagonal and off-diagonal elements of D^i of the GSF model could be written, using Eq. (7), as

$$MD_{xx}^{i}=8\{(\tfrac{1}{3})\beta_1+(\epsilon_1+\epsilon_2+\epsilon_3+\epsilon_4)+(\gamma_1+\gamma_2+\gamma_3+\gamma_4)\}\times[1-C_xC_yC_z]+4\beta_2[S_x^2]+8\{(\epsilon_5+\epsilon_6)+(\gamma_5+\gamma_6)\}[S_y^2+S_z^2]+(\tfrac{16}{3})(\epsilon_7+2\gamma_7)[1-C_{2y}C_{2z}]+(\tfrac{2}{3})\{3\beta_3+8\epsilon_7+4\gamma_7\}[2-C_{2x}(C_{2y}+C_{2z})] \tag{23}$$

and

$$MD_{xy}^{i}=4\{(\tfrac{2}{3})\beta_1-(\epsilon_1+\epsilon_2+\epsilon_3+\epsilon_4)-(\gamma_1+\gamma_2+\gamma_3+\gamma_4)\}\times[S_xS_yC_z]+(\tfrac{2}{3})\{3\beta_3-8\epsilon_7-4\gamma_7\}[S_{2x}S_{2y}]. \tag{24}$$

Corresponding elements of the CGW model could be written, using Eq. (8), as

$$MD_{xx}^{i}=(\tfrac{8}{3})\{\beta_1+4(\gamma_1+2\gamma_3)+6(\gamma_2+\gamma_4)\}[1-C_xC_yC_z]+4\{\beta_2+(\tfrac{8}{3})\gamma_1+4\gamma_6\}[S_x^2]+4\{-(\tfrac{2}{3})\gamma_1+\gamma_2+4\gamma_5+2\gamma_6\}[S_y^2+S_z^2]+2\{\beta_3+(\tfrac{2}{3})\gamma_3+4\gamma_7\}[2-C_{2x}(C_{2y}+C_{2z})]+4\{-(\tfrac{4}{3})\gamma_3-(\tfrac{1}{2})\gamma_4+2\gamma_7\}[1-C_{2y}C_{2z}] \tag{25}$$

and

$$MD_{xy}^{i}=(\tfrac{8}{3})\{\beta_1-2\gamma_1+3\gamma_2-4\gamma_3\}[S_xS_yC_z]+2\{\beta_3+(\tfrac{2}{3})\gamma_3+2\gamma_5+2\gamma_7\}[S_{2x}S_{2y}]. \tag{26}$$

When the range of ion-ion interactions is extended up to third nearest neighbors, the diagonal and off-diagonal elements of the matrix D^i of the GTF model are given by[20]

$$MD_{xx}^{i}=8\sigma_1[1-C_xC_yC_z]+4\sigma_2[S_x^2]+4\lambda_2[S_y^2+S_z^2]+4\lambda_3[1-C_{2y}C_{2z}]+4\sigma_3[2-C_{2x}(C_{2y}+C_{2z})] \tag{27}$$

and

$$MD_{xy}^{i}=8\nu_1[S_xS_yC_z]+4\nu_3[S_{2x}S_{2y}], \tag{28}$$

where σ_n, λ_n, and ν_n are the nth neighbor tensor force constants.

It is obvious from these expressions that the CGW model for bcc structures is not equivalent to the GSF model except for the contributions from central forces. Thus, the corresponding matrix elements of all these models contain the same number of terms that have nothing in common.

B. fcc structure

An atom at the origin forms 24 equilateral triangles each with its (i) first neighbors separated by first neighbor distance (E_1) and (ii) third neighbors separated by third neighbor distance (E_2), 12 isosceles triangles of S type and 24 isosceles triangles of M type, respectively, with its (i) first neighbors separated by second neighbor distance and first and second neighbors separated by first neighbor distance (I_1), (ii) first neighbors separated by third neighbor distance and first and third neighbors separated by first neighbor distance (I_2), (iii) third neighbors separated by first neighbor distance and third and first neighbors separated by third neighbor distance (I_3) and (iv) third neighbors separated by second neighbor distance and third and second neighbors separated by third neighbor distance (I_4) as well as 72 nonisosceles triangles with its first, second and third neighbor distances (T_1) when the short-range ion-ion interactions are restricted to first three nearest neighbors. An isosceles angle at the origin characterizes the M type triangles while a nonisosceles angle charac-

TABLE II. CGW angles and the characteristic unit vectors associated with the first, second, and third nearest neighbors of the fcc lattice.

Neighbor	Triangle	Angle	Unit vectors $\hat{\rho}$	$\hat{\sigma}$	$\hat{\tau}$
	E_1	θ_1	[110]	$[1\bar{1}2]$	$[1\bar{1}\bar{1}]$
	I_1	θ_3	[110]	$[1\bar{1}0]$	[001]
First	I_2	θ_5	[110]	$[11\bar{2}]$	$[\bar{1}\bar{1}1]$
	T_1	θ_8	[110]	$[00\bar{1}]$	$[1\bar{1}0]$
	I_3	θ_9	[110]	[332]	[113]
	I_1	θ_2	[200]	[010]	$[00\bar{1}]$
Second	T_1	θ_7	[200]	[011]	$[0\bar{1}\bar{1}]$
	I_4	θ_{11}	[200]	$[02\bar{1}]$	$[01\bar{2}]$
	I_2	θ_4	[211]	[011]	$[1\bar{1}\bar{1}]$
	T_1	θ_6	[211]	$[1\bar{1}\bar{1}]$	$[01\bar{1}]$
Third	I_3	θ_{10}	[211]	$[4\bar{7}\bar{1}]$	$[11\bar{3}]$
	I_4	θ_{12}	[211]	$[2\bar{5}\bar{1}]$	$[10\bar{2}]$
	E_2	θ_{13}	[211]	$[01\bar{1}]$	$[1\bar{1}\bar{1}]$

terizes the S type triangles. The directions of $\hat{\rho},\hat{\sigma},\hat{\tau}$ associated with first, second, and third neighbor distances as well as the angles θ_k they subtend in different triangles are given in Table II. The elements of the matrix D^i that are split in the manner described in Sec. II, obtained by summing over these seven sets of triangles, are given by

$$MD^{c}_{xx}=2\beta_1[2-C_x(C_y+C_z)]+4\beta_2[S_x^2]+(\tfrac{4}{3})\beta_3[6-C_x(C_{2y}C_z+C_yC_{2z})-4C_{2x}C_yC_z], \tag{29}$$

$$MD^{1s}_{xx}=4(\{(\tfrac{4}{3})(\epsilon_1+\epsilon_4+\epsilon_5)+3(\epsilon_6+\epsilon_7)\}[2-C_x(C_y+C_z)]+3(\epsilon_6+\epsilon_8)[S_y^2+S_z^2]+\{(\tfrac{4}{3})(\epsilon_1+\epsilon_4+\epsilon_5)+2(\epsilon_2+\epsilon_3)\}[1-C_yC_z]+4\{[(\epsilon_9+\epsilon_{10})/11]+[(\epsilon_{11}+\epsilon_{12})/5]+[(\epsilon_{13})/3]\}[1-C_{2x}C_yC_z]+\{(\epsilon_7+\epsilon_8)+4[(\tfrac{5}{11})(\epsilon_9+\epsilon_{10})+(\tfrac{2}{5})(\epsilon_{11}+\epsilon_{12})+(\tfrac{1}{3})\epsilon_{13}]\}[2-C_x(C_{2y}C_z+C_yC_{2z})]), \tag{30}$$

$$MD^{2s}_{xx}=(\tfrac{4}{3})(\{2(\gamma_1+\gamma_4+\gamma_5)+3(\gamma_2+\gamma_3)\}\times[2-C_x(C_y+C_z)]+9(\gamma_6+\gamma_8)[S_y^2+S_z^2]+2[\{4(\gamma_1+\gamma_4+\gamma_5)+9(\gamma_6+\gamma_7)\}[1-C_yC_z]+\{(\gamma_7+\gamma_8)+(\tfrac{16}{11})(\gamma_9+\gamma_{10})+(\tfrac{4}{5})(\gamma_{11}+\gamma_{12})\}[1-C_{2x}C_yC_z]+\{(\gamma_7+\gamma_8)+(\tfrac{25}{11})\times(\gamma_9+\gamma_{10})+(\tfrac{13}{5})(\gamma_{11}+\gamma_{12})+3\gamma_{13}\}\times[2-C_x(C_{2y}C_z+C_yC_{2z})]]), \tag{31}$$

$$MD^{3s}_{xx}=(\tfrac{4}{3})[\{-\gamma_1+\gamma_4+\gamma_5+3\gamma_8\}[2-C_x(C_y+C_z)]+6(2\gamma_7[S_x^2]-\gamma_8[S_y^2+S_z^2])+2(\{-2\gamma_1+2\gamma_4-\gamma_5-3\gamma_7\}[1-C_yC_z]+\{-3\gamma_7-(\tfrac{28}{11})\gamma_9+9\gamma_{10}+(\tfrac{4}{5})\gamma_{11}\}[1-C_{2x}C_yC_z])-3\{\gamma_8+(\tfrac{9}{11})\gamma_9+3\gamma_{10}+(\tfrac{8}{5})\gamma_{11}+\gamma_{13}\}[2-C_x(C_{2y}C_z+C_yC_{2z})]], \tag{32}$$

$$MD^{1m}_{xx}=MD^{1s}_{xx}+(\tfrac{96}{11})\epsilon_{10}[11-C_x(C_y+C_z)-9C_yC_z]+16(\epsilon_3+3\epsilon_{12})[S_y^2+S_z^2]+(\tfrac{32}{9})\epsilon_5[\{1-C_{2x}C_yC_z\}+\{2-C_x(C_{2y}C_z+C_yC_{2z})\}], \tag{33}$$

$$MD^{2m}_{xx}=MD^{2s}_{xx}+(\tfrac{48}{11})\gamma_{10}[9\{2-C_x(C_y+C_z)\}+4\{1-C_yC_z\}]+8(\gamma_3+6\gamma_{12})[S_y^2+S_z^2]+(\tfrac{16}{3})\gamma_5[2-C_x(C_{2y}C_z+C_yC_{2z})], \tag{34}$$

$$MD^{3m}_{xx}=MD^{3s}_{xx}+(\tfrac{8}{3})[\{2\gamma_1+(\tfrac{1}{11})(28\gamma_9-27\gamma_{10})\}\times[2-C_x(C_y+C_z)]-\{\gamma_1+(\tfrac{1}{11})(\gamma_9+12\gamma_{10})\}\times[1-C_yC_z]+\{3\gamma_2+10\gamma_{11}\}[S_x^2]-\{(\tfrac{3}{2})\gamma_2+3\gamma_3+\gamma_{11}+6\gamma_{12}\}[S_y^2+S_z^2]+\{\gamma_4+3\gamma_{13}\}\times[1-C_{2x}C_yC_z]-\{2\gamma_4+3\gamma_5\}\times[2-C_x(C_{2y}C_z+C_yC_{2z})]], \tag{35}$$

$$MD^{c}_{xy}=2\beta_1[S_xS_y]+(\tfrac{4}{3})\beta_3[2C_z(S_{2x}S_y+S_xS_{2y}) + S_xS_yC_{2z}], \tag{36}$$

$$\begin{aligned}MD^{1s}_{xy}=&-4\{(\tfrac{4}{3})(\epsilon_1+\epsilon_4+\epsilon_5)+3(\epsilon_6+\epsilon_7)\}[S_xS_y]\\&-4\{(\epsilon_7+\epsilon_8)+(\tfrac{12}{11})(\epsilon_9+\epsilon_{10})-(\tfrac{4}{3})\epsilon_{13}\}[S_xS_yC_{2z}]\\&-16\{[(\epsilon_9+\epsilon_{10})/11]+[(\epsilon_{11}+\epsilon_{12})/5]+[(\epsilon_{13})/3]\}\\&\times[C_z(S_{2x}S_y+S_xS_{2y})],\end{aligned} \tag{37}$$

$$\begin{aligned}MD^{2s}_{xy}=&-(\tfrac{4}{3})\{2(\gamma_1+\gamma_4+\gamma_5)+3(\gamma_2+\gamma_3)\}[S_xS_y]\\&+(\tfrac{8}{3})\{(\gamma_7+\gamma_8)+(\tfrac{7}{11})(\gamma_9+\gamma_{10})\\&-(\gamma_{11}+\gamma_{12}+3\gamma_{13})\}[S_xS_yC_{2z}]-(\tfrac{8}{3})\{(\gamma_7+\gamma_8)\\&+(\tfrac{16}{11})(\gamma_9+\gamma_{10})+(\tfrac{4}{5})(\gamma_{11}+\gamma_{12})\}\\&\times[C_z(S_{2x}S_y+S_xS_{2y})],\end{aligned} \tag{38}$$

$$\begin{aligned}MD^{3s}_{xy}=&(4/3)\{(\gamma_1-\gamma_4+2\gamma_5)+3(\gamma_3+\gamma_8)\}[S_xS_y]\\&-4\{\gamma_8-(\tfrac{1}{11})\gamma_9+2\gamma_{10}-2\gamma_{12}-\gamma_{13}\}[S_xS_yC_{2z}]\\&+4\{(\tfrac{56}{33})\gamma_9+5\gamma_{10}-(\tfrac{8}{15})\gamma_{11}\}[S_{2x}S_yC_z]\\&+4\{3\gamma_6+2\gamma_7+\gamma_8+(\tfrac{4}{11})\gamma_9-3\gamma_{10}\\&+(\tfrac{4}{5})\gamma_{11}+4\gamma_{12}\}[S_xS_{2y}C_z],\end{aligned} \tag{39}$$

$$MD^{1m}_{xy}=MD^{1s}_{xy}-(\tfrac{96}{11})\epsilon_{10}[S_xS_y]+(\tfrac{32}{9})\epsilon_5[S_xS_yC_{2z} - C_z(S_{2x}S_y+S_xS_{2y})], \tag{40}$$

$$MD^{2m}_{xy}=MD^{2s}_{xy}-(\tfrac{432}{11})\gamma_{10}[S_xS_y]-(\tfrac{16}{3})\gamma_5[S_xS_yC_{2z}] \tag{41}$$

and

$$\begin{aligned}MD^{3m}_{xy}=&MD^{3s}_{xy}+(\tfrac{4}{33})\{5(11\gamma_1+13\gamma_9)+54\gamma_{10}\}[S_xS_y]\\&+4\{(\tfrac{5}{3})\gamma_4+2\gamma_5+\gamma_{13}\}[S_xS_yC_{2z}]\\&+(\tfrac{4}{3})\{\gamma_4+3\gamma_{13}\}[(S_{2x}S_y+S_xS_{2y})C_z]\\&+4\{3\gamma_6+2\gamma_7+\gamma_8-(\tfrac{4}{3})(\gamma_9-\gamma_{11})\\&-4(2\gamma_{10}-\gamma_{12})\}[(S_{2x}S_y-S_xS_{2y})C_z],\end{aligned} \tag{42}$$

where $S_x=\sin(q_xa)$, $S_{2x}=\sin(2q_xa)$, $C_x=\cos(q_xa)$ and $C_{2x}=\cos(2q_xa)$ etc., $2a$ being the lattice parameter and M is the mass of the atom. The force constants ϵ_k and γ_k associated with the angle θ_k have been divided by a normalizing factor, square of the isosceles side of the appropriate triangle, in order to make them dimensionally equal to the central force constants β_n associated with the nth nearest-neighbor distance. In addition, using Eq. (7) the diagonal and off-diagonal elements of D^i of the GSF model could be written as

$$\begin{aligned}MD^{i}_{xx}=&\{2\beta_1+(\tfrac{8}{3})[2(\epsilon_1+\epsilon_4+\epsilon_5)+(\gamma_1+\gamma_4+\gamma_5)]+12(\epsilon_6+\epsilon_7)+4(\gamma_2+\gamma_3)\}[2-C_x(C_y+C_z)]+8\{(\tfrac{2}{3})[(\epsilon_1+\epsilon_4+\epsilon_5)\\&+2(\gamma_1+\gamma_4+\gamma_5)]+(\epsilon_2+\epsilon_3)+3(\gamma_6+\gamma_7)\}[1-C_yC_z]+4\beta_2[S_x^2]+12\{(\epsilon_6+\epsilon_8)+(\gamma_6+\gamma_8)\}[S_y^2+S_z^2]\\&+(\tfrac{16}{3})\{\beta_3+(\tfrac{3}{11})(\epsilon_9+\epsilon_{10})+(\tfrac{3}{5})(\epsilon_{11}+\epsilon_{12})+\epsilon_{13}+(\tfrac{1}{2})(\gamma_7+\gamma_8)+(\tfrac{8}{11})(\gamma_9+\gamma_{10})+(\tfrac{2}{5})(\gamma_{11}+\gamma_{12})\}[1-C_{2x}C_yC_z]\\&+(\tfrac{8}{3})\{(\tfrac{1}{2})\beta_3+(\tfrac{3}{2})(\epsilon_7+\epsilon_8)+(\tfrac{30}{11})(\epsilon_9+\epsilon_{10})+(\tfrac{12}{5})(\epsilon_{11}+\epsilon_{12})+2\epsilon_{13}+(\gamma_7+\gamma_8)+(\tfrac{25}{11})(\gamma_9+\gamma_{10})\\&+(\tfrac{13}{5})(\gamma_{11}+\gamma_{12})+3\gamma_{13}\}[2-C_x(C_{2y}C_z+C_yC_{2z})]\end{aligned} \tag{43}$$

and

$$\begin{aligned}MD^{i}_{xy}=&\{2\beta_1-(\tfrac{8}{3})[2(\epsilon_1+\epsilon_4+\epsilon_5)+(\gamma_1+\gamma_4+\gamma_5)]-4[(\gamma_2+\gamma_3)+3(\epsilon_6+\epsilon_7)]\}[S_xS_y]+(\tfrac{8}{3})(\{(\tfrac{1}{2})[\beta_3-3(\epsilon_7+\epsilon_8)]\\&-(\tfrac{18}{11})(\epsilon_9+\epsilon_{10})+2\epsilon_{13}+(\gamma_7+\gamma_8)+(\tfrac{7}{11})(\gamma_9+\gamma_{10})-(\gamma_{11}+\gamma_{12})-3\gamma_{13}\}[S_xS_yC_{2z}]+\{\beta_3-(\tfrac{6}{11})(\epsilon_9+\epsilon_{10})\\&-(\tfrac{6}{5})(\epsilon_{11}+\epsilon_{12})-2\epsilon_{13}-(\gamma_7+\gamma_8)-(\tfrac{16}{11})(\gamma_9+\gamma_{10})-(\tfrac{4}{5})(\gamma_{11}+\gamma_{12})\}[(S_{2x}S_y+S_xS_{2y})C_z]).\end{aligned} \tag{44}$$

Making use of Eq. (8), corresponding elements of the CGW model could be written as

$$\begin{aligned}MD^{i}_{xx}=&\{2\beta_1+8[(\gamma_1+\gamma_2+\gamma_3+\gamma_4+\gamma_5+\gamma_8)+(\tfrac{28}{33})\gamma_9+(\tfrac{45}{11})\gamma_{10}]\}[2-C_x(C_y+C_z]+8\{\gamma_1+4\gamma_4+2\gamma_5+6\gamma_6+4\gamma_7-(\tfrac{1}{11})\\&\times[(\tfrac{1}{3})\gamma_9-20\gamma_{10}]\}[1-C_yC_z]+4\{\beta_2+2\gamma_2+8\gamma_7+(\tfrac{20}{3})\gamma_{11}\}[S_x^2]+4\{-\gamma_2+6\gamma_6+2\gamma_8-(\tfrac{2}{3})\gamma_{11}+8\gamma_{12}\}[S_y^2+S_z^2]\\&+(\tfrac{8}{3})(\{2\beta_3+\gamma_4-2(2\gamma_7-\gamma_8)-(\tfrac{2}{11})(12\gamma_9-115\gamma_{10})+(\tfrac{8}{5})(2\gamma_{11}+\gamma_{12})+3\gamma_{13}\}[1-C_{2x}C_yC_z]\\&+\{(\tfrac{1}{2})\beta_3-2\gamma_4-\gamma_5+2\gamma_7-\gamma_8+(\tfrac{1}{11})(23\gamma_9-49\gamma_{10})+(\tfrac{2}{5})(\gamma_{11}+13\gamma_{12})+3\gamma_{13}\}[2-C_x(C_{2y}C_z+C_yC_{2z})])\end{aligned} \tag{45}$$

and

$$MD^{i}_{xy}=2\{\beta_1+2\gamma_1-4(\gamma_2+\gamma_4-\gamma_8)+(\tfrac{10}{11})[(\tfrac{13}{3})\gamma_9-18\gamma_{10}]\}[S_xS_y]+(\tfrac{4}{3})(\{\beta_3+5\gamma_4+2\gamma_5+2(2\gamma_7-\gamma_8)+(\tfrac{2}{11})(17\gamma_9-52\gamma_{10})-4\gamma_{11}+8\gamma_{12}-3\gamma_{13}\}\{S_xS_yC_{2z}\}+\{2\beta_3+\gamma_4+9\gamma_6+(2\gamma_7-\gamma_8)+(\tfrac{2}{11})(2\gamma_9+\gamma_{10})-(\tfrac{4}{5})(3\gamma_{11}-11\gamma_{12})+3\gamma_{13}\}[(S_{2x}S_y+S_xS_{2y})C_z]). \quad (46)$$

On the other hand, the diagonal and off-diagonal elements of the matrix D^i of the GTF model that incorporates the short-range interactions from the first three nearest neighbors, are given by[21]

$$MD^{i}_{xx}=4\sigma_1[2-C_x(C_y+C_z)]+4\lambda_1[1-C_yC_z]+4\sigma_2[S_x^2]+4\lambda_2[S_y^2+S_z^2]+8\sigma_3[1-C_{2x}C_yC_z]+8\lambda_3[2-C_x(C_{2y}C_z+C_yC_{2z})] \quad (47)$$

and

$$MD^{i}_{xy}=4\nu_1[S_xS_y]+8\nu_3[(S_{2x}S_y+S_xS_{2y})C_z]+8\mu_3[S_xS_yC_{2z}], \quad (48)$$

where σ_n, λ_n, ν_n, and μ_n are the nth neighbor tensor force constants.

These expressions invariably make it clear that the CGW model for fcc structures is not equivalent to the GSF model, except for the contributions from central forces. The only common feature among these three models that differ significantly is that the corresponding matrix elements have the same number of terms.

IV. DISCUSSION

It is obvious from the present analysis that the diagonal and off-diagonal matrix elements of the CGW model as well as those of the GSF model are expressed as a sum of five terms and two terms, respectively, in the case of the bcc lattice and as a sum of six terms and three terms, respectively, in the case of the fcc lattice. Each of these wave vector-dependent terms includes an algebraic sum of central and angular force constants. Corresponding matrix elements of the GTF model for the bcc lattice[20] and the fcc lattice[21] are obtained when either sum of scalar force constants is replaced by an appropriate second rank tensor force constant. In spite of the basic differences in their assumptions regarding the nature of ion-ion interactions, all these models give identical lattice dynamical results by simply adjusting the numerical values of their force constants. However, it is wrong to judge the equivalence between two models using this criterion. The apparent equivalence, based on the number of terms or independent force constants associated with their matrix elements, is therefore devoid of any significance.

The present analysis reveals that there is no means of expressing the three-body and mixed neighbor interactions in terms of two-body interactions, even in the case of first or second nearest neighbors of a bcc lattice and second nearest neighbors of a fcc lattice. Further, it is not at all essential to introduce additional force constants in order to incorporate the contributions from the former into the matrix elements of either lattice. In this context, use of extra force constants by Upadhyaya *et al.*[16] to express the three-body interactions is wrong and inconsistent with their own claim that these interactions can be expressed in terms of two-body interactions. The identical lattice dynamical results, obtained in the case of the bcc structure,[12,22] are cited in support of this spurious claim. However the procedure adopted by these authors is not capable of identifying the three-body contributions and the consequent superficial bifurcation of ion-ion interactions does not serve any purpose. Inclusion of terms with ''three-body'' force constants is an arbitrary means employed to match the dynamical matrix elements of the CGW model with those of the GTF model, ignoring the intrinsic differences between them. It was established in I that the corresponding (two-body) central force constants of the DAF and CGW models become unequal while assorted combination of central and angular force constants of the former become equal to those of the latter as a consequence of artificially matching the matrix elements of these models. The erroneous interpretation of the readjustments in the numerical values of the force constants together with the absurd presumption that the entire three-body contributions in the case of the bcc and fcc structures are incorporated using only one and three extra force constants, respectively, cast a serious doubt on the claims regarding the equivalence between CGW and GTF models.[14–16]

It may be recalled in this context that the nature of the GTF constants is quite different from that of central and angular force constants. The second derivative of the potential energy of a crystal with respect to atomic displacements is, in general, a tensor of second rank which can be represented by a 3×3 matrix. Most lattice dynamical models make use of some arbitrary assumptions regarding the nature of short-range ion-ion interactions whereas the GTF model exploits the symmetry elements associated with the crystal structure to reduce the number of independent parameters associated with each set of nearest neighbors. As a consequence, the central and angular force constants of the DAF and CGW models as well as the radial and tangential force constants of the AS and MAS models become scalar quantities while the GTF constants retain the characteristics of a second rank tensor. The matrices representing these tensors associated with the first, second, and third nearest neighbors of the bcc structure and the fcc structure are given, respectively, in Appendixes A and B. However, it is essential to reduce these matrices to their diagonal form, by means of appropriate unitary transformations, in order to express the GTF constants in terms of the central and angular force constants. The eigenvalues and the eigenvectors of the diagonal matrices corresponding to different sets of neighbors, determined by exploiting their transformational properties, are also included in Appendixes A and B. It is obvious from these results that one of these eigenvectors, X_n, which is oriented along the line joining the reference atom with its nth nearest neighbor, is identical with the corresponding unit vector $\hat{\rho}_k$ given in Tables I or II, in each and every case. As a consequence, the remaining orthogonal eigenvectors, Y_n and Z_n, are confined to a plane that passes through the unit

vectors $\hat{\sigma}_k$ and $\hat{\tau}_k$. Besides, a coordinate axes transformation that rotates $\hat{\sigma}_k$ and $\hat{\tau}_k$ through an angle α_k about $\hat{\rho}_k$ orients these vectors along Y_n and Z_n, respectively.[23] The σ and τ components of atomic displacements, which are, respectively, parallel and perpendicular to the plane of the CGW triangle, are resolved along the eigenvectors Y_n and Z_n. Thus the central and angular force constants that are equivalent to these eigenvalues of diagonal matrix are determined, in all cases, by invoking the invariance of the former with respect to coordinate axes rotations. The physically meaningful relations between the GTF constants and the scalar force constants, deduced by adopting this procedure in the case of bcc and fcc structures, are given in Appendix C.

It should therefore be clear from these relations that the elements of the dynamical matrix, D^i of the GTF model are transformed into those of the GSF model in the case of bcc and fcc structures, so long as the latter makes no other assumptions regarding the nature of ion-ion interactions. Notwithstanding the invariance of individual scalar force constants with respect to coordinate axes transformations, the assorted sums of central and angular force constants of the GSF model transform as the elements of a second rank tensor whereas those of the CGW model or any other sums of scalar force constants do not. Hence the present investigations reveal that the GTF model for cubic structures is equivalent to the corresponding GSF model in all respects. Further, the irreconcilable differences between Eqs. (7) and (8) make it abundantly clear that there is hardly any equivalence between the GTF model and the CGW model. Corresponding expressions for GTF constants, obtained by matching the matrix elements of the former with those of the latter,[14,16] do not comply with the transformation properties of a second rank tensor. Thus it is wrong to equate the GTF constants to the algebraic sums of central and angular force constants of the CGW model or to ignore the basic differences between these two models. Under these circumstances, the claim of Moore and Upadhyaya[14] and Upadhyaya *et al.*[16] that the GTF model is identical to the CGW model or their assertion that the GTF model incorporates three-body interactions, based on the investigations that are incapable of separating three-body interactions from two-body interactions and mixed neighbor interactions from same neighbor interactions, is of no consequence. On the contrary, the elastic inconsistency of the GTF model in the case of noncubic structures[8] unequivocally establishes that this model does not incorporate any contributions from the three-body interactions or mixed neighbor interactions and hence it is not invariant with respect to rigid body rotations. Such a model cannot be equivalent to the CGW model, even though the cubic symmetry restores the elastic consistency to all lattice dynamical models. It should therefore follow from this discussion that the GTF model is equivalent to the GSF model and the DAF, AS, MAS, CPP, and other models that do not incorporate three-body or mixed neighbor interactions, are approximate forms of the GSF model. The relations between their force constants acquire their physical significance from the fact that different two-body forces associated with these models are inter-related.

V. CONCLUSIONS

It is obvious from this analysis that neither the GTF model nor the GSF model is equivalent to the CGW model, so long as the two-body contributions perpendicular to the plane of the CGW triangle are not equal to the three-body and mixed neighbor contributions confined to the plane. The assorted sums of central and angular force constants of the GSF model for bcc and fcc structures transform as the elements of a second rank tensor whereas those of the CGW model do not, and hence the former is equivalent to the GTF model. All the previous claims regarding the equivalence between the GTF and CGW models for cubic structures as well as the presumption that the former incorporates the three-body interactions are inconsistent with the transformation properties of tensor force constants and therefore have no physical significance. Nevertheless, all models give identical lattice dynamical results by readjusting the numerical values of their force constants.

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APPENDIX A: FORCE CONSTANT MATRICES AND EIGEN VECTORS OF THE BCC LATTICE

Neighbor	Representative atom	Force constant matrix: Crystallographic axes (x,y,z)	Force constant matrix: Principal axes $(X<Y<Z)$	Eigenvectors $[X]$, $[Y]$, $[Z]$
First	(a,a,a)	$\begin{pmatrix} \sigma_1 & \nu_1 & \nu_1 \\ \nu_1 & \sigma_1 & \nu_1 \\ \nu_1 & \nu_1 & \sigma_1 \end{pmatrix}$	$\begin{pmatrix} (\sigma_1+2\nu_1) & 0 & 0 \\ 0 & (\sigma_1-\nu_1) & 0 \\ 0 & 0 & (\sigma_1-\nu_1) \end{pmatrix}$	$[111]$ $[\bar{2}11]$ $[0\bar{1}1]$
Second	$(2a,0,0,)$	$\begin{pmatrix} \sigma_2 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_2 \end{pmatrix}$	$\begin{pmatrix} \sigma_2 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_2 \end{pmatrix}$	$[200]$ $[010]$ $[001]$
Third	$(2a,2a,0)$	$\begin{pmatrix} \sigma_3 & \nu_3 & 0 \\ \nu_3 & \sigma_3 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}$	$\begin{pmatrix} (\sigma_3+\nu_3) & 0 & 0 \\ 0 & (\sigma_3-\nu_3) & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}$	$[220]$ $[\bar{1}10]$ $[001]$

APPENDIX B: FORCE CONSTANT MATRICES AND EIGENVECTORS OF THE FCC LATTICE

Neighbor	Representative atom	Force constant matrix: Crystallographic axes (x,y,z)	Force constant matrix: Principal axes $(X<Y<Z)$	Eigenvectors $[X]$, $[Y]$, $[Z]$
First	$(a,a,0)$	$\begin{pmatrix}\sigma_1 & \nu_1 & 0\\ \nu_1 & \sigma_1 & 0\\ 0 & 0 & \lambda_1\end{pmatrix}$	$\begin{pmatrix}(\sigma_1+\nu_1) & 0 & 0\\ 0 & (\sigma_1-\nu_1) & 0\\ 0 & 0 & \lambda_1\end{pmatrix}$	$[110]$ $[\bar{1}10]$ $[001]$
Second	$(2a,0,0)$	$\begin{pmatrix}\sigma_2 & 0 & 0\\ 0 & \lambda_2 & 0\\ 0 & 0 & \lambda_2\end{pmatrix}$	$\begin{pmatrix}\sigma_2 & 0 & 0\\ 0 & \lambda_2 & 0\\ 0 & 0 & \lambda_2\end{pmatrix}$	$[200]$ $[010]$ $[001]$
Third	$(2a,a,a)$	$\begin{pmatrix}\sigma_3 & \nu_3 & \nu_3\\ \nu_3 & \lambda_3 & \mu_3\\ \nu_3 & \mu_3 & \lambda_3\end{pmatrix}$	$\begin{pmatrix}(\sigma_3+\nu_3) & 0 & 0\\ 0 & (\lambda_3+\mu_3-\nu_3) & 0\\ 0 & 0 & (\lambda_3-\mu_3)\end{pmatrix}$	$[211]$ $[\bar{1}11]$ $[0\bar{1}1]$

APPENDIX C: EQUIVALENCE BETWEEN THE GTF CONSTANTS AND THE SCALAR FORCE CONSTANTS

(a) bcc structure:

$$\sigma_1=(\tfrac{1}{3})\beta_1+[\epsilon_1+\epsilon_2+\epsilon_3+\epsilon_4]+[\gamma_1+\gamma_2+\gamma_3+\gamma_4], \tag{C1}$$

$$\nu_1=(\tfrac{1}{3})\beta_1-(\tfrac{1}{2})[\epsilon_1+\epsilon_2+\epsilon_3+\epsilon_4]-(\tfrac{1}{2})[\gamma_1+\gamma_2+\gamma_3+\gamma_4], \tag{C2}$$

$$\sigma_2=\beta_2, \tag{C3}$$

$$\lambda_2=2[\epsilon_5+\epsilon_6]+2[\gamma_5+\gamma_6], \tag{C4}$$

$$\sigma_3=(\tfrac{1}{2})\beta_3+(\tfrac{2}{3})[2\epsilon_7+\gamma_7], \tag{C5}$$

$$\nu_3=(\tfrac{1}{2})\beta_3-(\tfrac{2}{3})[2\epsilon_7+\gamma_7] \tag{C6}$$

and

$$\lambda_3=(\tfrac{4}{3})[\epsilon_7+2\gamma_7]. \tag{C7}$$

(b) fcc structure:

$$\sigma_1=(\tfrac{1}{2})\beta_1+(\tfrac{2}{3})\{2[\epsilon_1+\epsilon_4+\epsilon_5]+[\gamma_1+\gamma_4+\gamma_5]\}+[\gamma_2+\gamma_3]+3[\epsilon_6+\epsilon_7], \tag{C8}$$

$$\nu_1=(\tfrac{1}{2})\beta_1-(\tfrac{2}{3})\{2[\epsilon_1+\epsilon_4+\epsilon_5]+[\gamma_1+\gamma_4+\gamma_5]\}-[\gamma_2+\gamma_3]-3[\epsilon_6+\epsilon_7], \tag{C9}$$

$$\lambda_1=(\tfrac{4}{3})\{[\epsilon_1+\epsilon_4+\epsilon_5]+2[\gamma_1+\gamma_4+\gamma_5]\}+2[\epsilon_2+\epsilon_3]+6[\gamma_6+\gamma_7], \tag{C10}$$

$$\sigma_2=\beta_2, \tag{C11}$$

$$\lambda_2=3[\epsilon_6+\epsilon_8]+3[\gamma_6+\gamma_8], \tag{C12}$$

$$\sigma_3=(\tfrac{1}{3})\{2\beta_3+(\tfrac{6}{11})[\epsilon_9+\epsilon_{10}]+(\tfrac{6}{5})[\epsilon_{11}+\epsilon_{12}]+2\epsilon_{13}+[\gamma_7+\gamma_8]+(\tfrac{16}{11})[\gamma_9+\gamma_{10}]+(\tfrac{4}{5})[\gamma_{11}+\gamma_{12}]\}, \tag{C13}$$

$$\nu_3=(\tfrac{1}{3})\{\beta_3-(\tfrac{6}{11})[\epsilon_9+\epsilon_{10}]-(\tfrac{6}{5})[\epsilon_{11}+\epsilon_{12}]-2\epsilon_{13}-[\gamma_7+\gamma_8]-(\tfrac{16}{11})[\gamma_9+\gamma_{10}]-(\tfrac{4}{5})[\gamma_{11}+\gamma_{12}]\}, \tag{C14}$$

$$\lambda_3=(\tfrac{1}{6})\{\beta_3+3([\epsilon_7+\epsilon_8]+(\tfrac{20}{11})[\epsilon_9+\epsilon_{10}]+(\tfrac{8}{5})[\epsilon_{11}+\epsilon_{12}])+2(2\epsilon_{13}+[\gamma_7+\gamma_8]+(\tfrac{25}{11})[\gamma_9+\gamma_{10}]+(\tfrac{13}{5})[\gamma_{11}+\gamma_{12}])\}+\gamma_{13} \tag{C15}$$

and

$$\mu_3=(\tfrac{1}{6})\{\beta_3-3[\epsilon_7+\epsilon_8]\}-(\tfrac{6}{11})[\epsilon_9+\epsilon_{10}]+(\tfrac{1}{3})\{2\epsilon_{13}+[\gamma_7+\gamma_8]+(\tfrac{7}{11})[\gamma_9+\gamma_{10}]-[\gamma_{11}+\gamma_{12}]\}-\gamma_{13}. \tag{C16}$$

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