Symmetrization of Ritz approximation functions for vibrational analysis of trigonal cylinders

Ward L. Johnson
Materials Reliability Division, National Institute of Standards and Technology, 325 Broadway, Boulder, Colorado 80305

Paul R. Heyliger
Department of Civil Engineering, Colorado State University, Fort Collins, Colorado 80523

(Received 22 March 2002; revised 3 January 2003; accepted 5 January 2003)

In the Ritz method of calculating vibrational normal modes, a set of finite series approximation functions provides a matrix eigenvalue equation for the coefficients in the series and the resonant frequency. The matrix problem usually can be block-diagonalized by grouping the functions into subsets according to their properties under the symmetry operations that are common to the specimen geometry and crystal class. This task is addressed, in this study, for the case of cylindrical specimens of crystals belonging to one of the higher trigonal crystal classes. The existence of doubly degenerate resonant modes significantly complicates the analysis. Group-theoretical projection operators are employed to extract, from series approximation functions in cylindrical coordinates, the terms that transform according to each irreducible representation of the point group. This provides a complete symmetry-based block diagonalization and categorization of the modal symmetries. Off-diagonal projection operators are used to provide relations between the displacement patterns of degenerate modes. The method of analysis is presented in detail to assist in its application to other geometries, crystal structures, and/or forms of Ritz approximation functions. [DOI: 10.1121/1.1558372]

PACS numbers: 43.20.Ks, 43.40.Cw [ANN]

I. INTRODUCTION

The Ritz method is a variational analytic technique for calculating the vibrational normal-mode displacements and frequencies from the elastic constants and geometry of an object. This method is frequently employed in iterative inversion algorithms to determine unknown elastic constants from measured frequencies. By inserting a finite number of approximation functions into Hamilton's principle, the method leads to a matrix eigenvalue equation involving variable parameters of the approximation functions. The matrix equation usually can be block diagonalized by grouping the approximation functions into orthogonal subsets according to their general symmetry properties. In this way, computer code for solving the eigenvalue problem can be made significantly more efficient. Such categorization of approximation functions also provides insight into common symmetry characteristics of the various vibrational modes and facilitates the prediction of relative coupling strengths for a specified distribution of excitation.

The task of symmetrizing Ritz approximation functions for a given macroscopic geometry, crystal symmetry, and crystal orientation involves an analysis of the transformations of these functions under the symmetry operations of the object (the operations that leave both the crystal structure and the geometry unchanged). Such symmetrizations have been performed for a number of geometries and crystal systems.

Demarest[1] presented a classification of the symmetries of approximation functions for cubes of orthorhombic material (belonging to the crystallographic point group that is denoted by D_{2h} in the Schoenflies system and *mmm* in the international system) with the twofold crystal axes perpendicular to the cube faces. (For a an overview of the crystallographic point groups, including representative graphical objects, see Ashcroft and Mermin.[2]) Demarest derived restrictions on the parities of the three Cartesian components of displacement with respect to reflections across the three perpendicular mirror planes and, in this way, divided approximation functions into eight orthogonal sets. These eight sets correspond to the eight irreducible representations of D_{2h} derived from group theory and, therefore, provide a block diagonalization of the Ritz matrices with minimal sizes of the submatrices for this symmetry. (For a brief summary of some concepts from group theory, see Appendix A.) Reducing the macroscopic symmetry (geometry) of the specimen to orthorhombic (a rectangular parallelepiped with unequal sides) maintains the D_{2h} symmetry. Therefore, the same classification scheme is valid for this geometry, and it was employed by Ohno.[3] Ohno also presented a similar classification of approximation functions for monoclinic crystals (C_{2h} in the Schoenflies notation; $2/m$ in the international notation) in the form of rectangular parallelepipeds, which divided functions into two sets according to their parity with respect to the single mirror plane. Since this approach does not consider the effects of all the symmetry operations C_{2h}, it does not minimize the size of the submatrices. In a subsequent paper, Ohno *et al.*[4] extended the analysis of C_{2h} specimens to include restrictions derived from the two-fold rotation of this point group and, in this way, separated the approximation functions into four sets and completed the block diago-

nalization. This latter work actually focused on parallelepipeds of trigonal material, but the overall symmetry is the same as that of a parallelepiped of monoclinic material, because the rectangular geometry eliminates the threefold trigonal symmetry axis.

The symmetrization of approximation functions for D_{2h} and C_{2h} specimens is relatively easy to accomplish, because all of the normal-mode displacements are either unchanged or reversed in sign by the symmetry operations of the object. In other words, all vibrational normal modes are nondegenerate (no two modes have the same frequency), so that the application of symmetry operations does not transformation the displacement pattern of one mode into that of another mode. The normal modes remain nondegenerate for specimens with fewer symmetry operations. In terms of group theory, D_{2h} and lower-symmetry point groups (including C_{2h}) have only one-dimensional irreducible representations. The symmetrization of approximation functions for specimens belonging to the cubic, tetragonal, and hexagonal point groups is much more difficult. These point groups have irreducible representations with dimension greater than one, so that degenerate normal modes are transformed into one another under some of the symmetry operations.

Mochizuki[5] provided a solution to the problem of block diagonalizing Ritz matrices for all crystal classes in spherical coordinates, except for the lower tetragonal and trigonal classes. He took advantage of the fact that the complete analytical solution for the normal modes of an isotropic sphere are known.[6,7] Using these symmetrized solutions as approximation functions, Mochizuki derived restrictions on indices of the functions for various crystallographic point groups based on transformation properties of the elastic constants. Although this derivation was presented in the context of spherical specimens, the same functions and classification scheme could be used for any specimen with an overall symmetry (combination of geometry and material symmetry) equal to a crystal symmetry considered by Mochizuki, with the limits of volume integrals in the Ritz calculation adjusted to match the geometry.

Although Mochizuki's analysis provides a solution to the problem of block-diagonalizing Ritz matrices for most of the crystal classes, this solution, since it is expressed in terms of complicated functions of spherical coordinates, is unattractive for nonspherical geometries. In another publication, Mochizuki[8] considered the symmetry restrictions on approximation functions in Cartesian coordinates. Using group-theoretical projection operators, he categorized approximation functions for right square prisms of tetragonal crystals and cubes of cubic crystals, in addition to parallelepipeds of lower-symmetry crystals.

Trigonal and hexagonal crystals have received the least attention in past work. The complete symmetrization of approximation functions for such crystals in geometries that do not eliminate symmetry operations has been accomplished previously only by Mochizuki[5] in spherical coordinates.

In the present study, we address the problem of symmetrizing approximation functions, expressed in cylindrical coordinates, for vibrational modes of cylindrical crystals belonging to one of the higher-symmetry trigonal classes, C_{3v}, D_3, or D_{3d} ($3m$, 32, or $\bar{3}m$ in the international notation). This analysis has been used in the development of a Ritz algorithm for trigonal cylinders, which is described elsewhere.[9] Several factors have determined the direction of this work. The focus on trigonal crystal classes arises from the important technological role that piezoelectric materials with this symmetry (including quartz) have in electronic oscillators. Currently, there is a particular need for temperature-dependent measurements of the elastic constants of several trigonal crystals with the structure of langasite, which may provide characteristics superior to quartz in some oscillator applications.[10,11] The cylindrical geometry of specimens was chosen, instead of a rectangular geometry, partly because it can provide measurements of elastic constants with less uncertainty arising from crystal alignment (only one crystal axis needs to be aligned, instead of two). This geometry also has all the symmetry elements of the crystal, so that the overall symmetry of the specimen is the same as that of the crystal and the size of Ritz submatrices can be minimized. The problem is formulated in cylindrical coordinates, because the conditions on approximation functions arising from a consideration of the threefold rotations appear to be intractable in Cartesian coordinates. Cylindrical coordinates allow for a complete categorization of the symmetries of approximation functions and the associated minimization of submatrices. The complete description of modal symmetries was also pursued because of an interest in characterizing the resonant modes that are excited with a direct inductive piezoelectric transduction method recently employed with cylindrical specimens.[12]

Group-theoretical projection operators are employed to extract, from series approximation functions, the terms that transform according to each irreducible representation of the point group. This method is presented here in some detail. The aim is to illustrate the method completely, so that other researchers may be assisted in its application to other specimen geometries, crystal structures, and/or forms of Ritz approximation functions.

II. SYMMETRY OF D_{3d} CYLINDERS

The objective of this work is to symmetrize Ritz approximation functions for resonant modes of specimens with the symmetry of one of the higher trigonal crystal classes, C_{3v}, D_3, or D_{3d}. However, only the D_{3d} class needs to be considered. Since linear elastic vibrations are insensitive to a lack of inversion, the inversion operator can be added to the C_{3v} and D_3 point groups, making them equivalent to the trigonal point group with the greatest number of symmetry operations, D_{3d}. This effective equivalence of C_{3v}, D_3, and D_{3d} for linear elasticity can also be seen from the fact that the elastic constant matrices for these crystal classes, which contain all of the elastic symmetry information, have the same form.[13]

The symmetry of a D_{3d} crystal in the form of a cylinder with the trigonal axis oriented along the cylinder axis is shown in Fig. 1. The cylindrical geometry maintains all the elements of the D_{3d} point group, including rotations of $2\pi/3$ and $-2\pi/3$ (threefold rotations) about the vertical axis ($\hat{z}$),

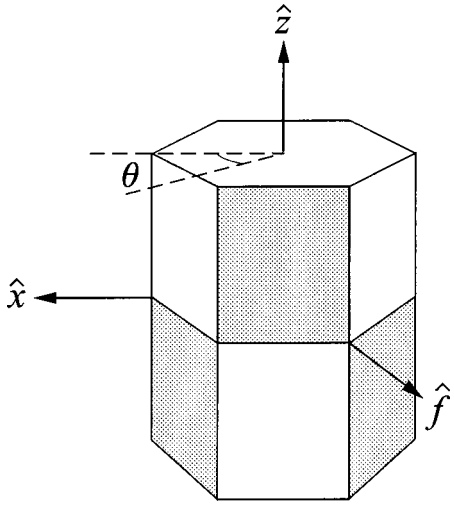

FIG. 1. Symmetry and definition of axes for an object belonging to the D_{3d} point group.

rotations of π (twofold rotations) about $\hat{x}$, $\hat{f}$, and $\hat{d}$ (where $\hat{d}$, on the back side of the object, is in the same plane as $\hat{x}$ and $\hat{f}$ and halfway between them), inversion, and the products of inversion and the rotations. The labeling of the $\hat{f}$ and $\hat{d}$ axes corresponds to that of Cornwell's[14] Appendix D. However, the axis label δ employed by Cornwell has been changed to $\hat{z}$, and $\hat{b}$ has been changed to $\hat{x}$ to match the conventions used by Heyliger and Johnson,[9] which seem more appropriate for this geometry.

Corresponding to each of the symmetry operations T is a transformation operator $P(T)$ that acts on vector functions. These transformation operators, when applied to an arbitrary function, $\vec{u}(r,\theta,z)=u_r(r,\theta,z)\hat{r}+u_\theta(r,\theta,z)\hat{\theta}+u_z(r,\theta,z)\hat{z}$, yield the following functions:

$$P(E)\vec{u}=u_r(r,\theta,z)\hat{r}+u_\theta(r,\theta,z)\hat{\theta}+u_z(r,\theta,z)\hat{z}, \tag{1a}$$

$$P(C_{3z})\vec{u}=u_r\left(r,\theta+\frac{2\pi}{3},z\right)\hat{r}+u_\theta\left(r,\theta+\frac{2\pi}{3},z\right)\hat{\theta}+u_z\left(r,\theta+\frac{2\pi}{3},z\right)\hat{z}, \tag{1b}$$

$$P(C_{3z}^{-1})\vec{u}=u_r\left(r,\theta-\frac{2\pi}{3},z\right)\hat{r}+u_\theta\left(r,\theta-\frac{2\pi}{3},z\right)\hat{\theta}+u_z\left(r,\theta-\frac{2\pi}{3},z\right)\hat{z}, \tag{1c}$$

$$P(C_{2x})\vec{u}=u_r(r,-\theta,-z)\hat{r}-u_\theta(r,-\theta,-z)\hat{\theta}-u_z(r,-\theta,-z)\hat{z}, \tag{1d}$$

$$P(C_{2f})\vec{u}=u_r\left(r,-\theta+\frac{4\pi}{3},-z\right)\hat{r}-u_\theta\left(r,-\theta+\frac{4\pi}{3},-z\right)\hat{\theta}-u_z\left(r,-\theta+\frac{4\pi}{3},-z\right)\hat{z}, \tag{1e}$$

$$P(C_{2d})\vec{u}=u_r\left(r,-\theta-\frac{4\pi}{3},-z\right)\hat{r}-u_\theta\left(r,-\theta-\frac{4\pi}{3},-z\right)\hat{\theta}-u_z\left(r,-\theta-\frac{4\pi}{3},-z\right)\hat{z}, \tag{1f}$$

$$P(I)\vec{u}=u_r(r,\theta+\pi,-z)\hat{r}+u_\theta(r,\theta+\pi,-z)\hat{\theta}-u_z(r,\theta+\pi,-z)\hat{z}, \tag{1g}$$

where the unit vectors $\hat{r}$ and $\hat{\theta}$ are in the radial and azimuthal directions at a given point. E is the identity operation. C_{3z} and C_{3z}^{-1} are rotations about $\hat{z}$ by $2\pi/3$ and $-2\pi/3$, respectively. C_{2x}, C_{2f}, and C_{2d} are twofold rotations about $\hat{x}$, $\hat{f}$, and $\hat{d}$, respectively. I is the inversion operation. The effects of the additional transformation operators involving inversion (IC_{3z}, etc.) can be derived easily from the relation[14]

$$P(IT)=P(I)P(T). \tag{2}$$

III. RESTRICTIONS ON INDICES OF APPROXIMATION FUNCTIONS

Following Heyliger and Johnson,[9] the components of a normal-mode displacement $\vec{u}(r,\theta,z)$ of a D_{3d} cylinder are approximated in cylindrical coordinates by finite series of the form

$$u_r(r,\theta,z)=\sum_{\alpha,n,\beta} a^c_{\alpha n\beta} r^\alpha \cos(n\theta) z^\beta + \sum_{\kappa,m,\gamma} a^s_{\kappa m\gamma} r^\kappa \sin(m\theta) z^\gamma, \tag{3a}$$

$$u_\theta(r,\theta,z)=\sum_{\alpha,n,\beta} b^c_{\alpha n\beta} r^\alpha \cos(n\theta) z^\beta + \sum_{\kappa,m,\gamma} b^s_{\kappa m\gamma} r^\kappa \sin(m\theta) z^\gamma, \tag{3b}$$

$$u_z(r,\theta,z)=\sum_{\alpha,n,\beta} c^c_{\alpha n\beta} r^\alpha \cos(n\theta) z^\beta + \sum_{\kappa,m,\gamma} c^s_{\kappa m\gamma} r^\kappa \sin(m\theta) z^\gamma, \tag{3c}$$

where n, m, α, β, κ, and γ are non-negative integers. For a given material density and set of elastic constants, the coefficients $a^c_{\alpha n\beta}$, $a^s_{\kappa m\gamma}$, $b^c_{\alpha n\beta}$, $b^s_{\kappa m\gamma}$, $c^c_{\alpha n\beta}$, and $c^s_{\kappa m\gamma}$ for each vibrational mode can be determined through Ritz analysis by inserting the approximation functions and the specimen geometry into a variational equation derived from Hamilton's principle.[9]

According to group theory, the displacement field $\vec{u}$ of each of the normal modes is a basis function for one of the irreducible representations of D_{3d}, which are conventionally labeled A_{1g}, A_{2g}, A_{1u}, A_{2u}, E_g, and E_u.[14] (See Appendixes A and B.) Barring accidental degeneracies, modes transforming as one of the first four of these irreducible representations are nondegenerate, and those transforming as E_g or E_u are doubly degenerate. Since functions transforming according to different irreducible representations are or-

thogonal (even if they are not solutions of the elastic eigenvalue problem), solutions of the vibrational problem can be sought using a limited set of approximation functions of the form given by Eq. (3) with the indices in the functions restricted to values that provide the symmetry associated with a given irreducible representation. In other words, submatrices can be considered separately in the Ritz calculation, if approximation functions are grouped in this way.

The restrictions on the indices of approximation functions are determined here by applying group-theoretical projection operators, which are defined as[14]

$$\mathcal{P}_{ij}^{p} \equiv \frac{d_p}{g} \sum_{T \in G} \Gamma^{p}(T)_{ij}^{*} P(T), \tag{4}$$

where $\Gamma^p(T)$ is the matrix for a symmetry operation T in an irreducible representation of dimension d_p of a group G that contains g symmetry operations (elements). (See Appendix A.) The summation is over all elements in the group, and the asterisk denotes the complex conjugate. For D_{3d}, g is equal to 12, the $P(T)$ are given by Eq. (1), p assumes six arbitrarily assigned values corresponding to the six irreducible representations, and d_p is either 1 (for the nondegenerate representations) or 2 (for the doubly degenerate representations).[14] The matrices for D_{3d} are given in Appendix B. For this point group, all of the matrices are real, so that $\Gamma^p(T)_{ij}^{*} = \Gamma^p(T)_{ij}$.

A diagonal projection operator $\mathcal{P}_{ii}^{p}$ with a given value of i, when applied to an arbitrary function, extracts the part of the function that transforms as the ith row of the representation Γ^p. When applied to series approximation functions such as those given by Eq. (3), inspection of the extracted functions leads to a determination of restrictions on the indices for functions belonging to a given irreducible representation. For the doubly degenerate representations, the projection operators with $i \neq j$ can be used to determine the relationship between coefficients in the expansions of two degenerate modes.

The application of a projection operator to a series approximation $\vec{u}$ with the form of Eq. (3) yields a function $\vec{u}'$:

$$\mathcal{P}_{ij}^{p} \vec{u} = \vec{u}' = u_r'(r,\theta,z)\hat{r} + u_\theta'(r,\theta,z)\hat{\theta} + u_z'(r,\theta,z)\hat{z}, \tag{5}$$

with

$$\begin{aligned} u_r'(r,\theta,z) = {} & \frac{d_p}{g} \sum_{\alpha,n,\beta} [A_{n\beta}(z) a_{\alpha n\beta}^{c} r^{\alpha} \cos(n\theta) \\ & + B_{n\beta}(z) a_{\alpha n\beta}^{c} r^{\alpha} \sin(n\theta)] \\ & + \frac{d_p}{g} \sum_{\kappa,m,\gamma} [C_{m\gamma}(z) a_{\kappa m\gamma}^{s} r^{\kappa} \cos(m\theta) \\ & + D_{m\gamma}(z) a_{\kappa m\gamma}^{s} r^{\kappa} \sin(m\theta)], \end{aligned} \tag{6a}$$

$$\begin{aligned} u_\theta'(r,\theta,z) = {} & \frac{d_p}{g} \sum_{\alpha,n,\beta} [A_{n\beta}(z) b_{\alpha n\beta}^{c} r^{\alpha} \cos(n\theta) \\ & + B_{n\beta}(z) b_{\alpha n\beta}^{c} r^{\alpha} \sin(n\theta)] \\ & + \frac{d_p}{g} \sum_{\kappa,m,\gamma} [C_{m\gamma}(z) b_{\kappa m\gamma}^{s} r^{\kappa} \cos(m\theta) \\ & + D_{m\gamma}(z) b_{\kappa m\gamma}^{s} r^{\kappa} \sin(m\theta)], \end{aligned} \tag{6b}$$

$$\begin{aligned} u_z'(r,\theta,z) = {} & \frac{d_p}{g} \sum_{\alpha,n,\beta} [A_{n\beta}(z) c_{\alpha n\beta}^{c} r^{\alpha} \cos(n\theta) \\ & + B_{n\beta}(z) c_{\alpha n\beta}^{c} r^{\alpha} \sin(n\theta)] \\ & + \frac{d_p}{g} \sum_{\kappa,m,\gamma} [C_{m\gamma}(z) c_{\kappa m\gamma}^{s} r^{\kappa} \cos(m\theta) \\ & + D_{m\gamma}(z) c_{\kappa m\gamma}^{s} r^{\kappa} \sin(m\theta)], \end{aligned} \tag{6c}$$

where

$$\begin{aligned} A_{n\beta}(z) = {} & z^{\beta} + [\Gamma_{ij}(C_{3z})_{ij} + \Gamma(C_{3z}^{-1})_{ij}] \cos(2n\pi/3) z^{\beta} + \Delta_1 \Gamma(C_{2x})_{ij} (-z)^{\beta} + \Delta_1 [\Gamma(C_{2f})_{ij} + \Gamma(C_{2d})_{ij}] \cos(4n\pi/3)(-z)^{\beta} \\ & + \Delta_2 \Gamma(I)_{ij} \cos(n\pi)(-z)^{\beta} + \Delta_2 [\Gamma(IC_{3z})_{ij} + \Gamma(IC_{3z}^{-1})_{ij}] \cos(n\pi)\cos(2n\pi/3)(-z)^{\beta} + \Delta_1\Delta_2 \Gamma(IC_{2x})_{ij} \cos(n\pi) z^{\beta} \\ & + \Delta_1\Delta_2 [\Gamma(IC_{2f})_{ij} + \Gamma(IC_{2d})_{ij}] \cos(n\pi)\cos(4n\pi/3) z^{\beta}, \end{aligned} \tag{7a}$$

$$\begin{aligned} B_{n\beta}(z) = {} & [-\Gamma(C_{3z})_{ij} + \Gamma(C_{3z}^{-1})_{ij}] \sin(2n\pi/3) z^{\beta} + \Delta_1 [\Gamma(C_{2f})_{ij} - \Gamma(C_{2d})_{ij}] \sin(4n\pi/3)(-z)^{\beta} + \Delta_2 [-\Gamma(IC_{3z})_{ij} \\ & + \Gamma(IC_{3z}^{-1})_{ij}] \cos(n\pi)\sin(2n\pi/3)(-z)^{\beta} + \Delta_1\Delta_2 [\Gamma(IC_{2f})_{ij} - \Gamma(IC_{2d})_{ij}] \cos(n\pi)\sin(4n\pi/3) z^{\beta}, \end{aligned} \tag{7b}$$

$$\begin{aligned} C_{m\gamma}(z) = {} & [\Gamma(C_{3z})_{ij} - \Gamma(C_{3z}^{-1})_{ij}] \sin(2m\pi/3) z^{\gamma} + \Delta_1 [\Gamma(C_{2f})_{ij} - \Gamma(C_{2d})_{ij}] \sin(4m\pi/3)(-z)^{\gamma} + \Delta_2 [\Gamma(IC_{3z})_{ij} \\ & - \Gamma(IC_{3z}^{-1})_{ij}] \cos(m\pi)\sin(2m\pi/3)(-z)^{\gamma} + \Delta_1\Delta_2 [\Gamma(IC_{2f})_{ij} - \Gamma(IC_{2d})_{ij}] \cos(m\pi)\sin(4m\pi/3) z^{\gamma}, \end{aligned} \tag{7c}$$

$$\begin{aligned} D_{m\gamma}(z) = {} & z^{\gamma} + [\Gamma(C_{3z})_{ij} + \Gamma(C_{3z}^{-1})_{ij}] \cos(2m\pi/3) z^{\gamma} - \Delta_1 \Gamma(C_{2x})_{ij} (-z)^{\gamma} - \Delta_1 [\Gamma(C_{2f})_{ij} + \Gamma(C_{2d})_{ij}] \cos(4m\pi/3)(-z)^{\gamma} \\ & + \Delta_2 \Gamma(I)_{ij} \cos(m\pi)(-z)^{\gamma} + \Delta_2 [\Gamma(IC_{3z})_{ij} + \Gamma(IC_{3z}^{-1})_{ij}] \cos(m\pi)\cos(2m\pi/3)(-z)^{\gamma} - \Delta_1\Delta_2 \Gamma(IC_{2x})_{ij} \cos(m\pi) z^{\gamma} \\ & - \Delta_1\Delta_2 [\Gamma(IC_{2f})_{ij} + \Gamma(IC_{2d})_{ij}] \cos(m\pi)\cos(4m\pi/3) z^{\gamma}, \end{aligned} \tag{7d}$$

$$\Delta_1 \equiv \begin{cases} 1 & \text{for } u_r', \\ -1 & \text{for } u_\theta' \text{ and } u_z', \end{cases} \tag{8a}$$

$$\Delta_2 \equiv \begin{cases} 1 & \text{for } u_r' \text{ and } u_\theta', \\ -1 & \text{for } u_z'. \end{cases} \tag{8b}$$

To illustrate the way restrictions on indices of the approximation functions are determined, consider the relatively simple case of vibrational normal modes that transform according to the irreducible representation A_{1g}. The values of the Γ_{11} (characters) of this one-dimensional representation are all equal to 1 (Table II), which corresponds to basis functions being unchanged by any of the symmetry operations of D_{3d}. With these values, Eq. (7) reduces to

$$A_{n\beta}(z) = [z^\beta + \Delta_1(-z)^\beta][1 + 2\cos(2n\pi/3)] + \Delta_2[\Delta_1 z^\beta + (-z)^\beta]\cos(n\pi) \times [1 + 2\cos(2n\pi/3)], \tag{9a}$$

$$B_{n\beta}(z) = 0, \tag{9b}$$

$$C_{m\gamma}(z) = 0, \tag{9c}$$

$$D_{m\gamma}(z) = [z^\gamma - \Delta_1(-z)^\gamma][1 + 2\cos(2m\pi/3)] - \Delta_2[\Delta_1 z^\gamma - (-z)^\gamma]\cos(m\pi) \times [1 + 2\cos(2m\pi/3)], \tag{9d}$$

using the identity $\cos(4n\pi/3) = \cos(2n\pi/3)$. For u_r', Δ_1 and Δ_2 are equal to 1, and Eqs. (9a) and (9d) become

$$A_{n\beta}(z) = [z^\beta + (-z)^\beta][1 + 2\cos(2n\pi/3) + \cos(n\pi) + 2\cos(n\pi)\cos(2n\pi/3)], \tag{10a}$$

$$D_{m\gamma}(z) = [z^\gamma - (-z)^\gamma][1 + 2\cos(2m\pi/3) - \cos(m\pi) - 2\cos(m\pi)\cos(2m\pi/3)]. \tag{10b}$$

Inspection of Eq. (10a) reveals that $A_{n\beta}(z)$ is zero unless n and β are even and n is a multiple of 3. Similarly, $D_{m\gamma}(z)$ is zero unless m and γ are odd and m is a multiple of 3. Thus, only approximation functions with these indices for the radial component need to be considered when searching for solutions of the vibrational problem that transform as A_{1g}.

The restrictions on indices for the azimuthal and axial components of A_{1g} functions are obtained by inserting the corresponding values of Δ_1 and Δ_2 [Eq. (8)] into Eq. (9). Similarly, restrictions on each of the components of functions transforming according to the other irreducible representations of D_{3d} are obtained by inserting the corresponding values of Γ_{11}, Δ_1, and Δ_2 into Eq. (7). The results of this analysis are summarized in Table I. For the doubly degenerate irreducible representations, E_g and E_u, the restrictions on the indices for the second mode, obtained by inserting Γ_{22} into Eq. (7), are also included in this table. The first and second modes of E_g and E_u are labeled "1" and "2" in the second column of the table, corresponding to the row definitions implicit in the Γ matrices, Eq. (B2).

The expressions for $B_{n\beta}(z)$ and $C_{m\gamma}(z)$ [Eqs. (7b) and (7c)] provide explicit information about the relationship between coefficients in the expansions for the degenerate modes that transform as E_g or E_u. Once the displacement field $\vec{u}$ for a mode transforming according to the first row of E_g or E_u is found, the displacement field $\vec{u}'$ of the second mode of the degenerate pair is given by Eqs. (5)–(8) with $i = 2$ and $j = 1$. For example, inserting the values for Γ_{21} of E_g [Eq. (B2)] into Eq. (7),

TABLE I. Parities of indices of approximation functions [Eq. (3)] for each of the irreducible representations (i.r.) of D_{3d}. ($E \equiv$ even, $O \equiv$ odd.) The values of n and m also must be multiples of 3 for A_{1g}, A_{2g}, A_{1u}, A_{2u} and must not be multiples of 3 for E_g and E_u. The second column lists the row indices of the doubly degenerate irreducible representations [Eq. (B2)].

i.r.	Row	Component	n	β	m	γ
		u_r	E	E	O	O
A_{1g}		u_θ	O	O	E	E
		u_z	E	O	O	E
		u_r	O	O	E	E
A_{2g}		u_θ	E	E	O	O
		u_z	O	E	E	O
		u_r	O	O	E	E
E_g	1	u_θ	E	E	O	O
		u_z	O	E	E	O
		u_r	E	E	O	O
E_g	2	u_θ	O	O	E	E
		u_z	E	O	O	E
		u_r	O	E	E	O
A_{1u}		u_θ	E	O	O	E
		u_z	O	O	E	E
		u_r	E	O	O	E
A_{2u}		u_θ	O	E	E	O
		u_z	E	E	O	O
		u_r	E	O	O	E
E_u	1	u_θ	O	E	E	O
		u_z	E	E	O	O
		u_r	O	E	E	O
E_u	2	u_θ	E	O	O	E
		u_z	O	O	E	E

$$A_{n\beta}(z) = 0, \tag{11a}$$

$$B_{n\beta}(z) = -\sqrt{3}[z^\beta - \Delta_1(-z)^\beta]\sin(2n\pi/3) + \sqrt{3}\Delta_2[\Delta_1 z^\beta - (-z)^\beta]\cos(n\pi)\sin(2n\pi/3), \tag{11b}$$

$$C_{m\gamma}(z) = \sqrt{3}[z^\gamma + \Delta_1(-z)^\gamma]\sin(2m\pi/3) + \sqrt{3}\Delta_2[\Delta_1 z^\gamma + (-z)^\gamma]\cos(m\pi)\sin(2m\pi/3), \tag{11c}$$

$$D_{m\gamma}(z) = 0. \tag{11d}$$

These equations reduce to the same expressions for all three of the components, u_r', u_θ', and u_r':

$$B_{n\beta}(z) = -4\sqrt{3}z^\beta \sin(2n\pi/3) = \begin{cases} -6z^\beta & \text{if } n = 1 + 3h, \\ 6z^\beta & \text{if } n = 2 + 3h, \end{cases} \tag{12a}$$

$$C_{m\gamma}(z) = 4\sqrt{3}z^\gamma \sin(2m\pi/3) = \begin{cases} 6z^\gamma & \text{if } m = 1 + 3k, \\ -6z^\gamma & \text{if } m = 2 + 3k, \end{cases} \tag{12b}$$

where h and k are non-negative integers, and n and m are still restricted to the parities indicated in Table I. Equation (12) also applies to the transformation between degenerate functions of E_u. Note that the prefactor d_p/g in the general expressions for u_r', u_θ', and u_r' [Eq. (6)] is equal to 1/6 for E_g and E_u. Therefore, the expansion for the second function ($\vec{u}'$) in a degenerate pair is equal to that for the first function ($\vec{u}$) with sine functions replacing cosine functions, cosine functions replacing sine functions, and coefficients multiplied by 1 or -1 [depending on the values of n or m, according to Eq. (12)].

IV. CONCLUSION

Group-theoretical projection operators provide a straightforward, although somewhat cumbersome, approach for symmetrizing Ritz approximation functions for cylinders of crystals belonging to one of the higher trigonal classes. For nondegenerate vibrational modes, this approach actually does not need to be employed, since restrictions on the functions can be derived by considering, in turn, each symmetry operation and the corresponding entries in the character table. However, the doubly degenerate modes introduce a complexity that has been addressed here by employing the full power of group theory through the projection operators. The final results for the specific set of series approximation functions given by Eq. (3) are simple restrictions on the indices of the series coefficients (Table I) that divide the functions into subsets corresponding to the irreducible representations of D_{3d}. These results are used by Heyliger and Johnson[9] to formulate a Ritz algorithm for calculating the modal displacements and frequencies of trigonal cylinders.

APPENDIX A: GROUP-THEORETICAL TERMINOLOGY

A brief summary of several relevant concepts from group theory is presented here for the benefit of readers who have little familiarity with this theory. Readers interested in complete mathematically rigorous definitions of terms should refer to the cited literature.

A crystallographic point group G is the set of all symmetry operations (elements), not including translations, that leave a crystal structure unchanged. Depending on the crystal structure, these operations may include rotations about an axis, inversion through a fixed point, reflections across a plane, rotation reflections, and/or rotation inversions.[2]

A matrix representation Γ of G is a set of nonsingular square matrices with the properties that 1), for every element T_i of G, there is a corresponding matrix $\Gamma(T_i)$ and 2), for every pair of elements T_i and T_j, matrix multiplication corresponds to successive application of symmetry operations:[14]

$$\Gamma(T_iT_j)=\Gamma(T_i)\Gamma(T_j). \tag{A1}$$

All of the matrices in a representation have the same number of rows, and this number is the dimension d of the representation. The character of each matrix is defined to be the trace.

A set of functions $\psi_1,\psi_2,\ldots,\psi_d$ is a basis for a representation of G if

TABLE II. Character table for D_{3d}.

	χ_1	χ_2	χ_3	χ_4	χ_5	χ_6
A_{1g}	1	1	1	1	1	1
A_{2g}	1	1	−1	1	1	−1
E_g	2	−1	0	2	−1	0
A_{1u}	1	1	1	−1	−1	−1
A_{2u}	1	1	−1	−1	−1	1
E_u	2	−1	0	−2	1	0

$$P(T)\psi_n(\vec{r})=\sum_{m=1}^{d}\Gamma(T)_{mn}\psi_m(\vec{r}), \tag{A2}$$

where $P(T)$ is an operator that transforms the coordinates of $\psi_n(\vec{r})$ according to the symmetry operation T. The function ψ_n is said to transform as the nth row of G.

There are an infinite number of representations of each crystallographic point group. However, almost all of these are reducible, which means that all the matrices in such a representation can be simultaneously block diagonalized through the application of an appropriate similarity transformation. For each crystallographic point group, there are only a few submatrices that appear in any completely block diagonalized representation (apart from similarity transformations of the submatrices). These submatrices are the irreducible representations of the point group.

For a given point group, basis functions which belong to different irreducible representations or different rows of the same irreducible representation are orthogonal. This group-theoretical result is central to the current paper, because the sorting of series approximation functions according to their irreducible representations (and rows, for two-dimensional representations) leads to a block diagonalization of the Ritz matrices.

APPENDIX B: IRREDUCIBLE REPRESENTATIONS OF D_{3d}

There are six irreducible representations of the crystallographic point group D_{3d}: four one-dimensional representations, which normally are labeled A_{1g}, A_{2g}, A_{1u}, A_{2u}, and two two-dimensional representations labeled E_g and E_u.[14] The subscripts "g" and "u" indicate that the corresponding basis functions are even and odd, respectively, under inversion.

Abbreviated information on the symmetries of basis functions for the irreducible representations is given by the characters, which are presented in Table II. The column labels in this table designate the classes, which are defined to include the following elements:[14]

$$\chi_1\equiv E, \tag{B1a}$$

$$\chi_2\equiv C_{3z},C_{3z}^{-1}, \tag{B1b}$$

$$\chi_3\equiv C_{2x},C_{2f},C_{2d}, \tag{B1c}$$

$$\chi_4\equiv I, \tag{B1d}$$

$$\chi_5\equiv IC_{3z},IC_{3z}^{-1}, \tag{B1e}$$

$$\chi_6\equiv IC_{2x},IC_{2f},IC_{2d}. \tag{B1f}$$

The effect of each symmetry operation on basis functions of the one-dimensional representations can be read directly from the table: the functions are either unchanged or reversed in sign by an operation, depending on whether the corresponding character is 1 or -1, respectively. For these representations, the single entry in the matrix $\Gamma(T)$ for each symmetry operation T is simply the character of that T.

The matrices for E_g, as presented by Cornwell,[14] are

$$\Gamma(E)=\Gamma(I)=\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}, \tag{B2a}$$

$$\Gamma(C_{3z})=\begin{bmatrix}-\frac{1}{2} & -\frac{1}{2}\sqrt{3}\\ \frac{1}{2}\sqrt{3} & -\frac{1}{2}\end{bmatrix}, \tag{B2b}$$

$$\Gamma(C_{3z}^{-1})=\begin{bmatrix}-\frac{1}{2} & \frac{1}{2}\sqrt{3}\\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2}\end{bmatrix}, \tag{B2c}$$

$$\Gamma(C_{2x})=\begin{bmatrix}-1 & 0\\ 0 & 1\end{bmatrix}, \tag{B2d}$$

$$\Gamma(C_{2f})=\begin{bmatrix}\frac{1}{2} & -\frac{1}{2}\sqrt{3}\\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2}\end{bmatrix}, \tag{B2e}$$

$$\Gamma(C_{2d})=\begin{bmatrix}\frac{1}{2} & \frac{1}{2}\sqrt{3}\\ \frac{1}{2}\sqrt{3} & -\frac{1}{2}\end{bmatrix}. \tag{B2f}$$

The additional matrices involving inversion [$\Gamma(IC_{3z})$, $\Gamma(IC_{3z}^{-1})$, etc.] are the same as the corresponding matrices above that do not involve inversion. The matrices for E_u are the same, except that those involving inversion have each matrix element reversed in sign.

[1] H. H. Demarest, Jr., "Cube-resonance method to determine the elastic constants of solids," J. Acoust. Soc. Am. **49**, 768–775 (1971).

[2] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Holt, Rinehart, and Winston, New York, 1976).

[3] I. Ohno, "Free vibration of a rectangular parallelepiped crystal and its application to determination of elastic constants of orthorhombic crystals," J. Phys. Earth **24**, 355–379 (1976).

[4] I. Ohno, Y. Shigeru, O. L. Anderson, and J. Noda, "Determination of elastic constants of trigonal crystals by the rectangular parallelepiped resonance method," Phys. Chem. Solids **47**, 1103–1108 (1986).

[5] E. Mochizuki, "Sphere-resonance method to determine elastic constants of crystal," J. Appl. Phys. **63**, 5668–5673 (1988).

[6] Y. Satô and T. Usami, "Basic study of the oscillations of a homogeneous elastic sphere, II. Distribution of Displacement," Geophys. Mag. **31**, 25–47 (1962).

[7] Y. Satô and T. Usami, "Basic study of the oscillations of a homogeneous elastic sphere, III. Boundary conditions and the generation of elastic waves," Geophys. Mag. **31**, 49–62 (1962).

[8] E. Mochizuki, "Application of group theory to free oscillations of an anisotropic rectangular parallelepiped," J. Phys. Earth **35**, 159–170 (1987).

[9] P. R. Heyliger and W. L. Johnson, "Traction-free vibrations of finite trigonal elastic cylinders," J. Acoust. Soc. Am. **113**, 1812–1825 (2003).

[10] D. C. Malocha, M. P. da Cunha, E. Adler, R. C. Smythe, S. Frederick, M. Chou, R. Helmbold, and Y. S. Zhou, "Recent measurements of material constants versus temperature for langatate, langanite, and langasite," *Proceedings of the 2000 IEEE/EIA International Frequency Control Symposium and Exhibition*, Kansas City (IEEE, Danvers, MA, 2000), pp. 200–205.

[11] J. A. Kosinski and R. A. Pastore, Jr., "A review of langasite material constants from BAW and SAW data: toward an improved data set," *Proceedings of the 2001 IEEE International Frequency Control Symposium and PDA Exhibition*, Seattle (IEEE, Danvers, MA, 2000), pp. 278–286.

[12] W. Johnson, S. Kim, and D. Lauria, "Anelastic loss in langatate," in *Proceedings of the 2000 IEEE/EIA International Frequency Control Symposium and Exhibition*, Kansas City (IEEE, Danvers, MA, 2000), pp. 186–190.

[13] B. A. Auld, *Acoustic Fields and Waves in Solids* (Krieger, Malabar, FL, 1990), Vol. I.

[14] J. F. Cornwell, *Group Theory in Physics* (Academic, New York, 1984), Vol. I.