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Interactions of collinear acoustic waves propagating along pure mode directions of crystals

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Previous studies on the interaction of collinear acoustic waves have been devoted to waves propagating along pure modes directions of cubic crystals. In this paper, we show that the calculations can be readily extended to all crystal point groups. Nonlinearity parameters characterizing the nonlinear interactions are defined here. The effective third order elastic constants involved in the parameters can be calculated by using the method presented in this paper. Our results are very useful for the study of elastic nonlinearity of crystals with any given symmetry. © *2014 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4865271]

I. INTRODUCTION

It is well known that interaction of collinear acoustic waves will generate their harmonic waves and waves with the sum and difference frequencies of the interacting waves. The nonlinear effects have been used to determine the third and higher order elastic constants of materials. Those higher order constants characterize the anharmonicity of crystal lattice and are important for understanding of many properties of crystals, such as thermal transportation, temperature and pressure dependence of second order elastic constants, attenuation of high frequency phonons, etc.

The interactions of elastic waves and harmonic generations have been studied theoretically and experimentally.[1–7] The third-order elastic constants (TOECs) and their temperature dependence of some cubic crystals have been determined by using ultrasonic second harmonic generation technique.[8,9] Anisotropic nonlinear elastic properties of an icosahedral quasicrystal were also studied.[10,11] Recently, the interactions of shear waves have been calculated and observed for cubic and other crystals although the interaction is prohibited for homogenous isotropic solids.[12–17] Nevertheless, most of those studies concentrate on longitudinal waves and isotropic solids or cubic crystals to which many useful materials, especially metals, belong to. It is known that many useful materials developed in recent decades belong to crystal systems other than cubic. For example, domain engineered PMN-PT single crystals will have 2 mm, 4 mm, or 3 m macroscopic symmetries when poled along the direction other than their natural polarization direction.[18] Investigations on the elasticity nonlinearity of these new crystals are needed for high power applications but have not been done up to date.

Here, we attempt to expand previous theories on interactions of collinear acoustic waves in cubic system to cover all crystal point groups in order to facilitate further experiments on crystals. First, the basic equations up to quadratic nonlinearity are given. It is known that among the 32 point groups, 20 are piezoelectric. But in the present calculations, only elastic nonlinearity has been taken into account. The nonlinear interactions of collinear acoustic waves propagating along pure mode directions of crystals are examined, which will simplify both the calculations and experiments. Nonlinearity parameters characterizing the interactions are defined. Some specific TOECs or their combinations will appear in the nonlinearity parameters, so that we can use these nonlinearity parameters to obtain the effective TOECs. Finally, the calculated results for tetragonal crystals (point group 422, 4 mm, $\bar{4}2$ m, 4/mmm) are listed as an example to demonstrate the procedure.

II. BASIC EQUATIONS

The basic equations involving interactions of collinear acoustic waves have been given in the literature as briefly described below.[7,17] Referring to un-deformed state, the stress equation of motion can be written as[19]

$$\delta_{iM}\rho_0\ddot{u}_M = \frac{\partial P_{Ji}}{\partial a_J}. \tag{1}$$

Here, ρ_0 is the mass density of the crystal in its un-deformed or natural state, δ_{iM} is a Kronecker delta employing to translate from the un-deformed state to deformed state or vice versa, P_{Ji} is the first Piola-Kirchhoff stress tensor, which is a two-point tensor, i.e., it represents the force per unit of area of an internal plane in un-deformed state and measured in the deformed state

$$P_{Ji} = \frac{\partial x_i}{\partial a_I}\frac{\partial \varphi}{\partial \eta_{IJ}}. \tag{2}$$

In Eq. (2), a_J and x_j are the positions of the same material particle before and after the deformation, φ is the strain energy density, which is invariant under allowed symmetry operations and can be written as the function of the Lagrangian strain tensor

$$\varphi = \frac{1}{2}c_{IJKL}\eta_{IJ}\eta_{KL} + \frac{1}{6}c_{IJKLMN}\eta_{IJ}\eta_{KL}\eta_{MN} + \cdots. \tag{3}$$

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Here, the subscripts are written in capital letters to emphasize that the quantities are evaluated in the un-deformed state. The Lagrangian strain is defined as

$$\eta_{KL} = \frac{1}{2}[u_{K,L} + u_{L,K} + u_{P,L}u_{P,K}]. \tag{4}$$

Thus, up to quadratic nonlinearity, the Piola-Kirchhoff stress tensor can be written as

$$P_{Ji} = \delta_{iI}\left[c_{IJKL}u_{K,L} + \left(\frac{1}{2}c_{IJNL}\delta_{MK} + c_{NJKL}\delta_{IM} + \frac{1}{2}c_{IJKLMN}\right)u_{K,L}u_{M,N}\right]. \tag{5}$$

Substituting the results into stress equation of motion, the displacement equation of motion, up to quadratic nonlinearity, can be written as

$$\rho_0 \ddot{u}_I = c_{IJKL}u_{K,LJ} + \tilde{c}_{IJKLMN}(u_{K,LJ}u_{M,N} + u_{K,L}u_{M,NJ}), \tag{6a}$$

$$\tilde{c}_{IJKLMN} = \frac{1}{2}c_{IJNL}\delta_{MK} + c_{NJKL}\delta_{IM} + \frac{1}{2}c_{IJKLMN}. \tag{6b}$$

Here, the translation Kronecker delta is eliminated. (Note: $\tilde{c}_{IJKLMN}$ do not have the same symmetry as c_{IJKLMN}.)

For calculation of plane wave propagation, it is often convenient to select the coordinate system in such a way that the direction of wave propagation is parallel to one axis of the coordinate system. When the a-axis is selected as the direction of wave propagation, the particle displacements are only spatially dependent on coordinate a. In this case, $\frac{\partial u}{\partial b} = \frac{\partial u}{\partial c} = 0$, Eqs. (6) can be rewritten as[7,17]

$$\rho_0 \ddot{u}_J - \gamma_{J111}u_{1,11} - \gamma_{J121}u_{2,11} - \gamma_{J131}u_{3,11} = f_J(u_1, u_2, u_3), \; (J = 1-3), \tag{7}$$

where the a-axis is referred to as 1-axis. Here, coma in subscript means partial differential with respect to the spatial coordinate following the comma:

$$f_J = g_{J1}u_{1,11}u_{1,1} + g_{J2}u_{2,11}u_{2,1} + g_{J3}u_{3,11}u_{3,1} + g_{J6}(u_{1,11}u_{2,1} + u_{1,1}u_{2,11}) + g_{J5}(u_{1,11}u_{3,1} + u_{1,1}u_{3,11}) + g_{J4}(u_{2,11}u_{3,1} + u_{2,1}u_{3,11}) \tag{8}$$

and

$$g_{11} = (3\gamma_{11} + \gamma_{111}),\; g_{22} = (3\gamma_{16} + \gamma_{666}),\; g_{33} = (3\gamma_{15} + \gamma_{555}),$$
$$g_{12} = g_{26} = (\gamma_{11} + \gamma_{166}),\; g_{13} = g_{35} = (\gamma_{11} + \gamma_{155}),$$
$$g_{14} = g_{25} = g_{36} = \gamma_{156},\; g_{15} = g_{31} = (\gamma_{15} + \gamma_{115}),$$
$$g_{16} = g_{21} = (\gamma_{16} + \gamma_{116}),$$
$$g_{23} = g_{34} = (\gamma_{16} + \gamma_{556}),\; g_{24} = g_{32} = (\gamma_{15} + \gamma_{566}).$$

Instead of c_{IJ} and c_{IJK} in Eq. (7), the γ_{IJ} and γ_{IJK} are used to emphasis those constants referred to the calculation coordinates. Also abbreviated indices are used. Usually, the right-hand-side of Eq. (7) is considered as a perturbation, the nonlinear equations can be solved by successive approximation method, i.e., let

$$u_I = \delta u_I^{(I)} + \delta^2 u_I^{(II)} + \cdots. \tag{9}$$

Here, $\delta \le 1$ indicates the order of magnitude of the successive terms in Eq. (9). Then, the first-order and second-order approximate equations will be given by

$$\rho_0 \begin{bmatrix} \ddot{u}_1^{(I)} \\ \ddot{u}_2^{(I)} \\ \ddot{u}_3^{(I)} \end{bmatrix} - \begin{bmatrix} \gamma_{11} & \gamma_{16} & \gamma_{15} \\ \gamma_{16} & \gamma_{66} & \gamma_{56} \\ \gamma_{15} & \gamma_{56} & \gamma_{55} \end{bmatrix} \begin{bmatrix} u_{1,11}^{(I)} \\ u_{2,11}^{(I)} \\ u_{3,11}^{(I)} \end{bmatrix} = 0, \tag{10a}$$

$$\rho_0 \begin{bmatrix} \ddot{u}_1^{(II)} \\ \ddot{u}_2^{(II)} \\ \ddot{u}_3^{(II)} \end{bmatrix} - \begin{bmatrix} \gamma_{11} & \gamma_{16} & \gamma_{15} \\ \gamma_{16} & \gamma_{66} & \gamma_{56} \\ \gamma_{15} & \gamma_{56} & \gamma_{55} \end{bmatrix} \begin{bmatrix} u_{1,11}^{(II)} \\ u_{2,11}^{(II)} \\ u_{3,11}^{(II)} \end{bmatrix} = \begin{bmatrix} g_{11} & g_{12} & g_{13} & g_{14} & g_{15} & g_{16} \\ g_{21} & g_{22} & g_{23} & g_{24} & g_{25} & g_{26} \\ g_{31} & g_{32} & g_{33} & g_{34} & g_{35} & g_{36} \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \\ h_5 \\ h_6 \end{bmatrix}, \tag{10b}$$

where g_{IJ} is given by Eq. (8) and

$$h_J = u_{J,1}^{(I)}u_{J,11}^{(I)} \quad (\text{for} \quad J = 1,2,3)$$
$$h_\alpha = u_{I,1}^{(I)}u_{J,11}^{(I)} + u_{I,11}^{(I)}u_{J,1}^{(I)} \quad [\text{for}\ \alpha = 4(I,J=2,3),\; 5(I,J=1,3), 6(I,J=1,2)]. \tag{10c}$$

It is seen that the first-order approximation equations are just the unperturbed linear ones. For plane wave solutions, the equations are the same as the Christoffel equations.[20] There are three acoustic wave modes: one quasi-longitudinal and two quasi-shear waves, all can propagate along the a-direction in crystals. Usually, the particle displacement component u_J includes contributions of all three quasi-longitudinal and quasi-shear waves. That is, three displacement components may be coupled to each other. Obviously, when $\gamma_{15} = \gamma_{16} = 0$, the displacement u_1 will not be coupled to u_2 and u_3. In this case, the direction of wave propagation is the first kind of pure mode direction. If the axes 2 and 3 of calculation coordinate system are selected to be coincident with polarization directions of two pure shear waves, then $\gamma_{56} = 0$.[20] Therefore, crystals having the first kind of pure mode directions are those with certain symmetries for which $\gamma_{15} = \gamma_{16} = \gamma_{56} = 0$. For the second kind of pure mode directions, the following conditions must be satisfied:[20] $\gamma_{15} \neq 0,\ \gamma_{16} = \gamma_{56} = 0$ or $\gamma_{16} \neq 0,\ \gamma_{15} = \gamma_{56} = 0$.

In ultrasonic measurements, the first kind of pure mode or simply the pure mode direction is preferred, since the interpretation of experimental results becomes simpler. Since there is no coupling between displacement components, it can be assumed that $u_1^{(I)} \neq 0,\ u_2^{(I)} = u_3^{(I)} = 0$ when dealing with longitudinal waves and $u_2^{(I)} \neq 0, u_1^{(I)} = u_3^{(I)} = 0$, or $u_3^{(I)} \neq 0,\ u_1^{(I)} = u_2^{(I)} = 0$ or $u_1^{(I)} = 0,\ u_2^{(I)} \neq 0,\ u_3^{(I)} \neq 0$

when dealing with shear waves. Besides, it is known that the second harmonic or waves with sum or difference frequencies (it will be called mix frequency wave hereafter) can reach the intensity strong enough to be detected in the measurements only when the interaction are said to be synchronous, that is, propagation velocities of the wave involved in the interaction are the same as the freely propagating second harmonic or mix frequency waves. Therefore, the second harmonic or mix frequency wave of shear waves generated through nonlinear interaction of longitudinal wave or vice versa is not relevant in practical experiments. Ignoring the non-synchronous interactions, the successive approximation equations for pure mode directions can be simplified. For the pure longitudinal wave, it is given by

$$\rho_0 \ddot{u}_1^{(I)} - \gamma_{11} u_{1,11}^{(I)} = 0, \tag{11a}$$

$$\rho_0 \ddot{u}_1^{(II)} - \gamma_{11} u_{1,11}^{(II)} = (3\gamma_{11} + \gamma_{111}) u_{1,1}^{(I)} u_{1,11}^{(I)}. \tag{11b}$$

Along a pure mode direction, the velocities of the two shear waves may or may not be the same. For the latter case, the successive approximate equations can be written as

$$\rho_0 \ddot{u}_2^{(I)} - \gamma_{66} u_{2,11}^{(I)} = 0, \tag{12a}$$

$$\rho_0 \ddot{u}_2^{(II)} - \gamma_{66} u_{2,11}^{(II)} = \gamma_{666} u_{2,1}^{(I)} u_{2,11}^{(I)}, \tag{12b}$$

or

$$\rho_0 \ddot{u}_3^{(I)} - \gamma_{55} u_{3,11}^{(I)} = 0, \tag{13a}$$

$$\rho_0 \ddot{u}_3^{(II)} - \gamma_{55} u_{3,11}^{(II)} = \gamma_{555} u_{3,1}^{(I)} u_{3,11}^{(I)}. \tag{13b}$$

For the former case, which is often referred to degenerate case, the self-action as well as cross-action between two shear waves are all synchronous. Thus, the equations are written as

$$\rho_0 \ddot{u}_2^{(I)} - \gamma u_{2,11}^{(I)} = 0, \tag{14a}$$

$$\rho_0 \ddot{u}_3^{(I)} - \gamma u_{3,11}^{(I)} = 0, \tag{14b}$$

$$\begin{aligned}\rho_0 \ddot{u}_2^{(II)} - \gamma u_{2,11}^{(II)} = {} & \gamma_{666} u_{2,1}^{(I)} u_{2,11}^{(I)} + \gamma_{556} u_{3,1}^{(I)} u_{3,11}^{(I)} \\ & + \gamma_{566} (u_{2,1}^{(I)} u_{3,11}^{(I)} + u_{2,11}^{(I)} u_{3,1}^{(I)}),\end{aligned} \tag{15a}$$

$$\begin{aligned}\rho_0 \ddot{u}_3^{(II)} - \gamma u_{3,11}^{(II)} = {} & \gamma_{566} u_{2,1}^{(I)} u_{2,11}^{(I)} + \gamma_{555} u_{3,1}^{(I)} u_{3,11}^{(I)} \\ & + \gamma_{556} (u_{2,1}^{(I)} u_{3,11}^{(I)} + u_{2,11}^{(I)} u_{3,1}^{(I)}).\end{aligned} \tag{15b}$$

Here, $\gamma = \gamma_{55} = \gamma_{66}$.

III. GENERATIONS OF SECOND HARMONIC AND MIX FREQUENCY WAVES

Since there is no mode coupling for pure mode directions, the second-order approximate equations can be solved separately for longitudinal and shear waves. For example, let the solution of Eq. (11a) be

$$u_1^{(I)} = A_1 \sin(\omega_1 t - k_1 a) + A_2 \sin(\omega_2 t - k_2 a). \tag{16}$$

Here, $k_j^2 = \rho_0 \omega_j^2 / \gamma_{11}$ ($j = 1, 2$). Then (11b) becomes

$$\begin{aligned}\rho_0 \ddot{u}_1^{(II)} - \gamma_{11} u_{1,11}^{(II)} = {} & \frac{1}{2}(3\gamma_{11} + \gamma_{111})\{k_1^3 A_1^2 \sin[2(\omega_1 t - k_1 a)] \\ & + k_2^3 A_2^2 \sin[2(\omega_2 t - k_2 a)] \\ & + k_1 k_2 (k_1 + k_2) A_1 A_2 \sin \\ & \times [(\omega_1 + \omega_2)t - (k_1 + k_2)a] \\ & + k_1 k_2 (k_1 - k_2) A_1 A_2 \sin \\ & \times [(\omega_1 - \omega_2)t - (k_1 - k_2)a]\}.\end{aligned} \tag{17}$$

Equation (17) is a linear inhomogeneous differential equation. The terms in the right-hand-side of the equation represents the self-action and cross-action of the fundamental waves, which can be considered as the driving force for the generation of the second harmonic and mix frequency waves. Since Eq. (17) becomes linear, the particular solutions for the second harmonic and mix frequency waves can be written separately as

$$\begin{aligned} u_1^{(II)} &= U_{2\omega_1} \cos[2(\omega_1 t - k_1 a)] \text{ or} \\ u_1^{(II)} &= U_{2\omega_2} \cos[2(\omega_2 t - k_2 a)],\end{aligned} \tag{18a}$$

$$U_{2\omega_1} = \frac{1}{8}\beta_L k_1^2 A_1^2 a \quad \text{or} \quad U_{2\omega_2} = \frac{1}{8}\beta_L k_2^2 A_2^2 a, \tag{18b}$$

for the second harmonic wave and

$$u_1^{(II)} = U_{\omega_1 \pm \omega_2} \cos[(\omega_1 \pm \omega_2)t - (k_1 \pm k_2)a], \tag{18c}$$

$$U_{\omega_1 \pm \omega_2} = \frac{1}{4}\beta_L k_1 k_2 A_1 A_2 a, \tag{18d}$$

for waves with sum or difference frequency. Here,

$$\beta_L = -\frac{3\gamma_{11} + \gamma_{111}}{\gamma_{11}} \tag{19}$$

is the so-called nonlinearity parameter.[21] It is seen that the amplitude of the second harmonic or mix frequency waves driven by the synchronous interactions will increase with propagation distance a. So their energy will be accumulated with propagation to reach a measurable intensity when the sample is long enough. Both the second order elastic constants (SOECs) and TOECs are involved in the defined nonlinearity parameter. The former represents the contribution from the induced nonlinearity due to the finite strain while the latter is the contribution of the intrinsic nonlinearity of the materials.

Similar results can be obtained for shear waves. The non-degenerate shear waves can have exactly the same solutions as the longitudinal wave but with the corresponding nonlinearity parameters given by

$$\beta_{S1} = -\frac{\gamma_{555}}{\gamma_{55}} \quad \text{or} \quad \beta_{S2} = -\frac{\gamma_{666}}{\gamma_{66}}. \tag{20a,b}$$

For degenerated shear waves, the setup in an experiment may be in such a way that the transducers with angular frequencies ω_1 and ω_2 are used to generate the fundamental shear waves simultaneously. In this case, the solutions of the first order approximate equations (14a) and (14b) can be written as

$$u_2^{(I)} = A_1 \sin(\omega_1 t - k_1 a) + A_2 \sin(\omega_2 t - k_2 a), \tag{21a}$$

$$u_3^{(I)} = B_1 \sin(\omega_1 t - k_1 a) + B_2 \sin(\omega_2 t - k_2 a), \tag{21b}$$

where $k_{1,2} = \omega_{1,2}\sqrt{\rho/\gamma}$ are the wave number of the fundamental shear waves. Substituting Eqs. (21) into Eqs. (15a) and (15b) gives

$$\begin{aligned}\rho_0 \ddot{u}_2^{(II)} - \gamma u_{2,11}^{(II)} = {} & \frac{1}{2}k_1^3(\gamma_{666}A_1^2 + \gamma_{556}B_1^2 + 2\gamma_{566}A_1B_1)\sin[2(\omega_1 t - k_1 a)] \\ & + \frac{1}{2}k_2^3(\gamma_{666}A_2^2 + \gamma_{556}B_2^2 + 2\gamma_{566}A_2B_2)\sin[2(\omega_2 t - k_2 a)] \\ & + \frac{1}{2}k_1k_2(k_1+k_2)[(\gamma_{666}A_1A_2 + \gamma_{556}B_1B_2 + \gamma_{556}(A_1B_2 + A_2B_1)]\sin[(\omega_1+\omega_2)t - (k_1+k_2)a] \\ & + \frac{1}{2}k_1k_2(k_1-k_2)[(\gamma_{666}A_1A_2 + \gamma_{556}B_1B_2 + \gamma_{556}(A_1B_2 + A_2B_1)]\sin[(\omega_1-\omega_2)t - (k_1-k_2)a],\end{aligned} \tag{22a}$$

$$\begin{aligned}\rho_0 \ddot{u}_3^{(II)} - \gamma u_{3,11}^{(II)} = {} & \frac{1}{2}k_1^3(\gamma_{566}A_1^2 + \gamma_{555}B_1^2 + 2\gamma_{556}A_1B_1)\sin[2(\omega_1 t - k_1 a)] \\ & + \frac{1}{2}k_2^3(\gamma_{566}A_2^2 + \gamma_{555}B_2^2 + 2\gamma_{556}A_2B_2)\sin[2(\omega_2 t - k_2 a)] \\ & + \frac{1}{2}k_1k_2(k_1+k_2)[(\gamma_{566}A_1A_2 + \gamma_{555}B_1B_2 + \gamma_{556}(A_1B_2 + A_2B_1)]\sin[(\omega_1+\omega_2)t - (k_1+k_2)a] \\ & + \frac{1}{2}k_1k_2(k_1-k_2)[(\gamma_{566}A_1A_2 + \gamma_{555}B_1B_2 + \gamma_{556}(A_1B_2 + A_2B_1)]\sin[(\omega_1-\omega_2)t - (k_1-k_2)a].\end{aligned} \tag{22b}$$

In the case of two fundamental shear waves are with different amplitudes and polarizations, it may be assumed that

$$A_1 = A\cos\varphi,\ B_1 = A\sin\varphi,\ \ A_2 = B\cos\psi,\ \ B_2 = B\sin\psi, \tag{23}$$

where ϕ and ψ are the angles of the polarization directions of the driving transducers of the fundamental waves with the direction of displacement u_2, A and B the amplitudes of the shear waves with frequencies ω_1 and ω_2, respectively. Then Eqs. (22) can be rewritten as

$$\begin{aligned}\rho_0 \ddot{u}_2^{(II)} - \gamma u_{2,11}^{(II)} = {} & \frac{1}{2}k_1^3(\gamma_{666}\cos^2\varphi + \gamma_{556}\sin^2\varphi + \gamma_{566}\sin 2\varphi)A^2\sin[2(\omega_1 t - k_1 a)] \\ & + \frac{1}{2}k_2^3(\gamma_{666}\cos^2\psi + \gamma_{556}\sin^2\psi + \gamma_{566}\sin 2\psi)B^2\sin[2(\omega_2 t - k_2 a)] \\ & + \frac{1}{2}k_1k_2(k_1+k_2)[(\gamma_{666}\cos\varphi\cos\psi + \gamma_{556}\sin\varphi\sin\psi + \gamma_{556}\sin(\varphi+\psi)]AB\sin[(\omega_1+\omega_2)t - (k_1+k_2)a] \\ & + \frac{1}{2}k_1k_2(k_1-k_2)[(\gamma_{666}\cos\varphi\cos\psi + \gamma_{556}\sin\varphi\sin\psi + \gamma_{556}\sin(\varphi+\psi)]AB\sin[(\omega_1-\omega_2)t - (k_1-k_2)a],\end{aligned} \tag{24a}$$

$$\begin{aligned}\rho_0 \ddot{u}_2^{(II)} - \gamma u_{2,11}^{(II)} = {} & \frac{1}{2}k_1^3(\gamma_{566}\cos^2\varphi + \gamma_{555}\sin^2\varphi + \gamma_{556}\sin 2\varphi)A^2\sin[2(\omega_1 t - k_1 a)] \\ & + \frac{1}{2}k_2^3(\gamma_{566}\cos^2\psi + \gamma_{555}\sin^2\psi + \gamma_{556}\sin 2\psi)B^2\sin[2(\omega_1 t - k_1 a)] \\ & + \frac{1}{2}k_1k_2(k_1+k_2)[(\gamma_{566}\cos\varphi\cos\psi + \gamma_{555}\sin\varphi\sin\psi + \gamma_{556}\sin(\varphi+\psi)]AB\sin[(\omega_1+\omega_2)t - (k_1+k_2)a] \\ & + \frac{1}{2}k_1k_2(k_1-k_2)[(\gamma_{666}\cos\varphi\cos\psi + \gamma_{556}\sin\varphi\sin\psi + \gamma_{556}\sin(\varphi+\psi)]AB\sin[(\omega_1-\omega_2)t - (k_1-k_2)a].\end{aligned} \tag{24b}$$

It is seen that Eqs. (24) are similar to Eq. (17). The interactions of two degenerate shear waves will generate the second harmonic waves of each fundamental wave as well as mix frequency waves. Those waves can be expressed, respectively, by

$$
\begin{aligned}
u^{(II)}_{2\_2\omega_1} &= U_{2-2\omega_1}\cos[2(\omega_1 t - k_1 a)],\quad u^{(II)}_{2\_2\omega_2} = U_{2-2\omega_2}\cos[2(\omega_2 t - k_1 a)],\\
u^{(II)}_{2\_\omega_1\pm\omega_2} &= U_{2\_\omega_1\pm\omega_2}\cos[(\omega_1\pm\omega_2)t - (k_1\pm k_2)a],\\
u^{(II)}_{3\_2\omega_1} &= U_{3-2\omega_1}\cos[2(\omega_1 t - k_1 a)],\quad u^{(II)}_{3\_2\omega 2} = U_{3-2\omega_2}\cos[2(\omega_2 t - k_2 a)],\\
u^{(II)}_{3\_\omega_1\pm\omega_2} &= U_{3\_\omega_1\pm\omega_2}\cos[(\omega_1\pm\omega_2)t - (k_1\pm k_2)a)],
\end{aligned}
\tag{25a-f}
$$

where

$$
\begin{aligned}
U_{2-2\omega_1} &= \frac{1}{8}\beta_{S3}k_1^2A^2a,\quad U_{2-2\omega_2} = \frac{1}{8}\beta_{S4}k_2^2B^2a,\\
U_{3-2\omega_1} &= \frac{1}{8}\beta_{S5}k_1^2A^2a,\quad U_{3-2\omega_2} = \frac{1}{8}\beta_{S6}k_2^2B^2a,\\
U_{2-\omega_1\pm\omega_2} &= \frac{1}{4}\beta_{S7}k_1k_2ABa,\quad U_{3-\omega_1\pm\omega_2} = \frac{1}{4}\beta_{S8}k_1k_2ABa,
\end{aligned}
\tag{26a-f}
$$

and

$$
\begin{aligned}
\beta_{S3} &= -\frac{\gamma_{666}\cos^2\varphi + \gamma_{556}\sin^2\varphi + \gamma_{566}\sin 2\varphi}{\gamma},\\
\beta_{S4} &= -\frac{\gamma_{666}\cos^2\psi + \gamma_{556}\sin^2\psi + \gamma_{566}\sin 2\psi}{\gamma},\\
\beta_{S5} &= -\frac{\gamma_{566}\cos^2\varphi + \gamma_{555}\sin^2\varphi + \gamma_{556}\sin 2\varphi}{\gamma},\\
\beta_{S6} &= -\frac{\gamma_{566}\cos^2\psi + \gamma_{555}\sin^2\psi + \gamma_{556}\sin 2\psi}{\gamma},\\
\beta_{S7} &= -\frac{\gamma_{666}\cos\varphi\cos\psi + \gamma_{556}\sin\varphi\sin\psi + \gamma_{566}\sin(\varphi+\psi)}{\gamma},\\
\beta_{S8} &= -\frac{\gamma_{566}\cos\varphi\cos\psi + \gamma_{555}\sin\varphi\sin\psi + \gamma_{556}\sin(\varphi+\psi)}{\gamma}.
\end{aligned}
\tag{27a-f}
$$

In experiments, it is quite often that one single broadband transducer is used to generate two fundamental shear waves with slightly different frequencies. In this case, $\varphi = \psi$ and

$$
\begin{aligned}
\beta_{S3} = \beta_{S4} = \beta_{S7} &= -\frac{\gamma_{666}\cos^2\varphi + \gamma_{556}\sin^2\varphi + \gamma_{566}\sin 2\varphi}{\gamma},\\
\beta_{S5} = \beta_{S6} = \beta_{S8} &= -\frac{\gamma_{566}\cos^2\varphi + \gamma_{555}\sin^2\varphi + \gamma_{556}\sin 2\varphi}{\gamma}.
\end{aligned}
\tag{28a,b}
$$

Meanwhile, if one receiving transducer is used to detect one of the second harmonic or mix frequency waves, the amplitude detected by the receiving transducer may be expressed as

$$
U = U_2\cos\theta + U_3\sin\theta, \tag{29}
$$

where U_2 and U_3 represent the amplitudes of the second harmonic or mix frequency waves along the directions of displacements u_2 and u_3, respectively, ϕ is the angle between polarization direction of the receiving transducer and displacement u_2. Usually, $\theta = \varphi$.

It is seen from Eqs. (20a,b) and (27a–f) that only intrinsic nonlinearity of materials contributes to the quadratic nonlinear effects of pure shear waves.

IV. EFFECTIVE SOECS AND TOECS OF CRYSTALS

The above discussions show that the TOECs, which characterize the quadratic nonlinear interactions of collinear acoustic waves along pure mode directions of crystals, are γ_{111}, γ_{555}, γ_{666}, γ_{556}, and γ_{566}. Those constants are referred to the calculation coordinates, which may be different from the constitutive coordinates. They can be related to constants defined under constitutive coordinates through the following tensor transformation:

$$
\gamma_{IJKLMN} = \alpha_{IP}\alpha_{JQ}\alpha_{KR}\alpha_{LS}\alpha_{MT}\alpha_{NU}c_{PQRSTU}, \tag{30}
$$

where α_{AB} is the element of coordinate transformation matrix, i.e., the direction cosine of rotated A-axis with respect to the B-axis of original coordinate. Thus, γ_{IJKLMN} may be just a single c_{IJKLMN} constant or a combination of several c_{IJKLMN}, so that it is called an effective TOEC.

The pure mode directions for various crystals were researched by Brugger.[20] The relation between the calculation and constitutive coordinates, i.e., α_{AB} can be found in Ref. 20 where the *a*-axis (or 1-axis) of the calculation coordinate is always parallel to the direction of wave propagation, that is, to the displacement direction of the pure longitudinal mode wave. Other two axes are parallel to displacement directions of the two pure mode shear waves, as mentioned above.

The TOEC is a six-order tensor. There are total 729 elements, which means that there are 729 summations in Eq. (30). But the symmetries of TOECs make the maximum independent TOECs being 56. The 56 independent TOECs can be grouped by the possible ways for the index to permute their positions, as shown in Table I.

Now, for simplicity, we define the following coefficients, here the superscripts x,y,z in $A^{x,y,z}_{ijklmn}$ correspond to the lower indexes of the relevant third order elastic constants c_{xyz}:

TABLE I. The 56 independent TOECs (M indicates the number of the possible ways for indexes to permute their positions).

M	TOECs
1	$c_{111}, c_{222}, c_{333}$
3	$c_{112}, c_{113}, c_{122}, c_{133}, c_{223}, c_{233}$
6	$c_{114}, c_{115}, c_{116}, c_{224}, c_{225}, c_{226}, c_{334}, c_{335}, c_{336}, c_{123}$
8	$c_{444}, c_{555}, c_{666}$
12	$c_{124}, c_{125}, c_{126}, c_{134}, c_{135}, c_{136}, c_{234}, c_{235}, c_{236},$ $c_{144}, c_{155}, c_{166}, c_{344}, c_{355}, c_{366}, c_{254}, c_{255}, c_{266}$
24	$c_{145}, c_{146}, c_{156}, c_{245}, c_{246}, c_{256}, c_{345}, c_{346},$ $c_{356}, c_{445}, c_{446}, c_{455}, c_{466}, c_{556}, c_{566}$
48	c_{456}

$$\begin{aligned}
A_{ijklmn}^{(ppp)} &= a_p b_p c_p, \text{ for } c_{111}, c_{222}, c_{333} \\
A_{ijklmn}^{(ppq)} &= a_p b_p c_q + a_p b_q c_p + a_q b_p c_p \text{ for } c_{112}, c_{113}, c_{122}, c_{133}, c_{223}, c_{233} \\
A_{ijklmn}^{(ppQ)} &= a_p b_p c_Q + a_p b_Q c_p + a_Q b_p c_p \text{ for } c_{114}, c_{115}, c_{116}, c_{224}, c_{225}, c_{226}, c_{334}, c_{335}, c_{336} \\
A_{ijklmn}^{(pqQ)} &= a_p(b_q c_Q + b_Q c_q) + a_q(b_p c_Q + b_Q c_p) + a_Q(b_p c_q + b_q c_p) \\
&\quad \text{for } c_{124}, c_{125}, c_{126}, c_{134}, c_{135}, c_{136}, c_{234}, c_{235}, c_{236} \\
A_{ijklmn}^{(pQQ)} &= a_p b_Q c_Q + a_Q b_p c_Q + a_Q b_Q c_p, \text{ for } c_{144}, c_{155}, c_{166}, c_{244}, c_{255}, c_{266}, c_{344}, c_{355}, c_{366}, \\
A_{ijklmn}^{(pQR)} &= a_p(b_Q c_R + b_R c_Q) + b_p(a_Q c_R + a_R c_Q) + c_p(a_Q b_R + a_R b_Q) \\
&\quad \text{for } c_{145}, c_{146}, c_{156}, c_{245}, c_{246}, c_{256}, c_{345}, c_{346}, c_{356} \\
A_{ijklmn}^{(QQR)} &= a_Q b_Q c_R + a_Q b_R c_Q + a_R b_Q c_Q \text{ for } c_{445}, c_{446}, c_{455}, c_{466}, c_{556}, c_{566} \\
A_{ijklmn}^{(QQQ)} &= a_Q b_Q c_Q \text{ for } c_{444}, c_{555}, c_{666} \\
A_{ijklmn}^{(123)} &= a_1(b_2 c_3 + b_3 c_2) + a_2(b_1 c_3 + b_3 c_1) + a_3(b_1 c_2 + b_2 c_1) \text{ for } c_{123} \\
A_{ijklmn}^{(456)} &\to a_4(b_5 c_6 + b_6 c_5) + a_5(b_4 c_6 + b_6 c_4) + a_6(b_5 c_4 + b_4 c_5) \text{ for } c_{456}.
\end{aligned} \tag{31}$$

Here,

$$\begin{aligned}
&a_p = \alpha_{ip}\alpha_{jp}, \; b_p = \alpha_{kp}\alpha_{lp}, \; c_p = \alpha_{mp}\alpha_{np}, \\
&a_Q = \alpha_{ip}\alpha_{jq} + \alpha_{iq}\alpha_{jp} \\
&b_Q = \alpha_{kp}\alpha_{lq} + \alpha_{kq}\alpha_{lp} \;\; c_Q = \alpha_{mp}\alpha_{nq} + \alpha_{mq}\alpha_{np}, \\
&p, q = 1, 2, 3, \quad Q, R = \begin{cases} 4 & p, q = 2, 3 \\ 5 & p, q = 3, 1 \\ 6 & p, q = 1, 2. \end{cases}
\end{aligned} \tag{32}$$

Every $A_{ijklmn}^{()}$ includes the summation of M times of products $\alpha_{is}\alpha_{jt}\alpha_{ku}\alpha_{lv}\alpha_{mw}\alpha_{nx}$, Then, the summation in Eq. (30) can be grouped into N terms, where N is equal to the number of independent TOECs of the crystals determined by the crystal symmetry.

For example, the independent and non-zero TOECs of tetragonal point groups 422, 4 mm, $\bar{4}2$ m, and 4/mmm are 12 and 20, respectively, i.e., $c_{111} = c_{222}$, $c_{112} = c_{122}$, $c_{113} = c_{223}$, c_{123},$c_{133} = c_{233}$, $c_{144} = c_{255}$, $c_{155} = c_{244}$, $c_{166} = c_{266}$, c_{333}, $c_{344} = c_{355}$, c_{366}, c_{456}.

The TOEC under an arbitrary rotated coordinate can be written as

$$\begin{aligned}
\gamma_{ijklmn} = &(A_{ijklmn}^{(111)} + A_{ijklmn}^{(222)})c_{111} + (A_{ijklmn}^{(112)} + A_{ijklmn}^{(122)})c_{112} + (A_{ijklmn}^{(113)} + A_{ijklmn}^{(223)})c_{113} + A_{ijklmn}^{(123)}c_{123} \\
&+ (A_{ijklmn}^{(133)} + A_{ijklmn}^{(233)})c_{133} + (A_{ijklmn}^{(144)} + A_{ijklmn}^{(255)})c_{144} + (A_{ijklmn}^{(155)} + A_{ijklmn}^{(244)})c_{155} \\
&+ (A_{ijklmn}^{(166)} + A_{ijklmn}^{(266)})c_{166} + A_{ijklmn}^{(333)}c_{333} + (A_{ijklmn}^{(344)} + A_{ijklmn}^{(355)})c_{344} + A_{ijklmn}^{(366)}c_{366} + A_{ijklmn}^{(456)}c_{456}.
\end{aligned} \tag{33}$$

Obviously, the calculations of Eq. (33) can be implemented by computer. The calculated effective TOECs for pure mode directions of tetragonal point groups 422, 4 mm, $\bar{4}2$ m, and 4/mmm are shown in Table II. Here, the symbols for pure mode directions defined in Ref. 20 are used. For other point groups, the formula similar to Eq. (33) can be easily obtained.

Similarly, the effective SOECs involved in above equations can be written as

$$\gamma_{ijkl} = \alpha_{ip}\alpha_{jq}\alpha_{rk}\alpha_{sl}c_{pqrs}. \tag{34}$$

They can be calculated by the same method as that for effective TOECs given above or through M-matrix listed by Auld on the cover page of his book.[22] The calculated results for tetragonal crystals[20] (point group 422, 4 mm, $\bar{4}2$ m, and 4/mmm) are also shown in Table II.

V. DISCUSSION AND CONCLUSION

In this paper, interactions of collinear elastic waves propagating along pure mode directions of crystals have been investigated. The nonlinearity parameters describing the interactions are given. The effective TOECs involved in the parameters are γ_{111}, γ_{555}, and γ_{666} (when shear waves are non-degenerated) or γ_{111}, γ_{555}, γ_{666}, γ_{556}, and γ_{566} (when shear waves are degenerated). A computerized method to calculate those effective TOECs of crystals is presented. It is found that the calculation method presented in this paper

TABLE II. Effective SOECs and TOECs of tetragonal crystals (Tetragonal 422, 4 mm, $\bar{4}2$ m, and 4/mmm).

	TIα	TIβ[a]	TIπ[a]	TIγ	TIκ
γ_{11}	c_{33}	$\frac{1}{2}c_{11}\cos^4\mu+\frac{1}{2}c_{12}\cos^4\mu+c_{66}\cos^4\mu$ $+2c_{13}\cos^2\mu\sin^2\mu+2c_{14}\cos^2\mu\sin^2\mu$ $+c_{66}\sin^4\mu$	$c_{11}\cos^4\theta+2c_{13}\cos^2\theta\sin^2\theta$ $+4c_{44}\cos^2\theta\sin^2\theta$ $+c_{33}\sin^4\theta$	$\frac{1}{2}c_{11}+\frac{1}{2}c_{12}$ $+c_{66}$	c_{11}
γ_{55}	c_{44}	$\frac{1}{2}c_{11}\cos^2\mu\sin^2\mu+\frac{1}{2}c_{12}\cos^2\mu\sin^2\mu$ $-2c_{13}\cos^2\mu\sin^2\mu+c_{33}\cos^2\mu\sin^2\mu$ $+c_{66}\cos^2\mu\sin^2\mu+c_{44}\cos^2 2\mu$	$c_{11}\cos^2\theta\sin^2\theta-2c_{13}\cos^2\theta\sin^2\theta$ $+c_{33}\cos^2\theta\sin^2\theta+c_{44}\cos^2 2\theta$	c_{44}	c_{44}
γ_{66}	c_{44}	$\frac{1}{2}c_{11}\cos^2\mu-\frac{1}{2}c_{12}\cos^2\mu$ $+c_{44}\sin^2\mu$	$c_{44}\sin^2\theta+c_{66}\cos^2\theta$	$-\frac{1}{2}c_{12}+\frac{1}{2}c_{11}$	c_{66}
γ_{15}	0	$-\frac{1}{2}c_{11}\cos^3\mu\sin\mu-\frac{1}{2}c_{12}\cos^3\mu\sin\mu$ $-c_{66}\cos^3\mu\sin\mu+c_{33}\cos\mu\sin^3\mu$ $+2c_{44}\cos\mu\sin\mu\cos 2\mu$ $+c_{13}\cos\mu\sin\mu\cos 2\mu$	$-c_{11}\cos^3\theta\sin\theta+c_{33}\cos\theta\sin^3\theta$ $+2c_{44}\cos\theta\sin\theta\cos 2\theta$ $+c_{13}\cos\theta\sin\theta\cos 2\theta$	0	0
γ_{16}	0	0	0	0	0
γ_{56}	0	0	0	0	0
γ_{111}	c_{333}	$\frac{1}{4}c_{111}\cos^6\mu+\frac{3}{4}c_{112}\cos^6\mu$ $+3c_{166}\cos^6\mu+\frac{3}{2}c_{113}\cos^4\mu\sin^2\mu$ $+\frac{3}{2}c_{123}\cos^4\mu\sin^2\mu+6c_{144}\cos^4\mu\sin^2\mu$ $+6c_{155}\cos^4\mu\sin^2\mu+3c_{366}\cos^4\mu\sin^2\mu$ $+12c_{456}\cos^4\mu\sin^2\mu+3c_{133}\cos^2\mu\sin^4\mu$ $+12c_{344}\cos^2\mu\sin^4\mu+c_{333}\sin^6\mu$	$c_{111}\cos^6\theta+3c_{113}\cos^4\theta\sin^2\theta$ $+12c_{155}\cos^4\theta\sin^2\theta$ $+3c_{133}\cos^2\theta\sin^4\theta$ $+12c_{344}\cos^2\theta\sin^4\theta$ $+c_{333}\sin^6\theta$	$\frac{1}{4}C_{111}+\frac{3}{4}C_{112}$ $+3c_{166}$	c_{111}
γ_{555}	0	$-\frac{1}{4}c_{111}\cos^3\mu\sin^3\mu-\frac{3}{4}c_{112}\cos^3\mu\sin^3\mu$ $+\frac{3}{2}c_{113}\cos^3\mu\sin^3\mu+\frac{3}{2}c_{123}\cos^3\mu\sin^3\mu$ $-3c_{133}\cos^3\mu\sin^3\mu-3c_{166}\cos^3\mu\sin^3\mu$ $+c_{333}\cos^3\mu\sin^3\mu+3c_{366}\cos^3\mu\sin^3\mu$ $-\frac{3}{2}c_{144}\cos\mu\sin\mu\cos^2 2\mu-\frac{3}{2}c_{155}\cos\mu\sin\mu\cos^2 2\mu$ $+3c_{344}\cos\mu\sin\mu\cos^2 2\mu-3c_{456}\cos\mu\sin\mu\cos^2 2\mu$	$-c_{111}\cos^3\theta\sin^3\theta$ $+3c_{113}\cos^3\theta\sin^3\theta$ $-3c_{133}\cos^3\theta\sin^3\theta$ $+c_{333}\cos^3\theta\sin^3\theta$ $-3c_{155}\cos\theta\sin\theta\cos^2 2\theta$ $+3c_{344}\cos\theta\sin\theta\cos^2 2\theta$	0	0
γ_{666}	0	0	0	0	0
γ_{556}	0	0	0	0	0
γ_{566}	0	$-\frac{1}{4}c_{111}\cos^3\mu\sin\mu+\frac{1}{4}c_{112}\cos^3\mu\sin\mu$ $+\frac{1}{2}c_{113}\cos^3\mu\sin\mu-\frac{1}{2}c_{123}\cos^3\mu\sin\mu$ $+c_{344}\cos\mu\sin^3\mu+c_{456}\cos\mu\sin^3\mu$ $+c_{144}\left(-\frac{1}{2}\cos\mu\sin^3\mu-\cos\mu\sin\mu\cos 2\mu\right)$ $+c_{155}\left(-\frac{1}{2}\cos\mu\sin^3\mu+\cos\mu\sin\mu\cos 2\mu\right)$	$-c_{166}\cos^3\theta\sin\theta+c_{366}\cos^3\theta\sin\theta$ $-c_{144}\cos\theta\sin^3\theta+c_{344}\cos\theta\sin^3\theta$ $+2c_{456}\cos\theta\sin\theta\cos 2\theta$	0	0

[a]These are the second kind of pure mode directions. The shear wave with particle displacement along the 2-axis is a pure one. Another shear wave is coupled to the longitudinal wave.

will give the same results listed in Ref. 17 for cubic crystal, which testifies the validity of our method.

It is observed that γ_{111} never vanishes. Thus, quadratic nonlinear interaction of longitudinal waves is always present regardless of the direction of wave propagation. From Eq. (30),

$$\gamma_{111}=\gamma_{111111}=\alpha_{1p}\alpha_{1q}\alpha_{1r}\alpha_{1s}\alpha_{1t}\alpha_{1u}c_{pqrstu}$$
$$=\alpha_{11}^6c_{111}+\alpha_{12}^6c_{222}+\alpha_{13}^6c_{333}+\cdots. \tag{35}$$

It is known that c_{111}, c_{222}, and c_{333} are never zero for any crystal (including isotropic solids). Among α_{11}, α_{12}, and α_{13}, at least one of them is non-zero, hence, γ_{111} is never zero, which is at least equal to one of c_{111}, c_{222}, and c_{333}. But for γ_{555} and γ_{666}, the situation is different

$$\gamma_{555}=\gamma_{131313}=\alpha_{1p}\alpha_{3q}\alpha_{1r}\alpha_{3s}\alpha_{1t}\alpha_{3u}c_{porstu},$$
$$\gamma_{666}=\gamma_{121212}=\alpha_{1p}\alpha_{2q}\alpha_{1r}\alpha_{2s}\alpha_{1t}\alpha_{2u}c_{pqrstu}. \tag{36a,b}$$

They involve the product of elements of the transformation matrix in different rows. If one of α_{ij} is zero then the products $\alpha_{1p}\alpha_{2q}\alpha_{1r}\alpha_{2s}\alpha_{1t}\alpha_{2u}=0$, $\alpha_{1p}\alpha_{3q}\alpha_{1r}\alpha_{3s}\alpha_{1t}\alpha_{3u}=0$. Besides, c_{555} and c_{666} themselves are zero for some crystals due to symmetry. Thus, the probability for γ_{555} and γ_{666} to be zero is very high. Our calculations show that γ_{555} is zero for most of pure mode directions and γ_{666} is zero for all the calculated cases. The quadratic nonlinear interaction of shear waves is still prohibited for many pure mode directions.

Our results presented in this paper provide a general method to calculate effective TOECs, which can be used for any symmetry systems and will be very helpful for experimentally investigating the nonlinear elastic properties of crystals.

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APPENDIX: α_{AB} FOR TETRAGONAL CRYSTALS

Tetragonal (422, 4 mm, $\bar{4}$2 m, 422)

1. TIα

$$\alpha = \begin{bmatrix} 0 & 0 & 1 \\ \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \end{bmatrix} \quad (\text{Along } [001])$$

θ can have any value in the case of degenerate transverse waves.

2. TIβ $$\alpha = \begin{bmatrix} \sqrt{\frac{1}{2}}\cos\mu & \sqrt{\frac{1}{2}}\cos\mu & \sin\mu \\ -1/\sqrt{2} & 1/\sqrt{2} & 0 \\ -\sqrt{\frac{1}{2}}\sin\mu & -\sqrt{\frac{1}{2}}\sin\mu & \cos\mu \end{bmatrix}$$

$$\sqrt{\frac{2C}{2A-B+2C}} = \cos\mu, \quad \sqrt{\frac{2A-B}{2A-B+2C}} = \sin\mu$$

$$A = c_{11} - 2c_{44} - c_{13}, \quad B = c_{11} - 2c_{66} - c_{12},$$
$$C = c_{33} - 2c_{44} - c_{13}$$

μ has a special value.

3. TIπ

$$\alpha = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix}$$
$$\times\ (\text{Along a special direction on x-z plane})\text{t}$$
$$\cos\theta = \sqrt{C/(A+C)}$$

θ has a special value.

4. TIγ

$$\alpha = \begin{bmatrix} \sqrt{1/2} & \sqrt{1/2} & 0 \\ -\sqrt{1/2} & \sqrt{1/2} & 0 \\ 0 & 0 & 1 \end{bmatrix} \ (\text{Along diagonal of x-y plane})$$

5. TIκ

$$\alpha = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

(Along [100] or [010]).

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