Elastic properties of a two-dimensional model of crystals containing particles with rotational degrees of freedom

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We consider a discrete two-dimensional model of a crystal with particles having rotational degrees of freedom. We derive the equations of motion and analyze its continuum analog obtained in the long-wave limit. The continuum equations are shown to be the ones of the micropolar elasticity theory. The conditions when the micropolar elasticity equations can be reduced to the equations of conventional elasticity theory are discussed. We show that the rotational degrees of freedom are responsible for the anomalies in the elastic properties of some of the dielectric crystals.

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I. INTRODUCTION

In many dielectric crystals the atom clusters are put together to form a lattice and the forces that hold the clusters together are usually much weaker compared to intercluster forces. It is natural to assume for such crystals that atom clusters are rigid: that is, to neglect the high-frequency intercluster vibrations. The positions of a finite-size cluster is defined not only by the displacement vector but also by the orientation angles. Coupling of the translational and rotational degrees of freedom may result in the appearance of soft optic modes. Contributions of the rotational modes to the physics of dielectric crystals have been studied from a continuum viewpoint[1–4] and with the use of microscopic models.[2,5–9] The role of rigid unit modes (RUM's) in amorphous and crystalline silica has been studied in Ref. 10. The theory of the coupling of an electric field with a field of elastic strain has been developed by Sannikov.[11]

In the present paper we focus on unusual elastic properties exhibited by the crystals with particles having rotational degrees of freedom. Particularly, we examine the nature of the negative Poisson ratio (ν) in such crystals. The Poisson ratio characterizes the response of an elastic body to uniaxial stress and is defined as the negative ratio between the transverse strain and the corresponding axial strain. For most of the materials in nature ν lies in the range from 0 to 0.5 and normally it is nearly equal to 0.3. Practically zero ν is exhibited, for example, by cork, and $\nu=0.5$ (constant volume medium) is observed for rubber or for the plastic deformation of metals.

An elastic medium can be stable only if the Lame coefficients are positive.[12] This suggests that the Poisson ratio of an isotropic elastic medium can range from -1 to 0.5. For an anisotropic medium, ν can take any value in some particular directions. That is why the negative ν is often attributed to the anisotropy of medium.[13] The anisotropy is the reason for the negative ν in highly anisotropic crystals like arsenic, antimony, and bismuth[14] and also in many single crystals of cubic metals deformed in an oblique direction with respect to the cubic axis.[15] However, *isotropic* materials with negative ν are quite rare. Cubic metals in the polycrystalline (isotropic) state show ν of about 0.3. It seems that the negative ν in an isotropic medium can be explained through the rotational degrees of freedom. The examples are the foams[16,17] and quartz (isotropic in the XY plane) near the α-β phase transition.[18]

In auxetics the negative Poisson ratio can be explained by their special electronic structure.[19]

An anomaly in the Poisson ratio has been reported for an isotropic two-dimensional (2D) microscopic model by Wojciechowski.[8] In his model ν becomes negative at high densities. A negative Poisson ratio has been reported for a model with rigid and elastic links randomly placed on a 2D honeycomb network near the percolation threshold.[20] The possibility to obtain an arbitrary ν in an anisotropic 2D microscopic model has been proved in Ref. 21. The model studied in Ref. 21 is a 2D generalization of the elastically hinged molecule (EHM) model.[22–24]

Another anisotropic 2D model with particles having rotational degrees of freedom has been offered by Ishibashi and Iwata[25] in order to describe some properties of the KH_2PO_4 (KDP) family of crystals, which has been studied extensively in the last five decades.[26] Their model contains the rigid particles square in shape, which stand for PO_4 tetrahedra. The model explains the variation of ν from -1 to 0. Here we carry out a more elaborate study of this model. We analyze the elastic properties of the anisotropic model subjected to homogeneous strain; then we analyze the dispersion relations of the discrete model in comparison with the dispersion relations of two different continuum approximations.

The paper is organized as follows. In Sec. II we describe the model and in Sec. III the Hamiltonian and the equations of motion are given. Section IV is devoted to an analysis of the homogeneous strain. In Sec. V the dispersion relations of the microscopic model are derived, and in Sec. VI the discrete model is reduced to the continuum one and, under certain assumptions, to the anisotropic elasticity theory. In Sec. VII the dispersion relations for continuum models are de-

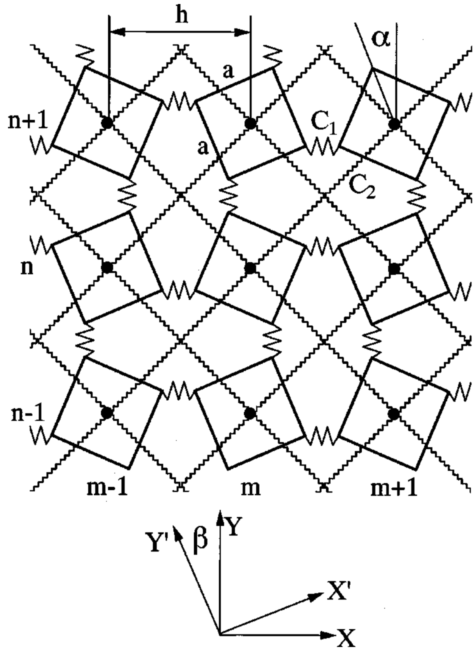

FIG. 1. The 2D microscopic model of a crystal. Absolutely rigid square particles are bound elastically and each particle experiences the action of the rotational background potential. The lattice spacing is *h*, and *a* and α are the size and the orientation angle of particles, respectively.

rived and, in Sec. VIII, they are compared to that of the discrete model.

II. DESCRIPTION OF THE MODEL

We consider the 2D microscopic model of a crystal shown in Fig. 1. The model consists of absolutely rigid elastically bound square particles and each particle experiences the action of the rotational background potential.

The geometry of the model can be described by the two parameters: the lattice spacing h and the parameter

$$A=\frac{\sqrt{2}}{2}a\sin\alpha, \tag{1}$$

where a and α are the size and the orientation angle of particles, respectively.

Particles have mass M and moment of inertia J. Each particle experiences the action of the rotational background potential with coefficient C. Elastic bonds with coefficient C_1 connect the vertices of each particle with the vertices of nearest neighbors. Elastic bonds with coefficient C_2 connect the center of each particle with the centers of next-nearest neighbors. We are interested here in the elastic properties of the model so that we do not introduce any anharmonic terms.

Particles are numbered with two indices m and n. Each particle has three degrees of freedom, namely, two components of displacement vector from the lattice point, $u_{m,n}, v_{m,n}$, and the angle of rotation, $\varphi_{m,n}$. A translational cell of the model [square area defined by the centers of particles $(m,n-1)$, $(m+1,n)$, $(m,n+1)$, and $(m-1,n)$] contains two particles. However, the primitive cell contains only one particle [square area defined by the centers of particles $(m-1,n-1)$, $(m,n-1)$, (m,n), and $(m-1,n)$].

III. HAMILTONIAN AND EQUATIONS OF MOTION

We introduce the new variables

$$\phi_{m,n}=(-1)^{m+n}\varphi_{m,n}. \tag{2}$$

Then, the energy of the model can be written as

$$\begin{aligned}H=\frac{1}{2}\sum_{m,n}\Big\{&M\dot{u}_{m,n}^2+M\dot{v}_{m,n}^2+J\dot{\phi}_{m,n}^2+C\phi_{m,n}^2\\&+C_1[u_{m,n}-u_{m-1,n}-A(\phi_{m,n}+\phi_{m-1,n})]^2\\&+C_1[v_{m,n}-v_{m,n-1}-A(\phi_{m,n}+\phi_{m,n-1})]^2\\&+\frac{C_2}{2}(u_{m,n}+v_{m,n}-u_{m-1,n-1}-v_{m-1,n-1})^2\\&+\frac{C_2}{2}(u_{m,n}-v_{m,n}-u_{m-1,n+1}+v_{m-1,n+1})^2\Big\},\end{aligned} \tag{3}$$

where the first three terms give the kinetic energy, the fourth term gives the energy of the rotational on-site potential, the following two terms give the energy of the vertex-to-vertex bonds, and the last two terms give the energy of center-to-center bonds.

Then, the equations of motion are

$$\begin{aligned}M\ddot{u}_{m,n}=&C_1(u_{m+1,n}-2u_{m,n}+u_{m-1,n})-C_1A(\phi_{m+1,n}\\&-\phi_{m-1,n})+\frac{C_2}{2}(u_{m+1,n+1}+u_{m-1,n-1}+u_{m+1,n-1}\\&+u_{m-1,n+1}-4u_{m,n})+\frac{C_2}{2}(v_{m+1,n+1}+v_{m-1,n-1}\\&-v_{m+1,n-1}-v_{m-1,n+1}),\end{aligned} \tag{4}$$

$$\begin{aligned}M\ddot{v}_{m,n}=&C_1(v_{m,n+1}-2v_{m,n}+v_{m,n-1})-C_1A(\phi_{m,n+1}\\&-\phi_{m,n-1})+\frac{C_2}{2}(u_{m+1,n+1}+u_{m-1,n-1}-u_{m+1,n-1}\\&-u_{m-1,n+1})+\frac{C_2}{2}(v_{m+1,n+1}+v_{m-1,n-1}\\&+v_{m+1,n-1}+v_{m-1,n+1}-4v_{m,n}),\end{aligned} \tag{5}$$

$$\begin{aligned}J\ddot{\phi}_{m,n}=&-C_1A^2(\phi_{m+1,n}+\phi_{m-1,n}+\phi_{m,n+1}+\phi_{m,n-1}\\&+4\phi_{m,n})+C_1A(u_{m+1,n}-u_{m-1,n}+v_{m,n+1}\\&-v_{m,n-1})-C\phi_{m,n}.\end{aligned} \tag{6}$$

The two first equations give the balance of force components and the third one gives the balance of moments acting on (m,n)th particle.

IV. HOMOGENEOUS STRAIN

Let us subject the model to the homogeneous strain with the components $\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{xy}$, and ε_{yx}. The displacements of particles in this case can be written as

$$u_{m,n} = hm\varepsilon_{xx} + hn\varepsilon_{xy}, \quad v_{m,n} = hn\varepsilon_{yy} + hm\varepsilon_{yx},$$

$$\phi_{m,n} = \phi. \tag{7}$$

The unknown angle of rotation ϕ can be found from Eq. (6) rewritten in view of Eq. (7) in the form

$$-8C_1A^2\phi + 2C_1Ah(\varepsilon_{xx} + \varepsilon_{yy}) - C\phi = 0. \tag{8}$$

The solution reads

$$\phi = \frac{2C_1Ah(\varepsilon_{xx} + \varepsilon_{yy})}{C + 8C_1A^2}. \tag{9}$$

Equations (7) and (9) define the displacements of particles in the model under homogeneous strain with components ε_{xx}, ε_{yy}, ε_{xy}, and ε_{yx}.

To analyze the anisotropy of the model let us calculate the components of the stress tensor in the coordinate system $X'Y'$ rotated with respect to the system XY by angle β (see Fig. 1). The result reads

$$\sigma_{x'x'} = c_{11}\varepsilon_{x'x'} + c_{12}\varepsilon_{y'y'} + c_{13}\varepsilon_{x'y'},$$

$$\sigma_{y'y'} = c_{21}\varepsilon_{x'x'} + c_{22}\varepsilon_{y'y'} + c_{23}\varepsilon_{x'y'},$$

$$\sigma_{x'y'} = \sigma_{y'x'} = c_{31}\varepsilon_{x'x'} + c_{32}\varepsilon_{y'y'} + c_{33}\varepsilon_{x'y'}, \tag{10}$$

where $c_{ij} = c_{ji}$ with

$$c_{11} = c_{22} = E_1(\cos^4\beta + \sin^4\beta) + 2(E_2 + 2E_3)\cos^2\beta\sin^2\beta,$$

$$c_{12} = 2(E_1 - 2E_3)\cos^2\beta\sin^2\beta + E_2(\cos^4\beta + \sin^4\beta),$$

$$c_{13} = -c_{23} = (-E_1 + E_2 + 2E_3)\sin\beta\cos\beta(\cos^2\beta - \sin^2\beta),$$

$$c_{33} = 2(E_1 - E_2)\cos^2\beta\sin^2\beta + E_3(\cos^2\beta - \sin^2\beta)^2, \tag{11}$$

and the macroscopic elastic constants are related to the microscopic parameters as follows:

$$E_1 = C_2 + \frac{CC_1 + 4C_1^2A^2}{C + 8C_1A^2}, \quad E_2 = C_2 - \frac{4C_1^2A^2}{C + 8C_1A^2},$$

$$E_3 = C_2. \tag{12}$$

In the coordinate system XY ($\beta = 0$), one has $E_1 = c_{11}$, $E_2 = c_{12}$, and $E_3 = c_{33}$.

Let us calculate the Poisson ratio, which characterizes the response of elastic body to uniaxial stress and is defined as the negative ratio between the transverse strain and the corresponding longitudinal strain. We put $\sigma_{x'x'} \neq 0$ and $\sigma_{y'y'} = \sigma_{x'y'} = \sigma_{y'x'} = 0$, and find from Eq. (10)

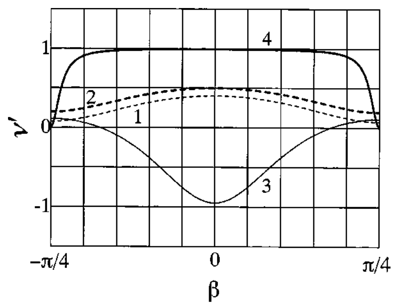

FIG. 2. Poisson ratio ν' as the function of orientation angle β of the applied uniaxial stress for $A = 0.5$ and different sets of C, C_1, C_2. Curve 1 corresponds to $C = 1$, $C_1 = 1$, $C_2 = 1$. Curve 2 is for $C = 100$, $C_1 = 1$, $C_2 = 1$. Relatively large C means that particles almost do not rotate. Curves 3 and 4 are for $C = 1$, $C_1 = 100$, $C_2 = 1$ and $C = 1$, $C_1 = 1$, $C_2 = 100$, respectively.

$$\nu' = -\frac{\varepsilon_{y'y'}}{\varepsilon_{x'x'}} = \frac{c_{12}c_{33} + c_{13}^2}{c_{11}c_{33} - c_{13}^2}. \tag{13}$$

Analysis of Eq. (13) shows that ν' is negative if and only if

$$CC_1^2\mathrm{tg}^2(2\beta) + 4CC_2^2 + 16C_1C_2(2C_2 - C_1)A^2 < 0. \tag{14}$$

One can see that this condition cannot be satisfied in the absence of the rotational degrees of freedom ($A = 0$ or $C \to \infty$).

Note that many crystals of KDP family demonstrate the negative Poisson ratio.[27]

It is possible to demonstrate that $-1 < \nu' < 1$ for any positive C, C_1, and C_2 and for any A and β. In Fig. 2 we plot ν' as the functions of β for $A = 0.5$ and different sets of C, C_1, and C_2. Curve 1 corresponds to $C = 1$, $C_1 = 1$, and $C_2 = 1$. Curve 2 is for $C = 100$, $C_1 = 1$, and $C_2 = 1$. Relatively large C means that particles almost do not rotate. Curve 3 is for $C = 1$, $C_1 = 100$, and $C_2 = 1$. In this case, the Poisson ratio is negative in a wide range of uniaxial stress orientations. Curve 4 is for $C = 1$, $C_1 = 1$, and $C_2 = 100$.

Uniaxial stress along two high-symmetry directions $\beta = 0$ and $\beta = \pi/4$ does not cause the appearance of shear strain. For, example, the Poisson ratio for uniaxial stress along $\beta = 0$ is

$$\nu_{\beta=0} = \frac{\bar{C}_2 - 4\bar{C}_1^2A^2 + 8\bar{C}_1\bar{C}_2A^2}{\bar{C}_1 + \bar{C}_2 + 4\bar{C}_1^2A^2 + 8\bar{C}_1\bar{C}_2A^2}, \tag{15}$$

where we have introduced $\bar{C}_1 = C_1/C$ and $\bar{C}_2 = C_2/C$. In the limiting case $\bar{C}_1 \gg \bar{C}_2$, one has $\nu \to -1$ if $\bar{C}_1 \gg 1$ and $\nu \to 0$ if $\bar{C}_1 \ll 1$. In the limiting case $\bar{C}_2 \gg \bar{C}_1$, one has $\nu \to 1$.

An interesting problem is to find the elastic constants of a polycrystal with randomly oriented microcrystals. We average the elastic constants c_{ij}, given by Eq. (11), over orientation angle β:

$$\langle c_{11} \rangle = \langle c_{22} \rangle = (3E_1 + E_2 + 2E_3)/4,$$

$$\langle c_{12}\rangle=(E_1+3E_2-2E_3)/4,$$
$$\langle c_{13}\rangle=\langle c_{23}\rangle=0,$$
$$\langle c_{33}\rangle=(\langle c_{11}\rangle-\langle c_{12}\rangle)/2. \tag{16}$$

One can see that after averaging there are only two independent elastic constants as it should be for an isotropic elastic body.

The Poisson ratio of the polycrystal becomes orientation independent and we can write it in the XY coordinate system:

$$\nu=-\frac{\varepsilon_{yy}}{\varepsilon_{xx}}=\frac{\langle c_{12}\rangle}{\langle c_{11}\rangle}=\frac{\overline{C}_1+2\overline{C}_2-8\overline{C}_1^2A^2+16\overline{C}_1\overline{C}_2A^2}{3\overline{C}_1+6\overline{C}_2+8\overline{C}_1^2A^2+48\overline{C}_1\overline{C}_2A^2}, \tag{17}$$

where $\overline{C}_1=C_1/C$ and $\overline{C}_2=C_2/C$.

In the limiting cases

$$\overline{C}_1\gg\overline{C}_2,\ \ \overline{C}_1\gg 1,\quad \text{then}\quad \nu\to-1,$$
$$\overline{C}_1\gg\overline{C}_2,\ \ \overline{C}_1\ll 1,\quad \text{then}\quad \nu\to 1/3,$$
$$\overline{C}_2\gg\overline{C}_1,\quad \text{then}\quad \nu\to 1/3. \tag{18}$$

The function $\nu(\overline{C}_1,\overline{C}_2)$, given by Eq. (17), was demonstrated to be a monotone one, so that it cannot take values smaller than -1 or greater than 1/3. Recall that the Poisson ratio of an isotropic solid must be in the range $-1\leqslant\nu\leqslant 1/2$.

Now suppose that particles cannot rotate. To consider this limit we put $C\gg C_1$ and $C\gg C_2$; that is, the rotational background potential is very rigid. The same limit can be achieved assuming that $A\to 0$ which means that the size of particles $a\to 0$ [see Eq. (1)]. In this limit, instead of E_1, E_2, and E_3, we have

$$E_1^*=C_1+C_2,\quad E_2^*=C_2,\quad E_3^*=C_2, \tag{19}$$

and the Poisson ratio becomes

$$\nu^*=-\frac{\varepsilon_{xx}}{\varepsilon_{yy}}=\frac{\langle c_{12}^*\rangle}{\langle c_{11}^*\rangle}=\frac{E_1^*+3E_2^*-2E_3^*}{3E_1^*+E_2^*+2E_3^*}=\frac{1}{3}. \tag{20}$$

One can see that if the rotations of particles are suppressed, the Poisson ratio of the polycrystal does not depend on microscopic parameters C_1 and C_2 and is equal to 1/3, which is the common value for many natural elastic bodies.

V. DISPERSION RELATION

Searching for the solution to Eqs. (4)–(6) in the form

$$u_{m,n}(t)=Ue^{i(\omega t+mhk_x+nhk_y)},$$
$$v_{m,n}(t)=Ve^{i(\omega t+mhk_x+nhk_y)},$$
$$\phi_{m,n}(t)=i\Phi e^{i(\omega t+mhk_x+nhk_y)}, \tag{21}$$

one obtains

$$(a_0+a_2+M\omega^2)U+a_3V+a_4\Phi=0,$$
$$a_3U+(a_1+a_2+M\omega^2)V+a_5\Phi=0,$$
$$a_4U+a_5V+(a_6+J\omega^2)\Phi=0, \tag{22}$$

where

$$a_0=2C_1[\cos(hk_x)-1],\quad a_1=2C_1[\cos(hk_y)-1],$$
$$a_2=2C_2[\cos(hk_x)\cos(hk_y)-1],$$
$$a_3=-2C_2\sin(hk_x)\sin(hk_y),$$
$$a_4=2C_1A\sin(hk_x),\quad a_5=2C_1A\sin(hk_y),$$
$$a_6=-4C_1A^2[\cos(hk_x)\cos(hk_y)+1]-C. \tag{23}$$

The dispersion relation can be obtained by setting the determinant of system, Eq. (22), equal to zero.

The dispersion curves, Eq. (22), can vanish only on the boundary of the first Brillouin zone. This fact suggests that, in the present form, our model does not support an incommensurate phase. However, it is not difficult to revise the model in a way that incommensurate phase would be possible.

Let us analyze the dispersion relations for two high-symmetry directions $k_x=k_y$ and $k_y=0$.

A. Case $k_x=k_y=k$

In this case $a_0=a_1$, $a_4=a_5$. The dispersion curves take the form

$$\omega_1^2(k)=\frac{a_3-a_0-a_2}{M},\quad \omega_{2,3}^2(k)=z_1\pm\sqrt{z_2^2+\frac{2a_4^2}{MJ}}, \tag{24}$$

where

$$z_1=-\frac{a_0+a_2+a_3}{2M}-\frac{a_6}{2J},\quad z_2=\frac{a_0+a_2+a_3}{2M}-\frac{a_6}{2J}. \tag{25}$$

Acoustic modes are ω_1, ω_3, and ω_2 is the optic mode.

B. Case $k_y=0$

In this case $a_1=a_3=a_5=0$ and we come to the following expressions for the dispersion curves:

$$\omega_1^2(k_x)=\frac{-a_2}{M},\quad \omega_{2,3}^2(k_x)=z_1\pm\sqrt{z_2^2+\frac{a_4^2}{MJ}}, \tag{26}$$

where

$$z_1=-\frac{a_0+a_2}{2M}-\frac{a_6}{2J},\quad z_2=\frac{a_0+a_2}{2M}-\frac{a_6}{2J}. \tag{27}$$

Modes ω_1 and ω_3 are the acoustic ones and ω_2 is the optic one.

VI. LONG-WAVE APPROXIMATION: ANISOTROPIC ELASTICITY THEORY

In the long-wave approximation Eqs. (4)–(6) become

$$\rho u_{tt}=(C_1+C_2)u_{xx}+C_2u_{yy}+2C_2v_{xy}-2C_1Ah^{-1}\phi_x, \tag{28}$$

$$\rho v_{tt}=C_2v_{xx}+(C_1+C_2)v_{yy}+2C_2u_{xy}-2C_1Ah^{-1}\phi_y, \tag{29}$$

$$J\phi_{tt}=-2C_1A^2h^2(\phi_{xx}+\phi_{yy})+2C_1Ah(u_x+v_y)-(C+8C_1A^2)\phi, \tag{30}$$

where $\rho=M/h^2$ is the density of the medium. These equations are often called the equations of micropolar elasticity, which generalize the equations of conventional elasticity theory. The main difference is that the micropolar elasticity can take into account the coupling of the field of microscopic rotations $\phi(x,y)$ with the displacement fields $u(x,y)$ and $v(x,y)$. It is important to note that, in our case, $\phi(x,y)$ is a slowly varying envelope function for the two-periodic-modulated structure [see Eq. (2)]. Rotational degrees of freedom appear in many models and those models are described by the equations similar to Eqs. (28)–(30). Equations (28)–(30) have the same form as the equations of 2D micropolar elasticity,[1] but in fact, the models do not coincide exactly because there is some difference in coefficients. The structural 2D model with orientable points jointed by extensible and flexible rods presented in Ref. 6 also has the structure identical to Eqs. (28)–(30) with coefficients different from our model and from the micropolar medium by Eringen.[1] Micropolar equations are used as continuum models for materials with beamlike microstructure.[7]

To obtain the equations of the conventional anisotropic elasticity theory we must neglect in Eq. (30) the inertia of rotations $J\phi_{tt}$ and the second derivatives ϕ_{xx} and ϕ_{yy}. Then,

$$\phi=\frac{2C_1Ah}{C+8C_1A^2}(u_x+v_y), \tag{31}$$

which coincides with Eq. (9).

Now we can eliminate ϕ from Eqs. (28) and (29) and write

$$\rho u_{tt}=E_1u_{xx}+E_3u_{yy}+(E_2+E_3)v_{xy}, \tag{32}$$

$$\rho v_{tt}=E_3v_{xx}+E_1v_{yy}+(E_2+E_3)u_{xy}, \tag{33}$$

where E_1, E_2, and E_3 are given by Eq. (12). Equations (32) and (33) are the equations of conventional two-dimensional elasticity for an anisotropic medium.

VII. DISPERSION RELATIONS FOR APPROXIMATE MODELS

First we calculate the dispersion relations for the continuum approximation given by Eqs. (28)–(30). We substitute

$$u=Ue^{i(\omega t+k_xx+k_yy)},\qquad v=Ve^{i(\omega t+k_xx+k_yy)},$$

$$\phi=i\Phi e^{i(\omega t+k_xx+k_yy)}, \tag{34}$$

and find that the set of homogeneous equations in U, V, and Φ has the form of Eq. (22) with

$$a_0=-C_1h^2k_x^2,\quad a_1=-C_1h^2k_y^2,\quad a_2=-C_2h^2(k_x^2+k_y^2),$$

$$a_3=-2C_2h^2k_xk_y,\quad a_4=2C_1Ahk_x,\quad a_5=2C_1Ahk_y,$$

$$a_6=2C_1A^2h^2(k_x^2+k_y^2)-8C_1A^2-C. \tag{35}$$

We note that the coefficients given by Eq. (35) coincide with the corresponding coefficients defined by Eq. (23) expanded in Taylor series with respect to k_x and k_y up to second order. This implies that the continuum model, Eqs. (28)–(30), can be used for the modeling of long-wave propagation. Dispersion curves in the particular directions $k_x=k_y$ and $k_y=0$ are given by Eqs. (24) and (26) with the parameters defined by Eq. (35).

To calculate the dispersion relations for the equations of anisotropic elasticity, we substitute the first two expressions of Eq. (34) into Eqs. (32) and (33) and obtain

$$(E_1k_x^2+E_3k_y^2-\rho\omega^2)U+(E_2+E_3)k_xk_yV=0,$$

$$(E_2+E_3)k_xk_yU+(E_3k_x^2+E_1k_y^2-\rho\omega^2)V=0. \tag{36}$$

Then the dispersion relations are

$$\rho\omega_{1,3}^2=z_1\mp\sqrt{z_2^2+(E_2+E_3)^2k_x^2k_y^2}, \tag{37}$$

where

$$2z_1=(E_1+E_3)(k_x^2+k_y^2),\quad 2z_2=(E_1-E_3)(k_x^2-k_y^2). \tag{38}$$

Note that the optic branch ω_2 is absent in the conventional elasticity theory.

Along the direction $k_x=k_y=k$ we have

$$\rho\omega_1^2(k)=(E_1-E_2)k^2,\quad \rho\omega_3^2(k)=(E_1+E_2+2E_3)k^2, \tag{39}$$

and along the direction $k_y=0$ we have

$$\rho\omega_1^2(k_x)=E_3k_x^2,\quad \rho\omega_3^2(k_x)=E_1k_x^2. \tag{40}$$

VIII. DISCUSSION

In the above, we have derived the exact equations of motion for the discrete model, Eqs. (4)–(6), their long-wave micropolar-type approximation, Eqs. (28)–(30), and the conventional elasticity theory, Eqs. (32) and (33).

Let us compare the dispersion relations for these three models. For purpose of illustration, we will consider a particular high-symmetry direction of the Brillouin zone, $k_y=0$, but all the conclusions made will be valid in general.

In Fig. 3, the dispersion curves for $M=J=h=1$, $A=0.5$, $C=4$, $C_1=1$, and $C_2=2$ are presented. The three thick solid lines are the dispersion curves for the discrete model [Eq. (26) with coefficients defined by Eq. (23)]. The

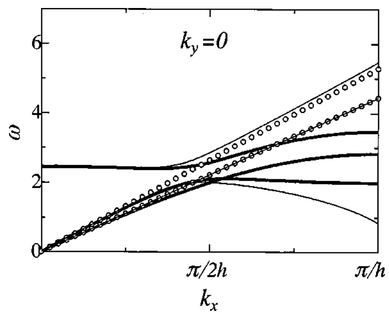

FIG. 3. The dispersion curves for $M=J=h=1$, $A=0.5$, $C=4$, $C_1=1$, and $C_2=2$. The three thick solid lines are the dispersion curves for the discrete model [Eq. (26) with coefficients defined by Eq. (23)]. The three thin solid lines correspond to the micropolar-type approximation [Eq. (26) with coefficients defined by Eq. (35)]. Open circles present the two branches of the conventional elasticity theory, Eq. (40).

three thin solid lines correspond to the micropolar-type approximation [Eq. (26) with coefficients defined by Eq. (35)]. Open circles present the two branches of the conventional elasticity theory, Eq. (40).

One can see that the two linear branches of the conventional elasticity (open circles) are tangent to the acoustic branches for the discrete model (thick solid lines) at $k_x=0$. The conventional elasticity does not describe the optic vibrations of the discrete model.

The micropolar elasticity (thin solid lines) gives a good approximation for all three branches of the discrete model in the range of $k<\pi/4h$.

In Fig. 4 we show the same as in Fig. 3 but instead of $C=4$ we put $C=40$ in order to suppress the rotations of particles. In this case the optic branch goes up and the two continuum models (thin solid lines and open circles) give almost the same approximations of the acoustic branches of the discrete model (thick solid lines).

One can see from Figs. 3 and 4 that the continuum approximations derived for the discrete model give an excellent approximation in the range of the long waves and the accuracy is not good for the short waves. This is a usual problem for the continuum models of structural media. When deriving the continuum analog to the discrete equations, we use the Taylor expansion, and the influence of high-order gradient terms is small for long waves but it is not small for a wavelength comparable with the size of a periodicity cell. To improve the approximation in the short-wave range one can take into account the fourth-order terms in the Taylor expansion. An alternative approach is the so-called many-field approximation when one uses more than one continuum field for the description of the generalized displacements. This approach was successfully used in Ref. 23 where the short-wave soliton solution for a nonlinear discrete model has been obtained.

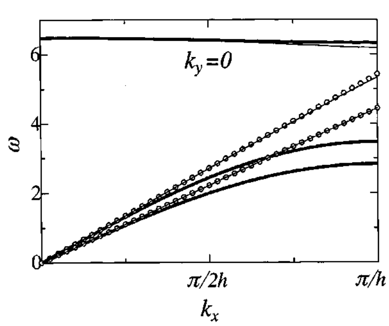

FIG. 4. Same as in Fig. 3 but instead of $C=4$ we put $C=40$ in order to suppress the rotations of particles.

Now let us turn to the discussion of the role of rotational degrees of freedom. If particles cannot rotate (the limit of $C\to\infty$ or, equivalently, $A\to 0$), then $\phi(x,t)$ disappears from the system, Eqs. (28)–(30), and we come to the following equations of conventional elasticity for the medium without microrotations:

$$\rho u_{tt}=(C_1+C_2)u_{xx}+C_2u_{yy}+2C_2v_{xy}, \tag{41}$$

$$\rho v_{tt}=C_2v_{xx}+(C_1+C_2)v_{yy}+2C_2u_{xy}. \tag{42}$$

If the rotations of particles are not suppressed, the model, discussed in this paper, presents a micropolar medium and the equation for $\phi(x,t)$ must be introduced. However, even in this case, under the assumption that ϕ_{xx}, ϕ_{yy}, and $J\phi_{tt}$ are small, we could derive Eqs. (32) and (33) which have the same structure as Eqs. (41) and (42) with coefficients redefined in order to take into account the rotations of particles.

The terms ϕ_{xx} and ϕ_{yy} are not small in the vicinity of crystal defects like the domain wall, dislocation, free surface, or tip of a crack. They also cannot be neglected in the modulated or incommensurate phase. In all these cases micropolar-type elasticity should be used.

Formally, the function $\phi(x,t)$ can be eliminated from Eqs. (28) and (29) even when ϕ_{xx} and ϕ_{yy} are not small and $J\phi_{tt}$ is negligible but, in this case, the higher-order spatial derivatives of u and v will appear in the equations. It is well known that the incommensurate phase cannot be described without taking into account the higher-order gradient terms. We have just demonstrated that these terms can appear in the media with microscopic rotations. Thus, microscopic rotations can be responsible for the appearance of incommensurate phase in crystals.

We can easily imagine the physical situation where ϕ_{xx} and ϕ_{yy} are small but the inertia of the rotations $J\phi_{tt}$ cannot be neglected. This can happen, for example, under an applied high-frequency electric field with possible resonance with the optic branch. The coupling with the rotational mode can play an important role in the ultrasonic-wave propagation. Effects of this kind cannot be studied in the framework of conventional elasticity because the rotational optic branch is absent in this theory. Here again the equation for $\phi(x,t)$ must be involved in the analysis.

Finally, we have shown in Sec. IV that the rotational degrees of freedom are responsible for the negative Poisson ratio in a polycrystal.

As pointed out above, our model in the present form does not support an incommensurate phase. But, for example, the introduction of a third-neighbor interaction will make the vanishing of a dispersion curve inside the first Brillouin zone possible. An additional nonlinear term can make the incommensurate structure stable. Besides, the model with a nonlinearity will support solutions in the form of a domain wall or soliton and comparison with the results of Pouget and Maugin[28] will become possible.

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