Journal of Theoretical Physics

Founded and Edited by M. Apostol **3** (1995)

ISSN 1453-4428

Elastic waves in a uniaxial solid

B.-F. Apostol
Department of Theoretical Physics,
Institute of Atomic Physics, Magurele-Bucharest MG-6,
POBox MG-35, Romania

Abstract

The elastic waves are derived in a uniaxially anisotropic model, which may be relevant for quasi-one-dimensional solids.

1 Elastic energy

A quasi-one-dimensional solid may be modelled as a uniaxially anisotropic continuum,*i.e.* an elastic body which is homogeneous in the x, y-plane and has an anisotropy axis along the z-direction. We shall use indistinctly the coordinate labels x, y, z and , respectively, $1, 2, 3$. In order to establish the elastic energy we start with the infinitesimal length given by

$$dl^2 = dx_i^2 + dx_3^2 \tag{1}$$

where $i = 1, 2$, which becomes

$$\begin{aligned} d\tilde{l}^2 = & [(1 + \partial u_1/\partial x_1)\, dx_1 + \partial u_1/\partial x_2 \cdot dx_2 + \partial u_1/\partial x_3 \cdot dx_3]^2 + \\ & + [\partial u_2/\partial x_1 \cdot dx_1 + (1 + \partial u_2/\partial x_2)\, dx_2 + \partial u_2/\partial x_3 \cdot dx_3]^2 + \\ & + [\partial u_3/\partial x_1 \cdot dx_1 + \partial u_2/\partial x_2 \cdot dx_2 + (1 + \partial u_3/\partial x_3)\, dx_3]^2 \end{aligned} \tag{2}$$

under the deformation field $x_i \rightarrow \tilde{x}_i = x_i + u_i$, $i = 1, 2, 3$. To the leading order in u_i (2) can be written as

$$d\tilde{l}^2 = dl^2 + 2u_{ij}dx_i dx_j + 2u_{i3}dx_i dx_3 + 2u_{33}dx_3^2 \quad , \tag{3}$$

where the deformation tensor

$$u_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \ , \ i, j = 1, 2 \quad , \tag{4}$$

the deformation vector

$$u_{i3} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_3} + \frac{\partial u_3}{\partial x_i}\right) \ \ i = 1, 2 \quad , \tag{5}$$

and the deformation scalar $u_{33} = \partial u_3/\partial x_3$ with respect to the rotations about the anisotropy axis have been introduced. According to the general principles of the elasticity theory[1] the density of the elastic energy includes the five quadratic invariants which can be constructed with the deformations given above, *i.e.* it may be written as

$$\mathcal{E}_{el} = \lambda u_{ii}^2 + \mu u_{ij}^2 + \tau u_{i3}^2 + \sigma u_{33}^2 + \nu u_{33} u_{ii} \quad , \tag{6}$$

where the Greek letters stand for the coupling (elastic) constants.

It is useful at this point to recall that, generally, we have 81 coupling constants $C_{ij,kl}$, which, however, are symmetric under the interchange of the ij and kl labels, and under the interchange of the ij and kl pairs of labels. The first two symmetries reduce the number of the coupling constants to 36, while the third symmetry effects a further reduction to 21. For these remaining elastic constants one employs usually the Voigt notation[2] $1 \rightarrow xx$, $2 \rightarrow yy$, $3 \rightarrow zz$, $4 \rightarrow yz(zy)$, $5 \rightarrow zx(xz)$, $6 \rightarrow xy(yx)$. The Cauchy relations $C_{12} = C_{66}$, $C_{13} = C_{55}$, $C_{23} = C_{44}$, $C_{45} = C_{36}$, $C_{56} = C_{14}$, $C_{46} = C_{25}$ further restrict the number of coupling constants, while the structure symmetry entails its own reduction.

It is known that the hexagonal symmetry has also five elastic constants. In fact, the elastic energy given by (6) looks very similar with that of the hexagonal symmetry. Indeed, (6) can be written as

$$\mathcal{E}_{el} = (\lambda + \frac{\mu}{2})u_{ii}^2 + \frac{\mu}{2}\left[(u_{11} - u_{22})^2 + 4u_{12}^2\right] + \tau u_{i3}^2 + \sigma u_{33}^2 + \nu u_{33}u_{ii} \quad , \tag{7}$$

which is exactly the elastic energy of the hexagonal symmetry, though the coordinates $x, y \rightarrow \xi, \zeta = x \pm y$, and the corresponding elastic field, are different.[3]

Using the notation

$$T = u_{ii} \tag{8}$$

for the trace of the deformation tensor we may write

$$u_{ij}^2 = \left(u_{ij} - \frac{1}{2}T\delta_{ij}\right)^2 + \frac{1}{2}T^2 = \frac{1}{2}\left(u_{11} - u_{22}\right)^2 + 2u_{12}^2 + \frac{1}{2}T^2 \tag{9}$$

and

$$\mathcal{E}_{el} = \mu\left(u_{ij} - \frac{1}{2}T\delta_{ij}\right)^2 + \left(\lambda + \frac{\mu}{2} - \frac{\nu^2}{4\sigma}\right)T^2 + \tau u_{i3}^2 + \sigma\left(u_{33} + \frac{\nu}{2\sigma}T\right)^2 \quad , \tag{10}$$

whence one can see the stability conditions

$$\mu, \tau, \sigma > 0, \quad \nu^2 < 2\sigma\left(2\lambda + \mu\right) \quad . \tag{11}$$

The elastic processes described by (10) can also be classified as follows. For $u_{11} = u_{22} = u_{i3} = u_{33} = 0$ we have the shear modes of the basal $(xy-)$ plane with the elastic energy density $2\mu u_{12}^2$; for $u_{ij} = u_{33} = 0$ we have the axial shear modes of energy τu_{i3}^2; for $u_{12} = u_{i3} = u_{33} = 0$ and $u_{11} = u_{22}$ we get the compression modes of the basal plane with the energy density $2\left(2\lambda + \mu\right)u_{11}^2$; the axial compression modes are easily obtained from $u_{ij} = u_{i3} = 0$, with the energy density σu_{33}^2; and finally, we have a special mode, which can be called a "pinch" mode, defined by $u_{12} = u_{i3} = 0$, $u_{11} = u_{22}$, $u_{33} + \frac{\nu}{2\sigma}T = u_{33} + \frac{\nu}{\sigma}u_{11} = 0$, of energy density $\left(\lambda + \frac{\mu}{2} - \frac{\nu^2}{4\sigma}\right)T^2 = 2\left(2\lambda + \mu\right)u_{11}^2 - \sigma u_{33}^2$.

2 Elastic waves

The kinetic energy is given by

$$E_{kin} = \frac{1}{2}\rho\int dV\left(\dot{u}_1^2 + \dot{u}_2^2 + \dot{u}_3^2\right) \quad , \tag{12}$$

where ρ is the mass density and V is the volume of the sample, while the elastic energy is obtained from (6) as

$$\begin{array}{c} E_{el} = \int dV \left[(\lambda+\mu) \left(\frac{\partial u_1}{\partial x_1}\right)^2 + \frac{1}{2}\mu \left(\frac{\partial u_1}{\partial x_2}\right)^2 + \frac{1}{4}\tau \left(\frac{\partial u_1}{\partial x_3}\right)^2 \right] + \\ + \int dV \left[\frac{1}{2}\mu \left(\frac{\partial u_2}{\partial x_1}\right)^2 + (\lambda+\mu) \left(\frac{\partial u_2}{\partial x_2}\right)^2 + \frac{1}{4}\tau \left(\frac{\partial u_2}{\partial x_3}\right)^2 \right] + \\ + \int dV \left(2\lambda \frac{\partial u_1}{\partial x_1} \cdot \frac{\partial u_2}{\partial x_2} + \mu \frac{\partial u_1}{\partial x_2} \cdot \frac{\partial u_2}{\partial x_1} \right) + \\ \int dV \left\{ \frac{\tau}{4} \left[\left(\frac{\partial u_3}{\partial x_1}\right)^2 + \left(\frac{\partial u_3}{\partial x_2}\right)^2 \right] + \sigma \left(\frac{\partial u_3}{\partial x_3}\right)^2 \right\} + \\ + \int dV \left[\frac{\tau}{2} \left(\frac{\partial u_1}{\partial x_3} \cdot \frac{\partial u_3}{\partial x_1} + \frac{\partial u_2}{\partial x_3} \cdot \frac{\partial u_3}{\partial x_2} \right) \right] + \nu \frac{\partial u_3}{\partial x_3} \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} \right) \quad . \end{array} \tag{13}$$

Introducing the Fourier transform

$$u_i(\mathbf{x}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{q}} u_{i\mathbf{q}} e^{i\mathbf{q}\mathbf{x}} \quad , \tag{14}$$

with $u_{i\mathbf{q}}^{\dagger} = u_{i-\mathbf{q}}$, $i = 1, 2, 3$, the kinetic energy becomes

$$E_{kin} = \frac{1}{2}\rho \sum_{\mathbf{q}} \left(\dot{u}_{1\mathbf{q}}^{\dagger} \dot{u}_{1\mathbf{q}} + \dot{u}_{2\mathbf{q}}^{\dagger} \dot{u}_{2\mathbf{q}} + \dot{u}_{3\mathbf{q}}^{\dagger} \dot{u}_{3\mathbf{q}} \right) \tag{15}$$

and the elastic energy

$$\begin{array}{c} E_{el} = \sum_{\mathbf{q}} \left[(\lambda+\mu) q_1^2 + \frac{1}{2}\mu q_2^2 + \frac{1}{4}\tau q_3^2 \right] u_{1\mathbf{q}}^{\dagger} u_{1\mathbf{q}} + \\ + \left[\frac{1}{2}\mu q_1^2 + (\lambda+\mu) q_2^2 + \frac{1}{4}\tau q_3^2 \right] u_{2\mathbf{q}}^{\dagger} u_{2\mathbf{q}} + \\ + (2\lambda+\mu) q_1 q_2 u_{1\mathbf{q}}^{\dagger} u_{2\mathbf{q}} + \left[\frac{1}{4}\tau (q_1^2 + q_2^2) + \sigma q_3^2 \right] u_{3\mathbf{q}}^{\dagger} u_{3\mathbf{q}} + \\ + \left(\frac{1}{2}\tau + \nu \right) q_1 q_3 u_{3\mathbf{q}}^{\dagger} u_{1\mathbf{q}} + \left(\frac{1}{2}\tau + \nu \right) q_2 q_3 u_{3\mathbf{q}}^{\dagger} u_{2\mathbf{q}} \quad . \end{array} \tag{16}$$

The orthogonal transform

$$\begin{array}{c} u_{1\mathbf{q}} = \cos\theta_{\mathbf{q}} \cdot v_{1\mathbf{q}} + \sin\theta_{\mathbf{q}} \cdot \widetilde{v}_{2\mathbf{q}} \quad , \\ u_{2\mathbf{q}} = -\sin\theta_{\mathbf{q}} \cdot v_{1\mathbf{q}} + \cos\theta_{\mathbf{q}} \cdot \widetilde{v}_{2\mathbf{q}} \quad , \end{array} \tag{17}$$

with

$$\sin\theta_{\mathbf{q}} = \frac{q_1}{\sqrt{q_1^2+q_2^2}} \quad , \quad \cos\theta_{\mathbf{q}} = \frac{q_2}{\sqrt{q_1^2+q_2^2}} \tag{18}$$

decouples the motions in the basal plane and leads to

$$E_{kin} = \frac{1}{2}\rho \sum_{\mathbf{q}} \left(\dot{v}_{1\mathbf{q}}^{\dagger} \dot{v}_{1\mathbf{q}} + \dot{\widetilde{v}}_{2\mathbf{q}}^{\dagger} \dot{\widetilde{v}}_{2\mathbf{q}} + \dot{u}_{3\mathbf{q}}^{\dagger} \dot{u}_{3\mathbf{q}} \right) \tag{19}$$

and

$$\begin{array}{c} E_{el} = \sum_{\mathbf{q}} \left[\frac{1}{2}\mu (q_1^2 + q_2^2) + \frac{1}{4}\tau q_3^2 \right] v_{1\mathbf{q}}^{\dagger} v_{1\mathbf{q}} + \\ + \left[(\lambda+\mu)(q_1^2 + q_2^2) + \frac{1}{4}\tau q_3^2 \right] \widetilde{v}_{2\mathbf{q}}^{\dagger} \widetilde{v}_{2\mathbf{q}} + \\ + \left[\frac{1}{4}\tau (q_1^2 + q_2^2) + \sigma q_3^2 \right] u_{3\mathbf{q}}^{\dagger} u_{3\mathbf{q}} + \\ + \left(\frac{1}{2}\tau + \nu \right) \mid q_3 \mid \sqrt{q_1^2 + q_2^2} u_{3\mathbf{q}}^{\dagger} \widetilde{v}_{2\mathbf{q}} \quad . \end{array} \tag{20}$$

We remark that the transform given by (17) and (18) amounts to a rotation of the polarizations around the anisotropy axis of angle $\theta_{\mathbf{q}}$, such that $\widetilde{v}_{2\mathbf{q}}$ is oriented along the transverse wavevector $\mathbf{q}_{\perp} = (q_1, q_2)$ and $v_{1\mathbf{q}}$ is perpendicular to it.

The hamiltonian given by (19) and (20) is brought to a sum of harmonic oscillators

$$H=\frac{1}{2}\rho\sum_{i\mathbf{q}}\left[\dot{v}_{i\mathbf{q}}^{\dagger}\dot{v}_{i\mathbf{q}}+\omega_i^2\left(\mathbf{q}\right)\cdot v_{i\mathbf{q}}^{\dagger}v_{i\mathbf{q}}\right] \tag{21}$$

$i=1,2,3$, with the frequencies given by

$$\omega_1^2\left(\mathbf{q}\right)=\frac{1}{2\rho}\left(2\mu q_\perp^2+\tau q_3^2\right)\quad , \tag{22}$$

and

$$\begin{gathered}\omega_{2,3}^2\left(\mathbf{q}\right)=\tfrac{1}{4\rho}([4\left(\lambda+\mu\right)+\tau]\,q_\perp^2+\left(\tau+4\sigma\right)q_3^2\pm\\ \pm\left[[[4\left(\lambda+\mu\right)-\tau]\,q_\perp^2+\left(\tau-4\sigma\right)q_3^2]^2+4\left(\tau+2\nu\right)^2q_3^2q_\perp^2\right]^{\frac{1}{2}})\end{gathered} \tag{23}$$

by a second orthogonal transform

$$\begin{aligned}u_{3\mathbf{q}}&=\cos\varphi_{\mathbf{q}}\cdot v_{3\mathbf{q}}+\sin\varphi_{\mathbf{q}}\cdot v_{2\mathbf{q}}\quad ,\\ \widetilde{v}_{2\mathbf{q}}&=-\sin\varphi_{\mathbf{q}}\cdot v_{3\mathbf{q}}+\cos\varphi_{\mathbf{q}}\cdot v_{2\mathbf{q}}\quad ,\end{aligned} \tag{24}$$

where

$$\tan 2\varphi_{\mathbf{q}}=\frac{2\left(\tau+2\nu\right)\mid q_3\mid q_\perp}{[4\left(\lambda+\mu\right)-\tau]\,q_\perp^2+\left(\tau-4\sigma\right)q_3^2}\quad . \tag{25}$$

Introducing the well-known creation and annihilation operators for phonons by

$$\begin{aligned}v_{i\mathbf{q}}&=\sqrt{\tfrac{\hbar}{2\rho\omega_i}}\left(a_{i\mathbf{q}}^{\dagger}+a_{i-\mathbf{q}}\right)\quad ,\\ \dot{v}_{i\mathbf{q}}&=i\sqrt{\tfrac{\hbar\omega_i}{2\rho}}\left(a_{i\mathbf{q}}^{\dagger}-a_{i-\mathbf{q}}\right)\quad ,\end{aligned} \tag{26}$$

the hamiltonian (21) acquires the usual diagonal form

$$H=\sum_{i\mathbf{q}}\hbar\omega_i\left(\mathbf{q}\right)\left(a_{i\mathbf{q}}^{\dagger}a_{i\mathbf{q}}+1/2\right)\quad . \tag{27}$$

3 Discussion

First, we remark that only $v_{1\mathbf{q}}$ is a purely transverse mode (*i.e.*, perpendicular to $\mathbf{q}$), $v_{2\mathbf{q}}$ and $v_{3\mathbf{q}}$ have both transverse and longitudinal components, to an extent prescribed by the angle $\varphi_{\mathbf{q}}$ .For any $\mathbf{q}$ there is a (local) trihedral frame $\mathbf{1},\mathbf{2},\mathbf{3}$, given by

$$\begin{gathered}u_{\mathbf{q}}=u_1\mathbf{i}+u_2\mathbf{j}+u_3\mathbf{k}=\\ =\left(\cos\theta\cdot\mathbf{i}-\sin\theta\cdot\mathbf{j}\right)v_1+\left(\sin\theta\cdot\cos\varphi\cdot\mathbf{i}+\cos\theta\cdot\sin\varphi\cdot\mathbf{j}+\sin\varphi\cdot\mathbf{k}\right)v_2+\\ +\left(-\sin\theta\cdot\sin\varphi\cdot\mathbf{i}-\cos\theta\cdot\sin\varphi\cdot\mathbf{j}+\cos\varphi\cdot\mathbf{k}\right)v_3=\\ =v_1\mathbf{1}+v_2\mathbf{2}+v_3\mathbf{3}\end{gathered} \tag{28}$$

which have the axes directed along the polarizations (polarization trihedron), the propagation vector $\mathbf{q}$ being in the $\mathbf{2},\mathbf{3}$-plane.

Secondly, we remark that if one assumes that the axial shear and the pinch modes are absent ($\tau=\nu=0$) then $\varphi_{\mathbf{q}}=0$ and we are left with the following three types of elastic waves:

$$\omega_1^2\left(\mathbf{q}\right)=\left(\mu/\rho\right)q_\perp^2 \tag{29}$$

with the polarization $v_{1\mathbf{q}}$ perpendicular to $\mathbf{q}_\perp$ and the anisotropy axis (chain axis in a quasi-one-dimensional solid);

$$\omega_2^2\left(\mathbf{q}\right)=\left[2\left(\lambda+\mu\right)/\rho\right]q_\perp^2 \tag{30}$$

with the polarization $v_{2\mathbf{q}}$ parallel to $\mathbf{q}_{\perp}$ (perpendicular to the chain axis); and

$$\omega_3^2\left(\mathbf{q}\right)=\left(2\sigma/\rho\right)q_3^2 \tag{31}$$

with the polarization $v_{3\mathbf{q}}=u_{3\mathbf{q}}$ parallel to the chain axis. This later mode couples to the electrons restricted to move only along the chains.

It seems that a resembling discussion can be found elsewhere.[4]

References

[1] L. Landau and E. Lifshitz, Theorie d'Elasticite, Moscow (1967).

[2] M. Born and K. Huang, Dynamical Theory of Crystal Lattices, Oxford (1954).

[3] See, for example, Ref.1.

[4] R. G. Payton, Elastic Waves Propagation in Transversely Isotropic Media, Nijhof (1983).