# Stresses Produced by a Continuous Distribution of Moving Dislocations in an Isotropic Continuum

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Kröner's equation for the stress field due to a continuous distribution of stationary dislocations is extended to the problem of moving dislocations. The equation governing the stress field takes the form $\Box_T\Box_L\chi=H$, where $\Box_T$ and $\Box_L$ are the d'Alembertian operators related to the velocities of the transverse and longitudinal sound waves, respectively. The expression for the stresses is also extended; it takes the form obtained from Kröner's equation by the substitution of d'Alembertian operators for the Laplacian.

The stresses due to continuous distributions of moving dislocations have been studied by several investigators.[1] They obtained the equation governing the stress field and, in some cases, obtained the stresses from its solution. In the present paper, we shall attack the problem from Kröner's point of view.[2] It will be shown that the stress field is governed by a repeated wave equation which is an extension of Kröner's for the problem of stationary dislocations.

When the body force is neglected, the stresses in an isotropic continuum satisfy the equation[3]

$$\Delta\sigma_{ij}+\frac{1}{1+\nu}\partial_i\partial_j\sigma_{kk}-\frac{\rho}{G}\frac{\partial^2\sigma_{ij}}{\partial t^2}-\frac{\nu}{1+\nu}\left(\Delta\sigma_{kk}-\frac{\rho}{G}\frac{\partial^2\sigma_{kk}}{\partial t^2}\right)\delta_{ij}=2G(\eta_{ij}-\delta_{ij}\eta_{kk})+2\rho\frac{\partial^2 e_{ij}{}^P}{\partial t^2}, \tag{1}$$

where $\sigma_{ij}$ is the stress tensor, $\eta_{ij}$ the incompatibility tensor, $e_{ij}{}^P$ the plastic strain tensor, $\rho$ the mass density of the material, $G$ the shear modulus, $\nu$ Poisson's ratio, $\delta_{ij}$ the Kronecker $\delta$, $\Delta$ the Laplacian operator, $\partial_i$ means $\partial/\partial x^i$, $x^i$ being the Cartesian coordinates which locate the material point, and $t$ the time. Throughout this paper, indices $i$, $j$, etc. take the values 1, 2 or 3, and Einstein's summation convention is used with respect to indices appearing twice in one expression.

The stresses satisfying the equilibrium equation can be expressed as

$$\sigma_{ij}=-\epsilon_{ikl}\epsilon_{jmn}\partial_k\partial_m\chi_{ln}+(\partial^2/\partial t^2)\psi_{ij}, \tag{2}$$

where $\epsilon_{ijk}$ is Eddington's $\epsilon$, $\chi_{ij}$ the Beltrami-Schaefer stress function tensor, and $\psi_{ij}$ a symmetric tensor which satisfies

$$\partial_j\psi_{ij}=\rho u_i, \tag{3}$$

$u_i$ being the vector of displacement of the material point. We use $\psi_{ij}'$ as is given from the following relations:

$$\psi_{ij}=2\rho(\psi_{ij}'-1-2\nu^{-1}\delta_{ij}\psi_{kk}'), \quad 2\rho\psi_{ij}'=\psi_{ij}-2\nu^{-1}\delta_{ij}\psi_{kk}, \tag{4}$$

and Kröner's $\chi_{ij}'$ from

$$\chi_{ij}=2G\{\chi_{ij}'+[\nu/(1-\nu)]\delta_{ij}\chi_{kk}'\}, \quad 2G\chi_{ij}'=\chi_{ij}-[\nu/(1+2\nu)]\delta_{ij}\chi_{kk}. \tag{5}$$

Substituting (2), (4), and (5) in (1), we have

$$\Box_T\Box_L(\chi_{ij}'-\delta_{ij}\chi_{kk}')+\Box_T\left[\frac{1}{1+\nu}\delta_{ij}\partial_k\partial_l\chi_{kl}'-\partial_i\partial_k\chi_{jk}'-\partial_j\partial_k\chi_{ki}'+\frac{1}{c_T{}^2}\frac{\partial^2}{\partial t^2}(\Phi_{ij}-\delta_{ij}\Phi_{kk})\right]$$
$$+\partial_i\partial_j\left(\frac{1}{1+\nu}\partial_k\partial_l\chi_{kl}'-\frac{2}{1-2\nu}\frac{1}{c_T{}^2}\frac{\partial^2}{\partial t^2}\Phi_{kk}\right)=\eta_{ij}-\delta_{ij}\eta_{kk}+\frac{1}{c_T{}^2}\frac{\partial^2}{\partial t^2}e_{ij}{}^P, \tag{6}$$

where

$$\Box_T=\Delta-\frac{1}{c_T{}^2}\frac{\partial^2}{\partial t^2}, \quad \Box_L=\Delta-\frac{1}{c_L{}^2}\frac{\partial^2}{\partial t^2}, \tag{7}$$

and

$$\Phi_{ij}=\psi_{ij}'+(c_T/c_L)^2\chi_{ij}', \tag{8}$$

$c_T$ and $c_L$ being the velocities of the transverse and longitudinal sound waves, respectively.

The stresses can be expressed in terms of three functions of position and time. On the other hand, we have twelve stress functions $\chi_{ij}$ and $\psi_{ij}$. Therefore, among those stress functions nine relations can be assumed. Three of those relations have been given by (3), and therefore six relations can be assumed arbitrarily. As those relations, we assume the following subsidiary condition:

$$\partial_i\partial_k\chi_{jk}' + \partial_j\partial_k\chi_{ki}' - \frac{1}{1+\nu}\delta_{ij}\partial_k\partial_l\chi_{kl}' - \frac{1}{c_T^2}\frac{\partial^2}{\partial t^2}(\Phi_{ij} - \delta_{ij}\Phi_{kk}) = 0. \tag{9}$$

With the use of this, the last two terms of the left-hand side of (6) vanish, and accordingly we have

$$\Box_T\Box_L(\chi_{ij}' - \delta_{ij}\chi_{kk}') = \eta_{ij} - \delta_{ij}\eta_{kk} + \frac{1}{c_T^2}\frac{\partial^2}{\partial t^2}e_{ij}{}^P. \tag{10}$$

This may be put into the form

$$\Box_T\Box_L\chi_{ij}' = \eta_{ij} + \frac{1}{c_T^2}\frac{\partial^2}{\partial t^2}(e_{ij}{}^P - \tfrac{1}{2}\delta_{ij}e_{kk}{}^P). \tag{11}$$

On the other hand, it follows from (2), (4), (5), (8), and (9) that

$$\sigma_{ij} = 2G[\Box_L\chi_{ij}' + (1-\nu)^{-1}(\partial_i\partial_j - \delta_{ij}\Box_2)\chi_{kk}'], \tag{12}$$

where

$$\Box_2 = \Delta - \frac{1}{2c_T^2}\frac{\partial^2}{\partial t^2}. \tag{13}$$

The incompatibility tensor is expressed in terms of the dislocation density tensor $S_{ij}$ as

$$\eta_{ij} = -\tfrac{1}{2}(\epsilon_{ikl}\partial_k S_{jl} + \epsilon_{jkl}\partial_k S_{il}) \tag{14}$$

(on distributed dislocations, see Kondo,[4] Kröner,[5] deWit,[6] and Mura.[7] The $\dot{e}_{ij}{}^P$ is given from the dislocation-flux density tensor $V_{ijk}$ through

$$\dot{e}_{ij}{}^P = \tfrac{1}{2}(\dot{\beta}_{ij}{}^P + \dot{\beta}_{ji}{}^P) \text{ and } \dot{\beta}_{ij}{}^P = -\epsilon_{imn}V_{mnj}, \tag{15}$$

where the dot means the derivative in regard to the time.

A field of moving dislocations is given by assigning $S_{ij}(\vec{x}, t)$ and $V_{ijk}(\vec{x}, t)$. $\eta_{ij}(\vec{x}, t)$ and $\dot{e}_{ij}{}^P(\vec{x}, t)$ are given from these tensors by means of (14) and (15). The stress functions are calculated from (11) after the substitution of $\eta_{ij}(\vec{x}, t)$ and $\dot{e}_{ij}{}^P(\vec{x}, t)$ in the right-hand side. The stress field due to the field of moving dislocations mentioned above is given from (12) by the substitution of these stress functions.[8]

If the field is independent of time, the d'Alembertian operators in (11) and (12) should be replaced by the Laplacian. Moreover, the last term on the fight-hand side of (11) vanishes. This is the case treated by Kröner.[9]

The expressions given in this Letter are analogous to those for a field in electrodynamics.[10] For instance, (2) is compared with the expression for an electric field in terms of the scalar and vector potentials, and (9) with the Lorentz condition which is assumed between those potentials. However, the terms appearing in the present Letter are tensors of second order, while those in the theory of electrodynamics are ordinarily vectors. Therefore, the expressions in the present theory become apparently more complicated than those in the theory of electrodynamics.

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[1]T. Mura, Phil. Mag. 8, 843 (1963), and Int. J. Eng. Sci. 1, 371 (1963), and Phil. Mag. 23, 235 (1971); H. Bross, Phys. Status Solidi 5, 329 (1964); G. Stenzel, Phys. Status Solidi 34, 351 (1969).

[2]E. Kröner, Z. Phys. 139, 175 (1954), and 142, 463 (1955).

[3]See, e.g., Eq. (3.13a) of Bross, Ref. 1.

[4]*RAAG Memoirs of the Unifying Study of Basic Problems in Engineering and Physical Sciences by Means of Geometry*, edited by K. Kondo (Gakujutsubunken-Fukyukai, Tokyo, 1955), Vol. I; *ibid.* (1958), Vol. II; *ibid.* (1962), Vol. III; *ibid.* (1968), Vol. IV.

[5]E. Kröner, *Kontinuumstheorie der Versetzungen und Eigenspannungen* (Springer, Berlin, 1958).

[6]R. deWit, Solid State Phys. 10, 249 (1960).

[7]*Mathematical Theory of Dislocations*, edited by T. Mura (American Society of Mechanical Engineering, New

York, 1969).
[8]On repeated wave equations, see, e.g., W. Nowacki, Z. Angew. Math. Mech. 51, T1 (1971).
[9]See Ref. 2 and Ref. 5, p. 54.
[10]One of the authors discussed the electromagnetic analogy for the field of moving dislocations [S. Minagawa, Phys. Status Solidi (b) 47, 197 (1971)].

# Bonding Bands, Lone-Pair Bands, and Impurity States in Chalcogenide Semiconductors*

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The origin of electronic states in two classes of semiconductors is explored: (i) semiconductors containing group-VI elements in twofold coordination, and (ii) tetrahedral semiconductors. In the first case the valence band arises from the unshared electron pair (lone pair) of the group-VI atom. We examine the effects of compositional variation on the distribution of states in amorphous semiconductors. It is predicted that an Anderson transition will occur in the band of lone-pair states when a group-VI element is added to a tetrahedral amorphous semiconductor.

This Letter points out the special role played by unshared electron pairs[1] in semiconductors which contain group-VI elements in twofold coordination. Examples of such semiconductors are the elements S, Se, and Te, IV-VI compounds ($GeTe_2$, $GeSe_2$, etc.), and V-VI compounds ($As_2S_3$, $As_2Se_3$, etc.), as well as many crystalline and glassy chalcogenide alloys. In contrast to the tetrahedral semiconductors (Si, Ge, III-V compounds, etc.) in which the bonding band forms the valence band and the antibonding band forms the conduction band, the situation is quite different in the chalcogenide semiconductors. If a chalcogen is a major constituent, the valence band in these materials is formed by the unshared-electron states.

In the following, the origin of states in Ge will be contrasted with that of states in Se. The electronic states of a solid may be considered, to first order, to be a broadened superposition of the molecular orbital states of the constituent bonds. Thus, Ge in fourfold coordination has hybridized $sp^3$ orbitals which are split into bonding ($\sigma$) and antibonding ($\sigma^*$) states. In the solid these molecular states are broadened into bands. Thus, in tetrahedral semiconductors the bonding band forms the valence band and the antibonding band forms the conduction band [see Fig. 1(a)]. In Se, on the other hand, the $s$ states lie well below the $p$ states and need not be considered. Because only two of the three $p$ states can be utilized for bonding, one normally finds Se in twofold coordination. This leaves one nonbonding electron pair. The situation is sketched in Fig. 1(b). In the solid these unshared or lone-pair (LP) electrons form a band near the original $p$-state energy. The $\sigma$ and $\sigma^*$ bands are split symmetrically with respect to this reference energy. Both the $\sigma$ and LP bands are occupied. Thus, the bonding band is no longer the valence band; this role is played by the LP band. Mooser and Pearson[2] correctly identified the valence band in Se with the nonbonding $p$ states. They used a molecular-orbital description to relate the semiconducting properties of many materials to their short-range order.

It is instructive to analyze the consequences of forming a dangling bond in the two classes of semiconductors. In both cases a filled state is

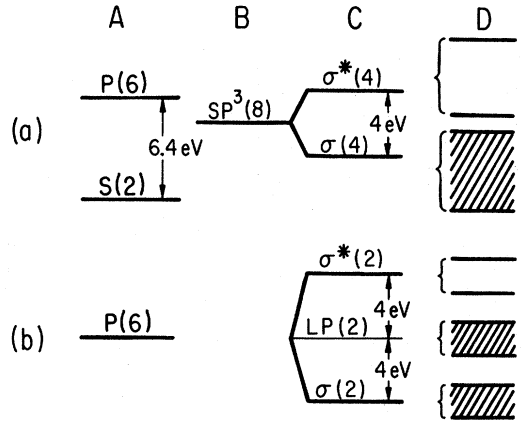


FIG. 1. Bonding in (a) Ge and (b) Se. (*A*) atomic states, (*B*) hybridized states, (*C*) molecular states, (*D*) broadening of states into bands in the solid.