NONLOCAL CONTINUUM DESCRIPTION OF LATTICE DYNAMICS AND APPLICATIONS

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Nonlocal Continuum Description of Lattice Dynamics and Applications

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Abstract

By means of a sampling theorem, the passage is made from lattice dynamics to nonlocal elasticity. Foundations of nonlinear (and linear) nonlocal elasticity is established on the basis of the nonlocal actions in continuum theory. The solutions are presented for the problems of screw-dislocation, anti-plane line crack and point defect in an elastic solid. Agreements with the atomic results and experiments are remarkable.

Keywords: fracture; Irving research

1. Introduction

All materials are made up of subbodies which constitute their substructure or microstructure. The size of subbodies may vary from atomic dimensions to the macroscopic scale such as grain size. Depending upon the nature and accuracy of the physical phenomena to be modelled, the average distance of subbodies play a central role. This distance may vary from the order of the lattice parameter a (10^{-8} cm in perfect crystals), to a few millimeters as in granular solids. The boundary and initial conditions brings into play another characteristic length A (e.g. thickness of a plate, wave length). The domain of applicability of a mathematical model depends on the ratio $e = a/A$. For classical continuum theory $e = 0$ and for the lattice dynamics $e = 1$. Since for real amorphous materials, lattice dynamic calculations are not possible or extremely costly, we may ask whether continuum theories can be constructed to cover the range $0 \leq e \leq 1$.

Indeed, such models entitled micropolar, micromorphic and nonlocal theories, have been proposed during the past two decades. Literature is fairly extensive on several sections of these theories (see [1,2]). The solutions of various critical problems have verified our hopes and expectations in that by means of nonlocal models, accurate predictions are

possible of the physical phenomena in submicroscopic scales. As a result, various long standing problems, such as crack tip singularity, dislocation core, point defects have been treated accurately [3-6]. Nonlocal plasticity [7], nonlocal fluid mechanics [8], nonlocal electromagnetism [9,10] are yet to be explored. Nevertheless, a few problems treated in these areas have already shown their power and potential, indicating that we are on the right path.

In this paper, first I present an account on linear nonlocal elasticity based on lattice dynamical models (Section 2). This shows us the firm physical foundations of the nonlocal elasticity. Next, I present a general theory of constitutive equations (Sections 3 and 4), which can be used to develop constitutive equations of memory-dependent materials (e.g. polymeric substances) undergoing finite deformations. Section 5 contains an account of some approximate models which can account for short nonlocality. These models are conducive to simpler mathematical treatments. The last three sections (Sections 6-8), contain solutions of some critical problems which fall outside of the domain of classical elasticity, since they give rise to stress singularities. The solution of the screw-dislocation problem (Section 6) leads to a finite maximum stress near the dislocation. The cohesive strength of perfect crystals based on this solution is in remarkably good agreement with those based on the atomic theories. The solution of the anti-plane crack problem presented in Section 7 contains no stress singularity so that the fracture criterium can be based on physically realistic maximum stress hypothesis. As shown in our other works (cf. [3,5,11]), it gives excellent agreement with experimental results. The last section contains the solution of the point defect problem.

2. Lattice Dynamical Foundation of Linear Elasticity

According to lattice dynamics, a perfect crystal consists of discrete atomic mass points attached to each other by springs (Fig. 1a). Let $\underset{\sim}{u}(n)$ denote the displacement vector of an atom located at a discrete point marked by n from the equilibrium position $x^o(n)$. If $\underset{\sim}{e}_k$ are a set of base vectors and $\underset{\sim}{e}^k$ are their reciprocals, i.e.

$$\underset{\sim}{e}^k \cdot \underset{\sim}{e}_\ell = \delta^k_\ell$$

We may write for the undeformed and deformed positions of an atom initially located at $\underset{\sim}{x}^o(\underset{\sim}{n})$ (Fig. 1b):

$$\underset{\sim}{x}^o(\underset{\sim}{n}) = n^k \underset{\sim}{e}_k , \quad \underset{\sim}{x}(\underset{\sim}{n}) = \underset{\sim}{x}^o(\underset{\sim}{n}) + \underset{\sim}{u}(\underset{\sim}{n}) \tag{2.1}$$

For a net consisting of atoms which are located at the "knots" of a parallelpiped with equal edge lengths (which are parallel to $\underset{\sim}{e}_k$) n^k may be taken to be integers. Such a lattice is called a simple lattice.

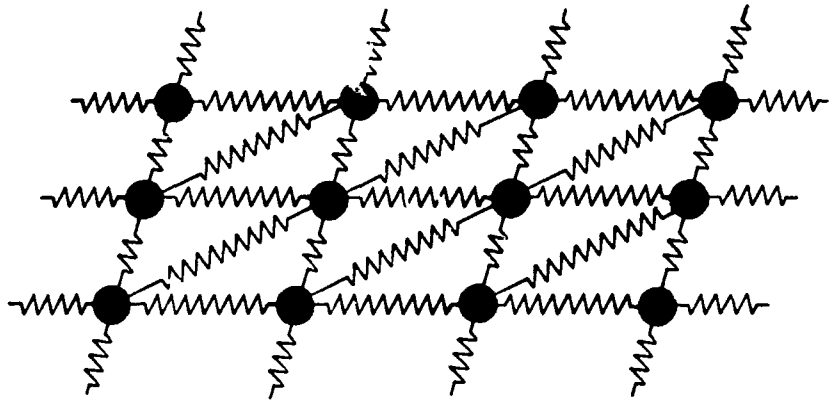
The potential energy (internal energy) of a lattice is a function only of the distance between atoms, e.g.

(2.2) $$V = \sum_{\underset{\sim}{n}\,\underset{\sim}{n}'} U[|\underset{\sim}{x}(\underset{\sim}{n}) - \underset{\sim}{x}(\underset{\sim}{n}')|]$$

A Mechanical analogy is a spring where the restoring force is a function of the change of length of the spring. For the harmonic approximation, it is simple to show that only quadratic terms in U, in the polynomial expansions of U about $\underset{\sim}{u} = \underset{\sim}{0}$ survives, and we have

(2.3) $$V = \frac{1}{2} \sum_{\underset{\sim}{n}\underset{\sim}{n}'} u^k(\underset{\sim}{n})\, \Phi_{k\ell}(\underset{\sim}{n},\underset{\sim}{n}')\, u^\ell(\underset{\sim}{n}')$$

(a)



(b)

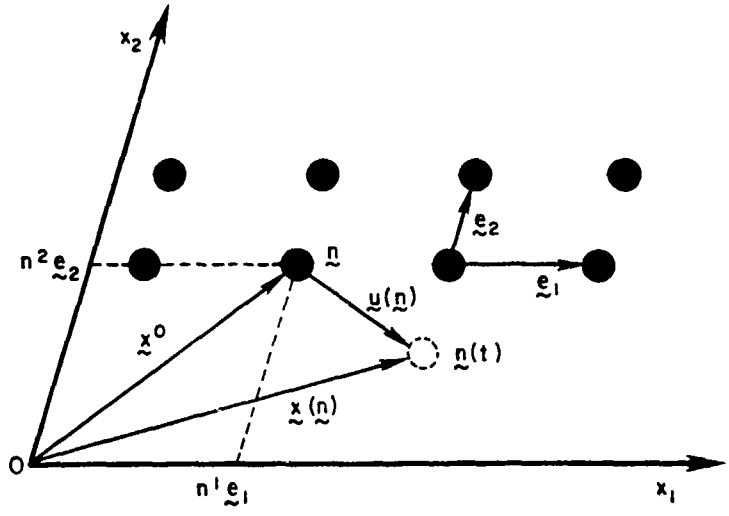


Figure 1: Atomic Model

where the constant potential energy corresponding to the equilibrium configuration is discarded and

$$\Phi_{k\ell}(\underset{\sim}{n},\underset{\sim}{n}') = U_{,k\ell}(|\underset{\sim}{x}(\underset{\sim}{n}) - \underset{\sim}{x}^{o}(\underset{\sim}{n}')|) \tag{2.4}$$

The Lagrangian of the system has the form

$$L = \frac{1}{2}\sum_{\underset{\sim}{n}} m(\underset{\sim}{n})\dot{\underset{\sim}{u}}(\underset{\sim}{n})\cdot\dot{\underset{\sim}{u}}(\underset{\sim}{n}) - \frac{1}{2}\sum_{\underset{\sim}{n}\underset{\sim}{n}'} \underset{\sim}{u}(\underset{\sim}{n})\cdot\underset{\approx}{\Phi}(\underset{\sim}{n},\underset{\sim}{n}')\cdot\underset{\sim}{u}(\underset{\sim}{n}') - \sum_{\underset{\sim}{n}} \underset{\sim}{q}(\underset{\sim}{n})\cdot\underset{\sim}{u}(\underset{\sim}{n}) \tag{2.5}$$

where $m(\underset{\sim}{n})$ is the mass of n^{th} atom and $\underset{\sim}{q}(\underset{\sim}{n})$ is the external force applied to it.

Lagrange's equation now reads

$$m(\underset{\sim}{n})\,\ddot{\underset{\sim}{u}} + \sum_{\underset{\sim}{n}'} \underset{\approx}{\Phi}(\underset{\sim}{n},\underset{\sim}{n}')\cdot\underset{\sim}{u}(\underset{\sim}{n}') = \underset{\sim}{q}(\underset{\sim}{n}) \tag{2.6}$$

This is the basic equation underlying the non-relativistic lattice dynamics.

To pass to the so-called quasicontinuum representation, we need to convert the summations in (2.5) and (2.6) to integrations. This is done by means of a sampling function based on a sampling theorem introduced by Shannon [12]. According to this theorem, if the Fourier transform $\tilde{f}(\underset{\sim}{k})$ of a function $f(\underset{\sim}{x})$ vanishes outside a region $|\underset{\sim}{k}| > k_o$, then this function is determined uniquely from its discrete values $f(\underset{\sim}{n}) = f(\underset{\sim}{x})$ at $\underset{\sim}{x} = \underset{\sim}{n}$. In fact, if

$$\tilde{f}(\underset{\sim}{k}) = v_o \sum_{\underset{\sim}{n}} f(\underset{\sim}{n})\, e^{i\underset{\sim}{n}\cdot\underset{\sim}{k}} \tag{2.7}$$

is the Fourier transform of $f(\underset{\sim}{x})$, then the inverse transform is given by

$$f(\underset{\sim}{x}) = v_o \sum_{\underset{\sim}{n}} f(\underset{\sim}{n})\, \delta_B(\underset{\sim}{x}-\underset{\sim}{n}), \tag{2.8}$$

where

$$\delta_B(\underset{\sim}{x}) = \frac{1}{(2\pi)^3}\int_B e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}\, d\underset{\sim}{k} \tag{2.9}$$

and v_o is the volume of an elementary cell constructed on the vector $\underset{\sim}{e}_k$. For a simple lattice with lattice parameter a, $|\underset{\sim}{e}_k| = a$. $v = a^3$ and the domain of $\underset{\sim}{k}$ is $0 < |\underset{\sim}{k}| < \frac{\pi}{a}$. It is clear that $\delta_B(0) = v_o^{-1}$ and $\delta_B(\underset{\sim}{n}) = 0$ for all other $\underset{\sim}{n} \neq 0$.

We note the important fact that $f(\underset{\sim}{x})$ given by (2.8) coincides exactly with $f(\underset{\sim}{n})$ at discrete points $\underset{\sim}{x} = \underset{\sim}{n}$, however being completely arbitrary elsewhere. Thus, we expect that the predictions of the nonlocal theory will agree with those of lattice dynamics at the atomic points, differing possibly in between.

Using the foregoing process, we obtain the nonlocal representation of (2.3) and (2.6)

$$(2.10) \qquad V = \frac{1}{2} \int_V \int_V \underset{\sim}{u}(\underset{\sim}{x}) \cdot \underset{\approx}{\Phi}(\underset{\sim}{x},\underset{\sim}{x}') \cdot \underset{\sim}{u}(\underset{\sim}{x}') \, dv(\underset{\sim}{x}) \, dv(\underset{\sim}{x}')$$

$$(2.11) \qquad \rho \ddot{\underset{\sim}{u}}(\underset{\sim}{x}) + \int_V \underset{\approx}{\Phi}(\underset{\sim}{x},\underset{\sim}{x}') \cdot \underset{\sim}{u}(\underset{\sim}{x}') \, dv(\underset{\sim}{x}') = \underset{\sim}{q}(\underset{\sim}{x})$$

where $\rho(x)$ is the mass density.

The invariance of Φ under rigid translations and rotations further shows that (cf. Kunin [6, p. 14], the Fourier transform of $\underset{\approx}{\Phi}$ can be written as:

$$(2.12) \qquad \Phi^{ij}(\underset{\sim}{k},\underset{\sim}{k}') = \tilde{c}^{\ell imj}(\underset{\sim}{k},\underset{\sim}{k}') \, k_\ell k'_m \, .$$

Consequently,

$$(2.13) \qquad V = \frac{1}{2} \int_V \int_V c^{\ell imj}(\underset{\sim}{x},\underset{\sim}{x}') \, e_{i\ell}(\underset{\sim}{x}) \, e_{mj}(\underset{\sim}{x}') \, dv \, dv' \, ,$$

$$(2.14) \qquad t^{k\ell}_{,k} + \rho(f^\ell - \ddot{u}^\ell) = 0$$

where we wrote $dv' \equiv dv(x')$ and

$$(2.15) \qquad t^{k\ell} = \frac{\delta V}{\delta e_{k\ell}} = \int_V c^{k\ell mn}(\underset{\sim}{x},\underset{\sim}{x}') \, e_{mn}(\underset{\sim}{x}') \, dv'$$

$$(2.16) \qquad q^\ell = \rho f^\ell \, , \qquad e_{mn} = \frac{1}{2}(u_{m,n} + u_{n,m})$$

Here $\delta V/\delta e_{k\ell}$ represents functional partial derivative. If the material properties vary slowly over a distance d, then

$$(2.17) \qquad c^{k\ell mn}(\underset{\sim}{x},\underset{\sim}{x}') = c_o^{k\ell mn}(\underset{\sim}{x}) \, \delta_B(\underset{\sim}{x}-\underset{\sim}{x}')$$

where $c_o^{k\ell mn}(\underset{\sim}{x})$ are the elastic moduli of zeroth-order, with respect to d. In the limit as the internal characteristic length (e.g. a) goes to zero, δ_B becomes Dirac delta measure and (2.15) gives classical Hooke's law. Now we are on familiar grounds.

The function $\delta_B(\underset{\sim}{x})$ given by (2.9) have been determined for various crystals. For cubic lattices, δ_B has the simple form

$$(2.18)\quad \delta_B(\underset{\sim}{x}-\underset{\sim}{x}') = \pi^{-3} \prod_{i=1}^{3} \frac{1}{x_i - x_i'} \sin\frac{\pi(x_i - x_i')}{a}$$

Another simple case is that of Debye continuum, which corresponds to the case of a spherical Brillouin zone, with radius $\kappa = \pi/a$. For this case, we have (cf. Kunin [6, p. 37])

$$(2.19)\quad \delta_B(\underset{\sim}{x}) = \frac{\kappa}{2\pi^2 r^2}\left(\frac{\sin(\kappa r)}{\kappa r} - \cos\kappa r\right), \qquad r = \sqrt{\underset{\sim}{x}\cdot\underset{\sim}{x}}$$

for the three-dimensional case and

$$(2.20)\quad \delta_B(\underset{\sim}{x}) = \frac{\kappa}{2\pi r} J_1(\kappa r)$$

for the two-dimensional case.

For engineering materials, it is useful to select other functions which give better match with the dispersion curves in the neighborhood of $\underset{\sim}{k} = \underset{\sim}{0}$. We make the following important observations:

i) In nonlocal elasticity, the total internal energy is a functional of the strain (eq. 2.13).

ii) The internal energy density coincides with those of the lattice dynamics at the discrete points occupied by the atoms.

iii) The displacement fields at the atomic points are the same for both the nonlocal elasticity and the lattice dynamics.

iv) Nonlocal elastic moduli can be determined from the interatomic potential.

v) In the limit, as the internal characteristic length (e.g. lattice parameter a) goes to zero, nonlocal elasticity reduces to classical (local) elasticity.

The development given above is for the so-called harmonic approximation (linear theory) and non-dissipative systems.

The interatomic potential is a nonlinear function of the distance. The harmonic approximation is valid only in the neighborhood of its minimum. When dislocations, holes and impurities exist (as in the case

of real materials), the dissipative effects come into play. In such situations, it is very difficult (if not impossible) to construct a nonlocal theory starting from lattice dynamics. Moreover, continuum approach make sense on its own grounds as an independent discipline. In Section 4, we present one such development.

3. Basic Axioms of Constitutive Theory

Some years ago (cf. Eringen [13]), I organized the basic elements of the constitutive theory of continuum mechanics into eight axioms:

(i) Axiom of Causality
(ii) Axiom of Determinism
(iii) Axiom of Equipresence
(iv) Axiom of Objectivity
(v) Axiom of Material Invariance
(vi) Axiom of Neighborhood
(vii) Axiom of Memory
(viii) Axiom of Admissibility

Of these (vi) and (vii) represents approximations that can be made because of the decay of interatomic interactions with distance and past times. Axiom (i) enunciate that the motion and temperatures of all material points are the cause of all physical phenomena. In fact, even the temperature can be discarded if the intrinsic motions of subbodies are taken into account. For example, according to the kinetic theory, the average kinetic energy of intrinsic motions is the absolute temperature.

Axiom (ii) and (iii) state that all other state variables (e.g. internal energy), at a point of the body, are functionals of the motions and temperatures of all points of the body. Here is the nonlocalidy!

Axiom (iv) and (v) expresses the invariance requirements for the response functionals, the first being the invariance under translations and rotations of the spatial frame and the second, under the material symmetry group.

Finally, Axiom (viii) imposes the compatibility of these functionals with the fundamental laws of motion and thermodynamics.

In Section 4, we proceed to show how these ideas can be used to develop a nonlocal continuum theory.

4. Theory of Nonlocal Elasticity

According to the axiom of causality, all state variables Z (Free energy ψ, entropy η, stress T_{KL}, heat Q_K) are functionals of the motions and temperatures of all points X' of the body, at all past times $-\infty < t' < t$. For simplicity, here we consider only isothermal elastic solids with no memory. Consequently, we have

$$\psi(\underset{\sim}{X},t) = \Psi[\underset{\sim}{x}(\underset{\sim}{X}',t),\underset{\sim}{X}'], \qquad X' \in V \tag{4.1}$$

where $\underset{\sim}{x}' = \underset{\sim}{x}(\underset{\sim}{X}',t)$ is the motion of a point $\underset{\sim}{X}'$ in the body V, and Ψ is a functional of the motion of all points $\underset{\sim}{X}' \in V$. This is also postulated for all other members of Z. Applications of the invariance under rigid body translations and rotations shows that ψ is a functional of the distance between the reference point and all other points in the body

$$(4.2) \qquad \psi(\underset{\sim}{X},t) = \Psi[|\underset{\sim}{x}(\underset{\sim}{X}',t) - \underset{\sim}{x}(\underset{\sim}{X},t)|, \underset{\sim}{X}]$$

But we have, in rectangular coordinates (see [13, p. 45]),

$$(4.3) \qquad x_k(\underset{\sim}{X}',t) - x_k(\underset{\sim}{X},t) = \int_{\underset{\sim}{X}}^{\underset{\sim}{X}'} R_{kL}\, C_{LK}^{\frac{1}{2}}\, dX_K$$

where R_{kL} and C_{KL} are, respectively, the rotation and deformation tensors. Consequently, ψ can be considered a functional of $\underset{\sim}{R}$ and $\underset{\sim}{C}$. The dependence on $\underset{\sim}{R}$ is admissible only through the difference $\underset{\sim}{R}(\underset{\sim}{X}',t) - \underset{\sim}{R}(\underset{\sim}{X},t)$ on account of the objectivity. For non-polar materials (Axiom (v)), this dependence is eliminated completely so that we arrive at

$$(4.4) \qquad \psi(\underset{\sim}{X},t) = \psi[\underset{\sim}{C}(\underset{\sim}{X}',t),\underset{\sim}{X}' ; \underset{\sim}{C}(\underset{\sim}{X},t),\underset{\sim}{X}], \qquad \underset{\sim}{X}' \neq \underset{\sim}{X}$$

For non-heat conducting solids, the second law of thermodynamics states that

$$(4.5) \qquad \int_V [-\rho_o(\dot{\psi} + \eta\dot{\theta}) + T_{KL}\dot{C}_{LK}]\, dV \geq 0$$

where ρ_o, η, $\theta > 0$ and T_{KL} are, respectively, the mass density of the body at the natural state, the entropy density, the absolute temperature, and the Piola-Kirckhoff stress tensor of which T_{KL} is related to Cauchy stress tensor $t_{k\ell}$ by

$$(4.6) \qquad t_{k\ell} = \frac{\rho}{\rho_o} T_{KL}\, x_{k,K} x_{\ell,L}$$

Note that, as against classical (local) continuum theory, we posit that *the total* entropy of the body must be non-negative.

The axiom admissability (viii) requires that (4.4) must not violate (4.5). In order to calculate $\dot{\psi}$ we need some smoothness requirement for the functional Ψ. To this end, we can assume that $C(X',t)$ belongs to a Banach or Hilbert space. However, if we confine our appetite to a more limited class of functionals, namely the linear functionals, in the sense of Friedman and Katz [14], then we can write

$$(4.7) \qquad \rho_o\, \psi(\underset{\sim}{X},t) = \int_V F[\underset{\sim}{C}(\underset{\sim}{X}',t),\underset{\sim}{X}' ; \underset{\sim}{C}(\underset{\sim}{X},t),\underset{\sim}{X}]\, dV(\underset{\sim}{X}')$$

The total internal energy is given by

$$(4.8)\qquad \int_V \rho\psi(\underset{\sim}{X},t)\, dV = \int_V \int_V F[\underset{\sim}{C}',\underset{\sim}{X}' ; \underset{\sim}{C},\underset{\sim}{X}]\, dV'\, dV$$

Since the change of the order of integrations does not affect V, we assume that

$$(4.9)\qquad F[\underset{\sim}{C}',\underset{\sim}{X}' ; \underset{\sim}{C},\underset{\sim}{X}] = \overset{*}{F}, \qquad \overset{*}{F} \equiv F[\underset{\sim}{C},\underset{\sim}{X} ; \underset{\sim}{C}',\underset{\sim}{X}']$$

where and henceforth, a superposed asterisk indicates the interchange of $\underset{\sim}{X}$ and $\underset{\sim}{X}'$.

We assume that F is continuously differentiable with respect to $\underset{\sim}{C}'$ and $\underset{\sim}{C}$. Using (4.7), we calculate

$$(4.10)\qquad \rho_o \dot{\psi} = \int_V \left(\frac{\partial F}{\partial \underset{\sim}{C}'} \cdot \dot{\underset{\sim}{C}}' + \frac{\partial F}{\partial \underset{\sim}{C}} \cdot \dot{\underset{\sim}{C}}\right) dV'$$

$$= \int_V \left[\frac{\partial F}{\partial \underset{\sim}{C}} + \left(\frac{\partial F}{\partial \underset{\sim}{C}'}\right)^*\right] \cdot \dot{\underset{\sim}{C}}\, dV' + \mathcal{D}$$

where

$$(4.11)\qquad \mathcal{D} \equiv \int_V \left[\frac{\partial F}{\partial \underset{\sim}{C}'} \cdot \dot{\underset{\sim}{C}}' - \left(\frac{\partial F}{\partial \underset{\sim}{C}'}\right)^* \cdot \dot{\underset{\sim}{C}}\right] dV'$$

Clearly,

$$(4.12)\qquad \int_V \mathcal{D}\, dV = 0$$

since the integrand of $\mathcal{D}$ is skew-symmetric function of $\underset{\sim}{X}$ and $\underset{\sim}{X}'$.

Substituting (4.10) into (4.5), we have

$$(4.13)\qquad \int_V \left\{T_{KL} - \int_V \left[\frac{\partial F}{\partial C_{KL}} + \left(\frac{\partial F}{\partial C'_{KL}}\right)^*\right] dV'\right\} \dot{C}_{KL}\, dV \geq 0$$

If this is to be valid for all values of $\underset{\sim}{C}$ throughout the body, it follows that

$$(4.14)\qquad T_{KL} = \int_V \left[\frac{\partial F}{\partial C_{KL}} + \left(\frac{\partial F}{\partial C'_{KL}}\right)^*\right] dV'$$

Thus, we have proved

> *THEOREM:* *The stress constitutive equations given by Equation (4.14) is compatible with the second law of thermodynamics.*

Note that (4.14) is exact, and it is valid for arbitrarily large elastic

strains. By means of polynomial expansions of F in $\underset{\sim}{C}'$, we obtain various nonlinear theories and the linear theory.

Linear Theory

It is practical to introduce the linear strain measures

$$C_{KL} = \delta_{KL} + 2\,E_{KL}, \qquad E_{KL} = \frac{1}{2}\,(U_{K,L} + U_{L,K}) \tag{4.15}$$

where $\underset{\sim}{U}$ is the displacement vector. We write

$$F = C_0 + C_{KLMN} E_{KL} E'_{MN} \tag{4.16}$$

where

$$C_0 = \overset{*}{C}_0 \qquad C_{KLMN} = C_{LKMN} = C_{KLNM} = \overset{*}{C}_{MNKL} \tag{4.17}$$

Substituting (4.16) into (4.14), we obtain

$$T_{KL} = \int_V C_{KLMN}(\underset{\sim}{X},\underset{\sim}{X}')\; E'_{MN}(\underset{\sim}{X}',t)\; dV' \tag{4.18}$$

For the linear theory, (4.6) gives $t_{k\ell} \simeq T_{KL}\,\delta_{kK}\delta_{\ell L}$, consequently,

$$t_{k\ell} = \int_V c_{k\ell mn}(\underset{\sim}{x},\underset{\sim}{x}')\; e_{mn}(\underset{\sim}{x}',t)\; dv(\underset{\sim}{x}') \tag{4.19}$$

where

$$\begin{aligned} c_{k\ell mn} &= C_{KLMN}\,\delta_{Kk}\delta_{L\ell}\delta_{Mm}\delta_{Nn}, \\ e_{mn} &= \frac{1}{2}\,(u_{m,n} + u_{n,m}). \end{aligned} \tag{4.20}$$

Hence we obtained the constitutive equations of the linear theory of nonlocal elasticity again, without any resort to the atomic structure.

For homogeneous medium $\underset{\sim}{c} = \underset{\sim}{c}(\underset{\sim}{x}'-\underset{\sim}{x})$ and for the homogeneous and isotropic medium, $\underset{\sim}{c}$ will be an isotropic function of $\underset{\sim}{\kappa} = \underset{\sim}{x}'-\underset{\sim}{x}$, i.e.

$$\begin{aligned} c_{k\ell mn} = {} & \lambda_o\,\delta_{k\ell}\delta_{mn} + \mu_o(\delta_{km}\delta_{\ell n} + \delta_{kn}\delta_{\ell m}) \\ & + \lambda_1(\kappa_m\kappa_n\,\delta_{k\ell} + \kappa_k\kappa_\ell\delta_{mn}) \\ & + \lambda_2(\kappa_k\kappa_m\,\delta_{n\ell} + \kappa_k\kappa_n\delta_{m\ell} + \kappa_\ell\kappa_m\delta_{kn} + \\ & \qquad + \kappa_\ell\kappa_n\,\delta_{km}) \\ & + \lambda_3\,\kappa_k\kappa_\ell\,\kappa_m\kappa_n \quad , \end{aligned} \tag{4.21}$$

where λ_o, μ_o and λ_α are functions of $|\underset{\sim}{\kappa}|$

$$(4.22) \quad \{\lambda_o, \mu_o, \lambda_\alpha\} = \{\lambda_o(|\underset{\sim}{\kappa}|), \mu_o(|\underset{\sim}{\kappa}|), \lambda_\alpha(|\underset{\sim}{\kappa}|)\}, \qquad \alpha=1,2,3$$

The material moduli λ_α are the contributions of the interatomic orientations to the isotropy. They are not present in local elasticity. Because of the appearance of κ_i, we expect that these terms are generally much smaller than λ_o and μ_o. We also expect that λ_o and μ_o attenuate with distance in the same way. If these two assumptions are accepted, then (4.19) may be put into the simple form

$$(4.23) \quad t_{k\ell} = \int_V \alpha(|\underset{\sim}{x}'-\underset{\sim}{x}|)\, \sigma_{k\ell}(\underset{\sim}{x}')\, dv(\underset{\sim}{x}')$$

where $\sigma_{k\ell}$ is the classical (local) Hookean stress, i.e.,

$$(4.24) \quad \sigma_{k\ell} = \lambda\, e_{rr}\delta_{k\ell} + 2\mu e_{k\ell}$$

and λ and μ are the classical Lamé constants.

The kernel function $\alpha(|\underset{\sim}{x}'-\underset{\sim}{x}|)$ appearing in (4.23) is of the dimension length^{-3}. Consequently, it must depend on the internal characteristic length. In fact, according to Eq. (2.17),

$$(4.25) \quad \alpha(|\underset{\sim}{x}'-\underset{\sim}{x}|) = \delta_B(\underset{\sim}{x}'-\underset{\sim}{x})$$

5. Approximate Models

(i) If the fields are slowly varying over a characteristic distance d, we can replace the integral operators with differential operators. This simply means that we expand $\bar{\underset{\sim}{c}}(\underset{\sim}{k})$ or $\bar{\alpha}(\underset{\sim}{k})$ into power series of k_i, e.g.

$$(5.1) \quad \bar{c}_{k\ell mn}(\underset{\sim}{k}) = c_{k\ell mn\tau_1\ldots\tau_r}\, (i\,k_1)\,(ik_2)\ldots(ik_r)$$

With $c_{k\ell mn\tau_1\ldots\tau_r}$ being real constants, (4.19) gives couple stress theory involving r derivatives of e_{mn}.

(ii) A more useful case involves matching $\bar{c}$ or $\bar{\alpha}$ in the wave number space with the dispersion curves, based on atomic models. For example, according to the Born-Kármán lattice model,

$$(5.2) \quad \omega_j^2(k)/\omega_{oj}^2 = (2\kappa/\pi k)^2 \sin^2(\pi k/2\kappa)$$

where

$$(5.3) \quad \omega_{oj}^2 = k^2c_j^2, \quad c_1^2 = (\lambda+2\mu)/\rho, \quad c_2^2 = \mu/\rho$$

are, respectively, the classical circular frequencies of the irrotational and equivoluminal waves. Here κ is the upper limit of k (the boundary of the Brillouin zone), e.g., for one-dimensional lattice $\kappa = \pi/a$, where a is the lattice parameter.

If we use (4.23) with (4.24) in (2.14), with $\underset{\sim}{f} = \underset{\sim}{0}$ for the harmonic waves, we obtain

$$\omega_j^2(k)/\omega_{oj}^2 = \bar{\alpha}(k^2) \tag{5.4}$$

where $\bar{\alpha}$ is the Fourier transform of α. A polynomial form of $1/\bar{\alpha}$ is most convenient to approximate (5.2):

$$1/\bar{\alpha} = 1 + \beta_j(k/\kappa)^2 + \delta_j(k/\kappa)^4 \tag{5.5}$$

At $k = 0$, this gives classical value $\omega_j = \omega_{oj}$ and at $k = \kappa$, it satisfies the condition $d\omega(k)/dk = 0$ if $\delta_j = 1$. Hence, we have

$$\bar{\alpha} = [1 + \beta_j(k/\kappa)^2 + (k/\kappa)^4]^{-1} \tag{5.6}$$

$$\omega/\omega_{oj} = [1 + \beta_j(k/\kappa)^2 + (k/\kappa)^4]^{-1/2} \tag{5.7}$$

The parameter β_j may be connected with the ratio of the boundary frequency $\omega_j(\kappa)$ to the Debye frequency ω_j^d, i.e.

$$\omega_j(\kappa)/\omega_j^d = (2 + \beta_j)^{-1/2} \tag{5.8}$$

from which it follows that $-2 < \beta_j < \infty$. Fig. 2 displays the dispersion curve based on (5.7), along with that based on the Born-Kármán model (5.2).

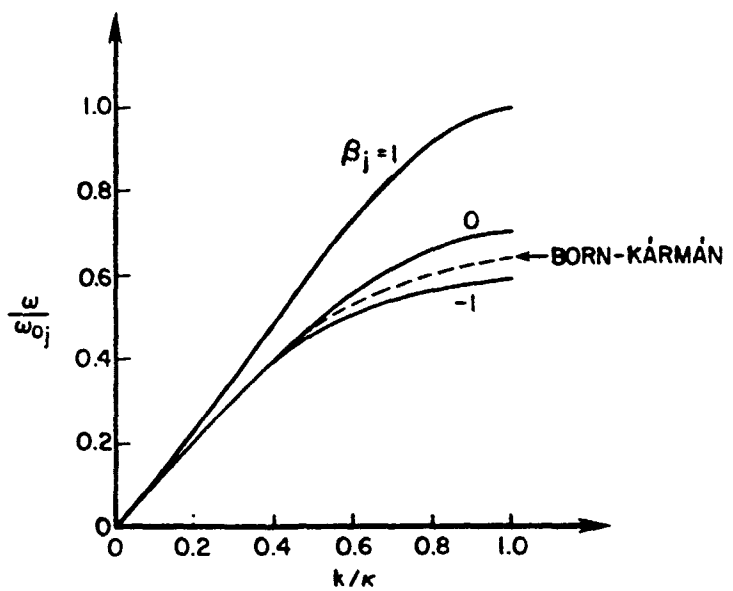


Figure 2: Dispersion Curves

It is more practical to leave β_j and δ_j free for a better fitting at a lower wave numbers for macroscopic engineering problems.

Therefore, we take

$$\bar{\alpha} = (1 + \varepsilon^2 k^2 + \gamma^4 k^4)^{-1} . \tag{5.9}$$

With this we have

$$(1 + \varepsilon^2 k^2 + \gamma^4 k^4)\, \bar{t}_{k\ell} = \bar{\sigma}_{k\ell} \tag{5.10}$$

The inverse Fourier transform of this gives

$$(1 - \varepsilon^2 \nabla^2 + \gamma^4 \nabla^4) t_{k\ell} = \sigma_{k\ell} \tag{5.11}$$

In terms of (4.23), this implies that

$$(1 - \varepsilon^2 \nabla^2 + \gamma^4 \nabla^4)\, \alpha(\underset{\sim}{x}'-\underset{\sim}{x}) = \delta(\underset{\sim}{x}'-\underset{\sim}{x}) \tag{5.12}$$

where $\delta(\underset{\sim}{x}'-\underset{\sim}{x})$ is the Dirac delta function. If we take the divergence of (5.11) and use (2.14), we obtain

$$\sigma_{k\ell,k} + (1 - \varepsilon^2 \nabla^2 + \gamma^4 \nabla^4)(\rho f_\ell - \rho \ddot{u}_\ell) = 0 \tag{5.13}$$

or, on using (4.24),

$$(\lambda + 2\mu)\, u_{k,\ell k} + \mu\, u_{\ell,kk} + (1 - \varepsilon^2 \nabla^2 + \gamma^4 \nabla^4)(\rho f_\ell - \rho \ddot{u}_\ell) = 0 \tag{5.14}$$

These equations replace the Navier equations of classical elasticity. They are singularly perturbed. Note that for the static problems and vanishing body forces (5.13) reduces to the equations of equilibrium of the classical elasticity and (5.14) to Navier's equations. However, since the real stress is not $\sigma_{k\ell}$ but $t_{k\ell}$, in order to determine the stress field, we must invert (5.10).

6. Screw Dislocation

A screw dislocation is a constant discontinuity in the displacement component u_3 at a point in the plane $x_3 = 0$. The discontinuity vector has a single component of magnitude b called, Burger's vector. In this case, $u_1 = u_2 = 0$ and $u_3 = u_3(x_1, x_2)$. Since all components of the stress tensor vanishes except t_{31} and t_{32}, the equations of equilibrium are satisfied by introducing the stress function $\phi(x_1, x_2)$ by

$$t_{13} = \phi_{,2}, \qquad t_{23} = -\phi_{,1} \tag{6.1}$$

Equations (5.11), in the simplest case $\gamma = 0$, gives

$$(1 - \varepsilon^2 \nabla^2)\phi_{,2} = \sigma_{13}, \qquad (1 - \varepsilon^2 \nabla^2)\phi_{,1} = -\sigma_{23} \tag{6.2}$$

For σ_{13} and σ_{23}, we have the expressions

(6.3) $$\sigma_{13} = \mu u_{3,1}, \qquad \sigma_{23} = \mu u_{3,2}$$

from which it follows that

(6.4) $$\sigma_{13,2} = \sigma_{23,1}$$

Using (6.2), this gives

(6.5) $$(1 - \varepsilon^2\nabla^2)\,\nabla^2\phi = 0$$

An appropriate solution of (6.5) vanishing as $r = (x_1^2 + x_2^2)^{\frac{1}{2}} \to \infty$ is given by

(6.6) $$\phi = C_0 + C_1 \ell n\, r + C_2\, K_0(r/\varepsilon)$$

where $K_0(z)$ is the modified Bessel's function, C_0, C_1 and C_2 are arbitrary constants, and (r,θ) are the plane polar coordinates, i.e.,

(6.7) $$x_1 = r\cos\theta, \qquad x_2 = r\sin\theta$$

The stress field referred to polar coordinates is given by

(6.8) $$t_{zr} = t_{31}\cos\theta + t_{32}\sin\theta,$$
$$t_{z\theta} = -t_{31}\sin\theta + t_{32}\cos\theta$$

It is simple to show that

(6.9) $$t_{zr} = \frac{1}{r}\frac{\partial\phi}{\partial\theta}, \qquad t_{z\theta} = -\frac{\partial\phi}{\partial r}$$

Employing (6.2), (6.3) and (6.6), we find that

(6.10) $$u_3 = C_1\theta$$

The jump discontinuity $u_3(2\pi) - u_3(0) = b$ is the Burger's vector b. Consequently, $C_1 = -b/2\pi$, and we have

(6.11) $$\phi = C_0 - (\mu b/2\pi)\,\ell n\, r + C_2 K_0(r/\varepsilon)$$

At the eye of the dislocation $r = 0$, $t_{z\theta}$ will vanish if $C_2 = -\mu b/2\pi\varepsilon$. Hence, the stress field is given by

(6.12) $$t_{z\theta} = \frac{\mu b}{2\pi r}\left[1 - \frac{r}{\varepsilon}K_1(r/\varepsilon)\right], \qquad t_{zr} = 0$$

This result was also found in another way in our previous works [5].

The non-dimensional stress field

$$(6.13) \qquad T \equiv (2\pi\epsilon/b)(t_{z\theta}/\mu) = \rho^{-1}[1 - \rho K_1(\rho)]$$

is plotted as a function of $\rho = r/\epsilon$ in Fig. 3. Unlike classical result $t_{z\theta}$ has no singularity at $\rho = 0$ and it approaches classical value $1/\rho$ for large ρ. It has a maximum at about $\rho = 1.1$, given by

$$(6.14) \qquad t_{z\theta\,max}/\mu \simeq 0.3993\,\frac{b}{2\pi\epsilon}$$

The strain energy per unit length L in the z-direction of a cylindrical tube of inner radius r_o and outer radius R, is given by

$$(6.15) \qquad \Sigma/L = 2\pi \int_{r_o}^{R} t_{z\theta}\, e_{z\theta}\, r\, dr = \frac{\mu b^2}{8\pi}\,[\ell n(R/r_o) + K_0(R/\epsilon) - K_0(r_o/\epsilon)]$$

Again, contrary to the classical result, this has no singularity at $r_o = 0$. For large R, the strain energy depends on the size of the solid, as expected.

By use of (6.14), we can determine the cohesive strength t_c of a perfect crystal. To this end, we write

$$(6.16) \qquad t_{z\theta\,max} = 0.3993\,\frac{b\mu}{2\pi\epsilon} = t_c$$

Based on phonon-dispersion, $\epsilon \simeq 0.39a$, where a is the lattice parameter. Using this for an aluminum crystal, we find that

$$(6.17) \qquad t_c/\mu \simeq 0.12 \qquad \{A\ell:\ [111]\langle 1\bar{1}0\rangle\}$$

This is very close to the theoretical strength $t_y/\mu = 0.11$, based on atomic models. For distributed dislocations macroscopic strength can be estimated. For such considerations, see [15].

7. Mode III Crack

A line crack located at $|x_1| < c$, $x_2 = 0$ in the plane $x_3 = 0$ is subject to a constant shear stress $t_{23} = -t_0$ along the upper surface of the crack and t_0 along the lower. The stress field is that of Mode III, i.e. the only non-vanishing stress components are t_{13} and t_{23}. To determine the stress field, we must obtain appropriate solutions of (6.5) and (6.3), subject to the boundary conditions

$$(7.1) \qquad \begin{aligned} &t_{23} = -\phi_{,1} = -t_0, && |x_1| < c, && x_2 = 0 \\ &u_3 = 0 && |x_1| > c, && x_2 = 0 \end{aligned}$$

$$(7.2) \qquad \{t_{23},\ u_3\} \to 0 \qquad \text{as} \qquad (x_1^2 + x_2^2)^{\frac{1}{2}} \to \infty$$

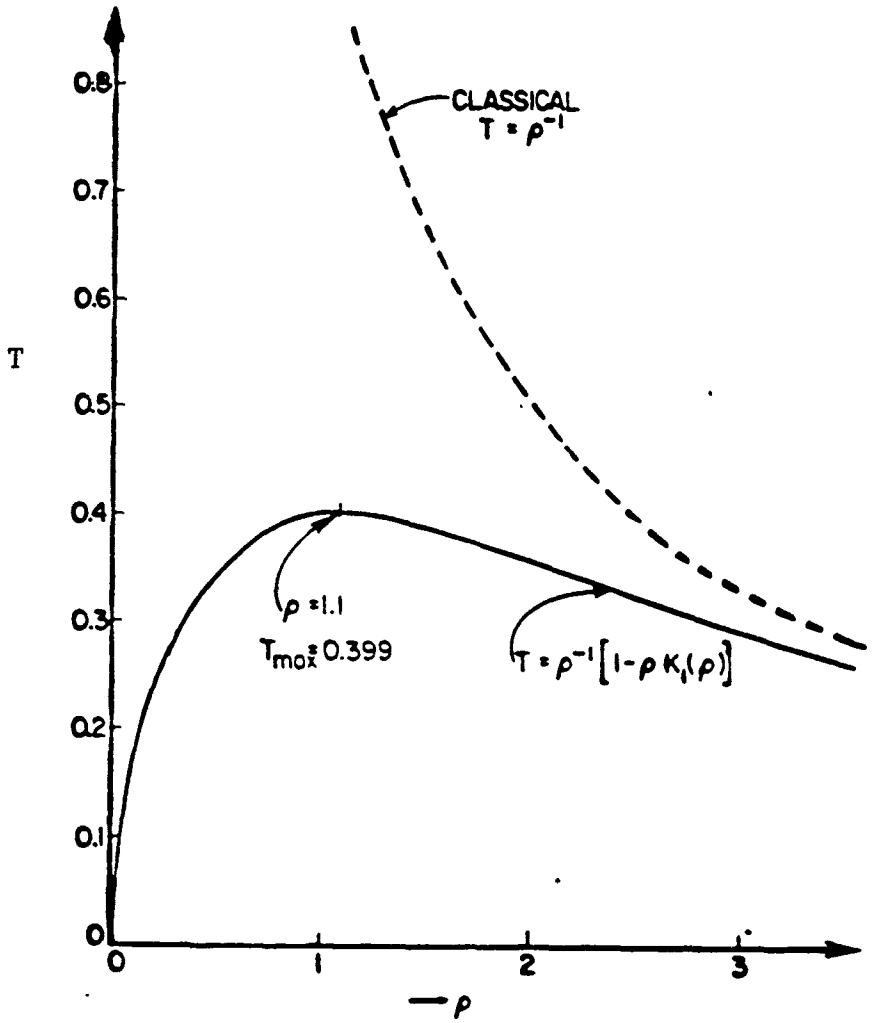


Figure 3: Non-Dimensional Hoop Stress for Screw Dislocation

$$(7.3) \qquad t_{13} = 0 \qquad |x_1| \to c \quad , \qquad x_2 = 0$$

Of these, (7.3) expresses the vanishing of the surface traction on the tip surfaces as these surfaces become two distinct points at $x_3 = 0$.

An appropriate solution of (6.5) vanishing at infinity in the upper plane $x_2 \geq 0$, is found by means of the Fourier transform technique

$$(7.4) \qquad \phi = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \mu \int_0^{\infty} [\xi A(\xi)\, e^{-\xi x_2} + B(\xi)\, e^{-\lambda x_2}] \sin(\xi x_1) d\xi$$

where $A(\xi)$ and $B(\xi)$ are to be determined from the boundary condition and

$$(7.5) \qquad \lambda \equiv (\xi^2 + \varepsilon^{-2})^{\frac{1}{2}}$$

Using (6.2) and (6.3), we find that

$$u_3 = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \int_0^\infty \xi A(\xi)\, e^{-\xi x_2} \cos(\xi x_1)\, d\xi \tag{7.6}$$

The stress field is given by

$$\begin{aligned} t_{13}/\mu &= -\left(\frac{2}{\pi}\right)^{\frac{1}{2}} \int_0^\infty [\xi^2 A(\xi)\, e^{-\xi x_2} + \lambda B(\xi)\, e^{-\lambda x_2}] \sin(\xi x_1) d\xi, \\ t_{23}/\mu &= -\left(\frac{2}{\pi}\right)^{\frac{1}{2}} \int_0^\infty [\xi^2 A(\xi)\, e^{-\xi x_2} + \xi B(\xi)\, e^{-\lambda x_2}] \cos(\xi x_1) d\xi \end{aligned} \tag{7.7}$$

At the tips of the crack, t_{13} vanishes if

$$B = A(\xi)\, \xi^2 A/\lambda \tag{7.8}$$

and we obtain

$$\begin{aligned} t_{13}/\mu &= -\left(\frac{2}{\pi}\right)^{\frac{1}{2}} \int_0^\infty \xi^2 A(\xi)(e^{-\xi x_2} - e^{-\lambda x_2}) \sin(\xi x_1)\, d\xi\,, \\ t_{23}/\mu &= -\left(\frac{2}{\pi}\right)^{\frac{1}{2}} \int_0^\infty \xi^2 A(\xi)(e^{-\xi x_2} - \frac{\xi}{\lambda} e^{-\lambda x_2}) \cos(\xi x_1)\, d\xi \end{aligned} \tag{7.9}$$

The remaining boundary conditions at $x_2 = 0$ read

$$\begin{aligned} &\int_0^\infty \zeta C(\zeta)[1 + k(\varepsilon\zeta)]\; J_{-\frac{1}{2}}(x\zeta) d\zeta = t_o/\mu\, x^{\frac{1}{2}}, \quad 0 < x < 1 \\ &\int_0^\infty C(\zeta)\, J_{-\frac{1}{2}}(x\zeta)\, d\zeta = 0, \qquad x > 1 \end{aligned} \tag{7.10}$$

where we set

$$\begin{aligned} k(\varepsilon\zeta) &= -\zeta[\zeta^2 + e^2]^{-1/2} \\ x &= x_1/c\,, \quad \zeta = c\xi \quad e = c/\varepsilon \\ C(\zeta) &= c^{-3}\, \zeta^{3/2}\, A(\zeta/c) \end{aligned} \tag{7.11}$$

and used $J_{-\frac{1}{2}}(z) = (2/\pi z)^{\frac{1}{2}} \cos z$, to replace $\cos(x\zeta)$ with its expression in terms of the Bessel's function $J_{-\frac{1}{2}}(z)$.

The solution of the dual integral equations (7.10) is not known. However, it is possible to reduce the problem to the solution of a Fredholm equation as shown in our previous work [11]. An approximate

solution for small ε can be obtained and it has the classical form

$$C_o(\zeta) = (\pi/2)^{\frac{1}{2}} (t_o/\mu)\ \zeta^{-\frac{1}{2}} J_1(\zeta) \tag{7.12}$$

This solution suffices for calculations when the crack size is larger than 100 atomic distances. Indeed it can be shown that the next perturbation is of order ε/c.

Substituting (7.12) into $(7.9)_2$, we obtain t_{23} along the crack line $x_2 = 0$:

$$t_{23}/t_o = -\int_0^\infty J_1(\zeta)[1 - \zeta(\zeta^2 + e^2)^{-\frac{1}{2}}] \cos(\zeta x)\, d\zeta \tag{7.13}$$

From (7.13), it can be deduced that as $\varepsilon \to \infty$ $(e = 0)$ t_{23} gives the classical elasticity solution. For $e = 0$ (no crack) $t_{23} = 0$ and for $e \neq 0$, there is no singularity along the x-axis. The non-dimensional stress $T \equiv t_{23}/t_0$ as a function of the non-dimensional distance x_1/c along the crack line is shown in Fig. 4 for two different values of $\varepsilon (= 0.1$ and $0.01)$. From these figures, it is clear that the boundary condition at the crack tip is satisfied very well, especially for $\varepsilon = 0.01$, as expected. Outside of the crack, the stress reaches a maximum, afterwards decaying with distance, to the classical elasticity solution. In our previous work [3,5,11], we have introduced a fracture criterium based, physically realistic, maximum stress hypothesis. This gave excellent agreement with the results of atomic theories and experiment. Further study of this problem may be necessary in order to take account of the inhomogeneity caused by the presence of the crack.

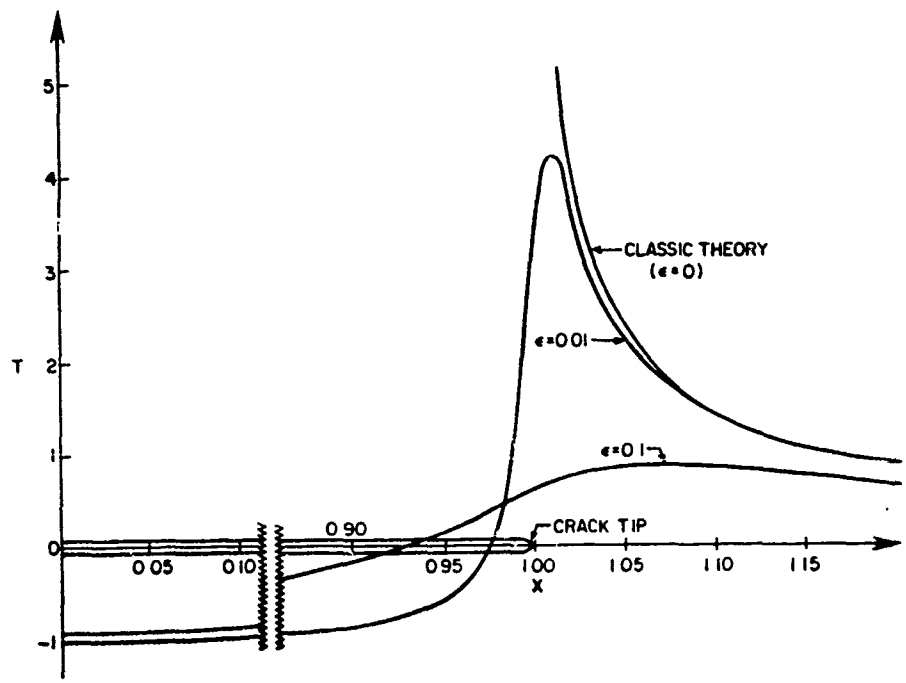


FIGURE 4: STRESS DISTRIBUTION

8. Cylindrical Hole (Defect)

A cylindrical hole of radius r_o with axis x_3 in an infinite elastic medium may be treated as a two-dimensional problem. In plane polar coordinates,

$$x_1 = r\cos\theta\,, \qquad r_2 = r\sin\theta \tag{8.1}$$

With the Airy stress function $\phi(x_1,x_2)$

$$t_{11} = \phi_{,22}\,, \qquad t_{22} = \phi_{,11}\,, \qquad t_{12} = -\phi_{,12} \tag{8.2}$$

equations of equilibrium are satisfied identically.

The strain tensor $e_{k\ell}$ must obey the compatibility equations

$$e_{11,22} + e_{22,11} - 2\,e_{12,12} = 0 \tag{8.3}$$

For $e_{k\ell}$, we have the relations

$$2\mu\, e_{k\ell} = \sigma_{k\ell} - \nu\,\sigma_{rr}\delta_{k\ell}\,, \qquad k,\ell = 1,2 \tag{8.4}$$

and for $\sigma_{k\ell}$ from (5.11) with $\gamma \equiv 0$,

$$(1 - \varepsilon^2\nabla^2)\, t_{k\ell} = \sigma_{k\ell}\,, \tag{8.5}$$

all of these being valid in rectangular coordinates.

Combining (8.2) to (8.5), we obtain

$$(1 - \varepsilon^2\nabla^2)\,\nabla^4\phi = 0 \tag{8.6}$$

But from (8.2) to (8.5), summing over k and ℓ, we have

$$(1 - \varepsilon^2\nabla^2)\,\nabla^2\phi = \frac{2\mu}{1-2\nu}\,\underset{\sim}{\nabla}\cdot\underset{\sim}{u} \tag{8.7}$$

Consequently

$$\nabla^2(\underset{\sim}{\nabla}\cdot\underset{\sim}{u}) = 0 \tag{8.8}$$

whose general solution is

$$\underset{\sim}{\nabla}\cdot\underset{\sim}{u} = C_1\,\ell n\, r + C_2 \tag{8.9}$$

Since $\underset{\sim}{\nabla}\cdot\underset{\sim}{u}$ can be replaced by its expression referred to polar coordinates,

$$\underset{\sim}{\nabla}\cdot\underset{\sim}{u} = \frac{1}{r}\frac{d}{dr}(r\,u)\,, \qquad \underset{\sim}{u} = u(r)\underset{\sim}{e}_r \tag{8.10}$$

(8.9) is integrated to give

$$r\,u = \frac{C_1}{4}\,r^2(2\,\ell n\, r - 1) + \frac{1}{2}\,C_2\,r^2 + C \tag{8.11}$$

Using the fact that u must vanish as $r \to \infty$, we obtain

$$r u = C \tag{8.12}$$

With this, $\nabla \cdot \underset{\sim}{u} = 0$ and (8.7) are integrated to give

$$\phi = A_1 + A_2 \ln r + A_3 I_0(r/\varepsilon) + A_4 K_0(r/\varepsilon) \tag{8.13}$$

where A_1 to A_4 are constants, and I_0 and K_0 are the modified Bessel's functions. To calculate the stress field in polar coordinates, we observe that

$$t_{rr} = t_{11}\Big|_{\theta=0} = \frac{1}{r}\frac{d\phi}{dr}, \qquad t_{\theta\theta} = \nabla^2\phi - t_{rr} \tag{8.14}$$

The stress field will vanish at $r = \infty$ if $A_3 = 0$, and it will have the classical elasticity value C for $\varepsilon = 0$ if $A_2 = -2\mu C$. Hence

$$\begin{aligned} t_{rr} &= -(2\mu C/\varepsilon^2\rho^2)[1 + A\rho K_1(\rho)], \\ t_{\theta\theta} &= (2\mu C/\varepsilon^2\rho^2)[1 + A\rho K_1(\rho) + A\rho^2 K_0(\rho)], \\ t_{r\theta} &= 0 \\ \rho\varepsilon u &= C \end{aligned} \tag{8.15}$$

where

$$\rho = r/\varepsilon, \qquad A = A_4/2\mu C \tag{8.16}$$

The constant C is connected with the volume change at $r = 0$, and constant A is left undetermined. By expanding $K_0(\rho)$ and $K_1(\rho)$ near $\rho = 0$, we find that for $A = -1$ the singularity of the stress field can be reduced from ρ^{-2} to $\ln\rho$ at $\rho = 0$, i.e. in the vicinity of $\rho = 0$, we have

$$\begin{aligned} t_{rr} &= (\mu C/\varepsilon^2)[\ln(\rho/2) - \tfrac{1}{2} - \psi(1)], \\ t_{\theta\theta} &= (\mu C/\varepsilon^2)[\ln(\rho/2) + \tfrac{1}{2} - \psi(1)] \end{aligned} \tag{8.17}$$

where

$$-\psi(1) = \underset{\sim}{C} = 0.5772\ldots$$

$\underset{\sim}{C}$ being the Euler constant. In terms of the displacement field, these read

$$\begin{aligned} t_{rr} &= (\mu\rho u/\varepsilon)[\ln(\rho/2) - \tfrac{1}{2} - \psi(1)], \\ t_{\theta\theta} &= (\mu\rho u/\varepsilon)[\ln(\rho/2) + \tfrac{1}{2} - \psi(1)]. \end{aligned} \tag{8.18}$$

On physical grounds, u must be finite at $r = 0$. Since interatomic distance is of the order of ε, we see that for finite u, t_{rr} and $t_{\theta\theta} \to 0$ as $\rho \to 0$.

Although $u \to \infty$ as $\rho \to 0$, we may assume that the lowest value of $r = \varepsilon$, i.e. $\rho = 1$. For this value of ρ, both t_{rr} and $t_{\theta\theta}$ are finite.

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