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SCREW DISLOCATION IN NONLOCAL HEXAGONAL ELASTIC CRYSTALS. (U)
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PRINCETON UNIVERSITY

Department of Civil Engineering

STRUCTURES AND MECHANICS

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SCREW DISLOCATION IN NONLOCAL HEXAGONAL ELASTIC CRYSTALS

by

A. Cemal Eringen
and
F. Balta

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ABSTRACT

The solution is given for the problem of screw dislocation in hexagonal crystals with long range interatomic interactions. The field equations of nonlocal elastic solids are employed to determine the anti-plane shear stresses and the elastic energy for a screw dislocation in the basal plane. Interestingly enough, none of the classical stress and energy singularities are present in the nonlocal solutions. Maximum shear stresses are calculated for several hexagonal crystals and compared with the isotropic materials. Theoretical shear stress to initiate a dislocation with a Burger's vector of one atomic distance is calculated and found to be in the acceptable range known from the lattice dynamic calculations.

1. INTRODUCTION

The classical elasticity solutions of Volterra dislocations are well documented (cf. [1]). The simplest among these is the screw dislocation in an isotropic elastic solid which exhibits a $1/r$-singularity for the shear stress and a logarithmic singularity for the elastic energy. The classical elasticity solutions, therefore, fail in a "core region" near the center line of a cylinder. In a previous paper [2] we have shown that such singularities are not present in the solutions based on the nonlocal elasticity theory. This, rather recent theory [3,4], models the solids much more

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[1] This work was supported by the office of Naval Research

satisfactorily in that the effect of long range interatomic interactions are taken into account in the stress constitutive equations. This in return allows the treatment of geometrical discontinuities and those associated with the physical inputs (force distributions, wave lengths, energy, etc.) in a more satisfactory manner. Yet, it is a continuum theory so that all problems can be formulated as boundary-value problems. The failure of classical elasticity theory in the dislocation core region has led physicists to invent various atomistic models to provide an estimate for the state of stress and energy in this region.

Encouraged with the results of our recent work on isotropic nonlocal elastic solids [2] we felt that the analysis should be extended to anisotropic solids, since in anisotropic materials the solution is influenced highly with the orientational effects. Hexagonal crystals represent technically an important class of materials with well-known stable dislocation patterns. Here we give the solution of the screw dislocation problem with the Burger's vector lying in the basal plane. In section 2 we present a brief summary of the field equations of the nonlocal elasticity theory. In section 3 we obtain the solution of the screw dislocation problem leading to expressions of the stress fields and the elastic energy. In section 4 some results of computer calculations are presented and the maximum shear stresses that cause a single dislocation in several hexagonal crystals (Mg, Apatite, Cd, Zn) are calculated. The shear stress distributions along a radial plane for these crystals display considerable differences from those for the isotropic solids. Gratifyingly no stress and energy singularity occur so that by use of the maximum shear stress hypothesis it is possible to calculate theoretical shear stress (cohesive stress).

2. FORMULATION

The basic equations of linear, homogeneous, nonlocal elastic solids, in the static case with vanishing body force, are [3,4]:

$$(2.1)\qquad t_{k\ell,k} = 0$$

$$(2.2)\qquad t_{k\ell} = \int_V a_{k\ell mn}(\underset{\sim}{x}',\underset{\sim}{x})e_{mn}(\underset{\sim}{x}')dv(\underset{\sim}{x}') \ ,$$

$$(2.3)\qquad e_{mn} = \tfrac{1}{2}(u_{m,n}+u_{n,m}) \ ,$$

where the only difference from the classical elasticity theory is in the stress constitutive equations (2.2) which state that the stress at a reference point $\underset{\sim}{x}$ is a function of strains at all points $\underset{\sim}{x}'$. As usual we use the summation convention for the repeated indices over the range (1,2,3) and denote the partial differentiation with respect to x_k by a comma, e.g.

$$t_{k\ell,m} \equiv \partial t_{k\ell}/\partial x_m \quad , \quad u_{k,\ell}(\underset{\sim}{x}') = \partial u_k/\partial x'_\ell \ .$$

The total strain energy of the body is given by

$$(2.4)\qquad \Sigma = \tfrac{1}{2}\int_V t_{k\ell}e_{\ell k}dv = \tfrac{1}{2}\int_V\int_V a_{k\ell mn}(\underset{\sim}{x}',\underset{\sim}{x})e_{k\ell}(\underset{\sim}{x})e_{mn}(\underset{\sim}{x}')dv(\underset{\sim}{x}')dv(\underset{\sim}{x})$$

From this expression and (2.2) it is clear that the nonlocal elastic moduli $a_{k\ell mn}(\underset{\sim}{x}',\underset{\sim}{x})$ possess the symmetry regulations

$$(2.5)\qquad a_{k\ell mn}(\underset{\sim}{x}',\underset{\sim}{x}) = a_{\ell kmn}(\underset{\sim}{x}',\underset{\sim}{x}) = a_{mnk\ell}(\underset{\sim}{x},\underset{\sim}{x}') = a_{nmk\ell}(\underset{\sim}{x},\underset{\sim}{x}')$$

Hence there are 21 independent functions for the nonlocal anisotropic solids that contribute to the total elastic energy. The translational invariance of (2.2) dictates that for homogeneous materials $a_{k\ell mn}$ must depend on $\underset{\sim}{x}'-\underset{\sim}{x}$. Hence

$$a_{k\ell mn}(\underset{\sim}{x}',\underset{\sim}{x}) = a_{k\ell mn}[(x_1'-x_1)^2,(x_2'-x_2)^2,(x_3'-x_3)^2] \tag{2.6}$$

In conformity with the phonon dispersion curves in lattice dynamics we can approximate $a_{k\ell mn}(\underset{\sim}{x}'-\underset{\sim}{x})$ by

$$a_{k\ell mn}(\underset{\sim}{x}'-\underset{\sim}{x}) = c_{k\ell mn}\alpha[(x_1'-x_1)^2,(x_2'-x_2)^2,(x_3'-x_3)^2], \tag{2.7}$$

where $c_{k\ell mn}$ are the elastic constants of the classical elasticity and $\alpha(\underset{\sim}{x}'-\underset{\sim}{x})$ is an <u>attenuation function</u> that depends on $\underset{\sim}{x}'-\underset{\sim}{x}$.

From the physics of solids the following properties of $\alpha(\underset{\sim}{x}'-\underset{\sim}{x})$ are obvious.

(a) $\alpha(\underset{\sim}{x}'-\underset{\sim}{x})$ attenuates rapidly with $x_k'-x_k$.

(b) In the classical elasticity limit $\alpha(\underset{\sim}{x}'-\underset{\sim}{x})$ must become a Dirac delta measure.

Based on these observations we assume that:

(i) $\alpha(\underset{\sim}{x}'-\underset{\sim}{x})$ is a continuous function of $\underset{\sim}{x}'-\underset{\sim}{x}$, with a bounded support Ω where $\alpha>0$.

(ii)

$$\int_\Omega \alpha(\underset{\sim}{x}'-\underset{\sim}{x})dv(\underset{\sim}{x}') = 1 \quad . \tag{2.8}$$

In an exactly similar fashion to our work [2] we can now prove that (2.1) and (2.2) are satisfied if and only if

$$\sigma_{k\ell,k} = 0 \qquad \text{in } V \ , \tag{2.9}$$

where

$$\sigma_{k\ell} = c_{k\ell mn} e_{mn} \tag{2.10}$$

is the classical Hookes' law. This result may be stated as:

Theorem of Correspondence:

The displacement field of the boundary-value problem of nonlocal, anisotropic elasticity, under the assumptions (i) and (ii), is identical to that of the classical anisotropic elasticity theory. The stress field is, however, given by

$$t_{k\ell}(\underset{\sim}{x}) = \int_V \alpha(\underset{\sim}{x}'-\underset{\sim}{x})\sigma_{k\ell}(\underset{\sim}{x}')dv(\underset{\sim}{x}') \ . \tag{2.11}$$

These results are valid for any kind of anisotropic solid.

For the hexagonal crystals the number of non-zero independent elastic constants $c_{k\ell mn}$ is five (cf. [1] p. 428) so that (2.10) has the form:

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{31} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{22} & c_{12} & 0 & 0 & 0 \\ c_{13} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{bmatrix} \begin{bmatrix} e_{11} \\ e_{22} \\ e_{33} \\ e_{23} \\ e_{31} \\ e_{12} \end{bmatrix} \tag{2.12}$$

where

$$c_{11} = c_{1111} \quad , \quad c_{12} = c_{1122} \quad , \quad c_{13} = c_{1133} \quad , \quad c_{22} = c_{2222} \quad ,$$

$$(2.13) \qquad c_{44} = c_{2323} \quad , \quad c_{55} = \tfrac{1}{2}(c_{11}-c_{13})$$

The attenuation function $\alpha(\underset{\sim}{x}'-\underset{\sim}{x})$ may also have different rates of decay in the basal plane perpendicular to the x_2-axis than in the x_2-direction. Considering the fact that in the basal plane, hexagonal crystals are isotropic and recalling (2.7) we must have

$$(2.14) \qquad \alpha = \alpha[(x'_\beta-x_\beta)(x'_\beta-x_\beta),\ (x'_2-x_2)^2] \quad , \quad \beta=1,3 \ .$$

The specific form of this function can be fixed by the dispersion curves available in lattice dynamics. A very useful one is the function[1]

$$(2.15) \qquad \alpha = \alpha_o \exp[-(k_1/a)^2(x'_\beta-x_\beta)(x'_\beta-x_\beta)-(k_2/a)^2(x'_2-x_2)^2], \ \beta=1,3$$

where α_o is determined by the normalization (2.8). The constants k_1 and k_2 are, respectively, the attenuation factors in the basal plane and along the x_2-axis and a is the lattice parameter.

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[1]While this function does not have finite support nevertheless it gives the Dirac delta measure in the limit $a\to 0$.

3. SCREW DISLOCATION

A pure screw dislocation in the z-direction in the basal plane of a hexagonal crystal is possible, Fig. 1. Referred to rectangular coordinates ($x_1=x$, $x_2=y$, $x_3=z$), the nonzero components of the displacement and stress fields are given by (cf. [1], p. 426)

$$u_z = \frac{b}{2\pi} \tan^{-1} (B^{-\frac{1}{2}} y/x), \tag{3.1}$$

$$\sigma_{xz} = -\frac{Ab}{2\pi} \frac{y}{Bx^2+y^2}, \tag{3.2}$$

$$\sigma_{yz} = \frac{ABb}{2\pi} \frac{x}{Bx^2+y^2} \tag{3.3}$$

where $\underset{\sim}{b}=(0,0,b)$ is the Burger's vector, and A and B are constants related to the classical elastic moduli c_{ij} by

$$A = [c_{44}(c_{11}-c_{13})/2]^{\frac{1}{2}} \quad , \quad B = 2c_{44}/(c_{11}-c_{13}) \tag{3.4}$$

The elastic energy per unit length of a cylinder, with inner and outer radii r_o and R, is given by

$$\Sigma/L = \frac{Ab^2}{4\pi} \ln \left(\frac{R}{r_o}\right) \quad . \tag{3.5}$$

From these results it is clear that the stress field has a 1/r-singularity and the energy has a logarithmic singularity as $r_o \to 0$. This, of course, is the troublesome state, well-known in classical elasticity.

According to the theorem of correspondence we can employ these results to obtain the solution in nonlocal elasticity. To this end we first calculate the classical stress fields in cylindrical coordinates. Thus,

$$(3.6)\quad \begin{aligned} \sigma_{\theta z} &= -\sigma_{xz}\sin\theta+\sigma_{yz}\cos\theta = \frac{Ab}{2\pi}\;\frac{1}{r} \;, \\ \sigma_{rz} &= \frac{A(B-1)b}{2\pi}\;\frac{1}{r}\;\frac{\tan\theta}{B+\tan^2\theta} \;, \end{aligned}$$

where

$$\cos\theta = x/(x^2+y^2)^{\frac{1}{2}} \quad , \quad \sin\theta = y/(x^2+y^2)^{\frac{1}{2}} \quad .$$

In curvilinear coordinates the physical components of the stress field $t^{(k)}_{\ (\ell)}$ is given by (see [2])

$$(3.7)\quad t^{(k)}_{\ (\ell)} = \int_V \alpha(\underset{\sim}{x}'-\underset{\sim}{x})\sigma^{(k')}_{\ (\ell')}(\underset{\sim}{x}')\delta^{\ell'}_{\ \ell}\delta^{k}_{\ k'}dv(\underset{\sim}{x}') \quad ,$$

where $\delta^{\ell'}_{\ \ell}$ and $\delta^{k}_{\ k'}$ are the direction cosines between the curvilinear coordinates x'^k and x^k. In this case we have

$$(3.8)\quad \begin{aligned} &\delta^1_{\ 1'} = \delta^2_{\ 2'} = \underset{\sim}{e}_r\cdot\underset{\sim}{e}'_r = \underset{\sim}{e}_\theta\cdot\underset{\sim}{e}'_\theta = \cos(\theta'-\theta) \quad , \quad \delta^3_{\ 3'} = \underset{\sim}{e}_z\cdot\underset{\sim}{e}'_z = 1 \;, \\ &\delta^2_{\ 1'} = \underset{\sim}{e}_\theta\cdot\underset{\sim}{e}'_r = \sin(\theta'-\theta) \quad , \quad \delta^1_{\ 2'} = \underset{\sim}{e}_r\cdot\underset{\sim}{e}'_\theta = -\sin(\theta'-\theta), \end{aligned}$$

where $(\underset{\sim}{e}_r, \underset{\sim}{e}_\theta, \underset{\sim}{e}_z)$ are the unit vectors of the cylindrical coordinates at $\underset{\sim}{x}$ and $(\underset{\sim}{e}'_r, \underset{\sim}{e}'_\theta, \underset{\sim}{e}'_z)$ are those at $\underset{\sim}{x}'$, Fig. 2.

Substituting (3.8) into (3.7) we obtain

$$(3.9)\quad \begin{aligned} t_{rz} &= \int_V \alpha(\underset{\sim}{x}'-\underset{\sim}{x})\;[-\sigma_{\theta z}(\underset{\sim}{x}')\sin(\theta'-\theta)+\sigma_{rz}(\underset{\sim}{x}')\cos(\theta'-\theta)]dv(\underset{\sim}{x}'), \\ t_{\theta z} &= \int_V \alpha(\underset{\sim}{x}'-\underset{\sim}{x})\;[\sigma_{\theta z}(\underset{\sim}{x}')\cos(\theta'-\theta)+\sigma_{rz}(\underset{\sim}{x}')\sin(\theta'-\theta)]dv(\underset{\sim}{x}') \quad . \end{aligned}$$

The normalization constant α_o in (2.15) is obtained by integrating over the infinite space. This gives

$$\alpha_o = \pi^{-3/2} k_1{}^2 k_2 a^{-3} \quad . \tag{3.10}$$

In cylindrical coordinates for the function α we have

$$\begin{aligned}\alpha(\underset{\sim}{x}'-\underset{\sim}{x}) = \alpha_o \; & \exp[-(k_1/a)^2(z'-z)^2]\cdot\exp[-(k_1/a)^2 r^2\cos^2\theta \\ & -(k_2/a)^2 r^2\sin^2\theta]\cdot\exp[-(k_1/a)^2(r'^2\cos^2\theta'-2rr'\cos\theta\cos\theta') \\ & -(k_2/a)^2(r'^2\sin^2\theta'-2rr'\sin\theta\sin\theta')]\end{aligned}$$

If we note that the function α is even in $(\theta'-\theta)$ the integrals in (3.9) take the forms

$$\begin{aligned} t_{rz} &= \frac{A(B-1)b}{2\pi}\int_{-\infty}^{\infty}\int_o^{\infty}\int_o^{2\pi}\alpha(\underset{\sim}{x}'-\underset{\sim}{x})\;\frac{\tan\theta'}{B+\tan^2\theta'}\;\cos(\theta'-\theta)d\theta'dr'dz' \quad , \\ t_{\theta z} &= \frac{Ab}{2\pi}\int_{-\infty}^{\infty}\int_o^{\infty}\int_o^{2\pi}\alpha(\underset{\sim}{x}'-\underset{\sim}{x})[\cos(\theta'-\theta)+(B-1)\;\frac{\tan\theta'}{B+\tan^2\theta'}\;\sin(\theta'-\theta)]d\theta'dr'dz' \, . \end{aligned} \tag{3.12}$$

Integration in (3.12) over r' and z' can be carried out leading to

$$\begin{aligned} t_{rz} &= \frac{Ak\kappa}{4\pi^{3/2}}\;\frac{b}{a}\int_o^{2\pi}[(B-1)\;\frac{\sin\theta'\cos\theta'}{1+(B-1)\cos^2\theta'}\;\cos(\theta'-\theta)f(\rho,\theta,\theta')d\theta' \quad , \\ t_{\theta z} &= \frac{Ak\kappa}{4\pi^{3/2}}\;\frac{b}{a}\int_o^{2\pi}[\cos(\theta'-\theta)+(B-1)\;\frac{\sin\theta'\cos\theta'}{1+(B-1)\cos^2\theta'}\;\sin(\theta'-\theta)]f(\rho,\theta,\theta')d\theta' \end{aligned} \tag{3.13}$$

where

$$(3.14)\quad \rho = kr/a \quad , \quad k=k_1 \quad , \quad k_2/k_1 = \kappa$$

$$f(\rho,\theta,\theta') = \exp\{-\rho^2[1+(\kappa^2-1)\sin^2\theta - \frac{(\cos\theta\cos\theta'+\kappa^2\sin\theta\sin\theta')^2}{1+(\kappa^2-1)\sin^2\theta'}]\}$$

$$\cdot\{1+\mathrm{erf}[\rho\ \frac{\cos\theta\cos\theta'+\kappa^2\sin\theta\sin\theta'}{[1+(\kappa^2-1)\sin^2\theta']^{\frac{1}{2}}}]\}$$

$$\cdot[1+(\kappa^2-1)\sin^2\theta']^{-\frac{1}{2}}$$

The displacement field is given by

$$(3.15)\quad u_r = u_\theta = 0 \quad , \quad u_z = \frac{b}{2\pi}\ \tan^{-1}(B^{-\frac{1}{2}}\tan\theta) \ ,$$

so that the only non-zero componenet of the strain tensor is

$$(3.16)\quad e_{\theta z} = \frac{B^{\frac{1}{2}}b}{4\pi}\ \frac{1}{r}\ [1+(B-1)\cos^2\theta]^{-1} \ .$$

The total strain energy per unit length in the z-direction is now calculated by

$$(3.17)\quad \Sigma/L = \frac{B^{\frac{1}{2}}b}{8\pi}\int_{r_o}^{R} [1+(B-1)\cos^2\theta]^{-1} t_{\theta z}(r,\theta)drd\theta$$

4. DISCUSSION

The shear stress $t_{\theta z}$ takes its maximum values at $\theta=\pi/2$. The non-dimensional shear stress,

$$(4.1)\quad \tau_{\theta z} = t_{\theta z}/t_o \quad , \quad t_o \equiv \frac{Ak}{2\pi}\ \frac{b}{a} \ ,$$

is plotted in Fig. 3 as a function of ρ for various hexagonal crystals. We have selected the value of κ as the ratio of elastic constants c_{22}/c_{11} with the consideration that the attenuation in a given direction is probably proportional to the elastic modulus in that direction. The elastic constants used are taken from [5] and they are listed in Table 1 together with κ and the maximum value of $\tau_{\theta z}$ and the $\rho=\rho_m$ at which it occurs. The $t_{\theta z}/t_o$ is also shown on Fig. 3 as a function of ρ for the isotropic crystals. It is clear that the maximum shear stress and its location is greatly affected by the anisotropy. In particular, for Cd and Zn the maximum shears are nearly one half of that for the isotropic solids. In Figs. 4 and 5 we display the non-dimensional shear stresses $t_{\theta z}$ and $\tau_{rz}=t_{rz}/t_o$ as functions of θ for magnesium. The maxima occurs at $\rho \simeq 1.10$, $\theta=\pi/2$ for $t_{\theta z}$ and $\rho \simeq 1.40$, $\theta=\pi/4$ for t_{rz}.

For engineering purposes it may be useful to give the ratios of shear stresses to those for the isotropic solids. These are shown in Fig. 6 as functions of ρ at $\theta=\pi/2$. These curves may be used to make estimates for other hexagonal crystals with different κ. Since t_{rz} is much smaller than $t_{\theta z}$ we have not provided corresponding curves for t_{rz}.

Unlike the results in the classical theory the shear stresses possess no singularity but acquire maxima. Consequently we can equate the maximum shear stress to the cohesive shear stress to obtain the condition to produce a dislocation of single atomic distance. Thus taking $b/a=1$ we have calculated the ratio of theoretical shear stress to the shear modulus c_{44}. These are listed in Table 2 for different attenuation constants k=1, 1.25 and 1.50. The value k=1.50 makes the dispersion curve for the plane shear waves obtained theoretically by using (2.15) nearly coincident with those obtained from experiments of Joynson[6]. It appears that the theoretical shear stress calculated is about twice the value based on lattice dynamics calculations (cf. [7], p. 19) for Zn. Considering the inaccuracies involved in the estimate of interatomic force laws, it is clear that the present results are in the right range. In fact, if one takes k somewhat smaller than 1 and κ slightly different, it is possible to lower these ratios. However, one cannot place any great faith in these values in the absence of experiments sufficiently accurate for the atomic scale phenomena.

The total energy given by (3.17) may be expressed as

$$(4.2) \qquad \Sigma = Ab^2 L\Sigma_o$$

where Σ_o depends on κ,B and P=kR/a. For various materials Σ_o is calculated and listed in Table 3. The case of isotropic materials agree very well with the result given in [2][1]. Σ_o grows indefinitely with the radius R becoming infinite for $R=\infty$ as expected.

[1] In [2] eqs. (4.2) and (4.3) contain a typographical error. Right-hand side of Σ should be multiplied by $\frac{1}{2}$ in both (4.2) and (4.3).

Table 1. Maximum Shear Stress

Material	Elastic Constants c_{11}	c_{12}	c_{13}	c_{22}	c_{44}	$\kappa = (c_{22}/c_{11})$	$\tau_{\theta z} = (t_{\theta z}/t_o)$	$\rho_m = (kr_m/a)$
	$\times 10^{11}$ dyn/cm^2							
Zn	16.5	5.0	3.1	6.2	3.96	0.376	0.3370	2.65
Mg	5.93	2.14	2.57	6.15	1.64	1.037	0.6555	1.08
Cd	11.4	4.0	3.94	5.08	2.0	0.446	0.3911	2.25
Apatite	16.7	6.6	1.31	14.0	6.63	0.838	0.5871	1.29
Ice	1.34	0.53	0.65	1.45	0.313	1.082	0.6824	1.03

Table 2. $t_{\theta z}/c_{44}$

Material	k = 1.00	1.25	1.50
Zn	0.0698	0.0872	0.1049
Mg	0.1056	0.1320	0.1584
Cd	0.0850	0.1062	0.1275
Apatite	0.1007	0.1258	0.1510
Ice	0.1140	0.1425	0.1710

Table 3: Coefficient Σ_o of Total Energy; $\Sigma_o = \Sigma / Ab^2 L$

Material \ $P = kR/a$	1.	2.	3.	5.	7.	10.
Isotropic (ref.[2])	0.0158	0.0400	0.0555	0.0755	0.0889	0.1031
Isotropic (Present: $B=\kappa=1$)	0.0159	0.0392	0.0553	0.0755	0.0894	0.1071
Zn	0.0061	0.0184	0.0304	0.0491	0.0622	0.0767
Mg	0.0164	0.0400	0.0560	0.0762	0.0902	0.1082
Cd	0.0072	0.0212	0.0342	0.0535	0.0667	0.0813
Apatite	0.0137	0.0356	0.0515	0.0717	0.0853	0.1019
Ice	0.0169	0.0408	0.0568	0.0771	0.0911	0.1095

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FIGURE CAPTIONS

Fig. 1 Screw Dislocation in Hexagonal Crystals

Fig. 2 Coordinates in (x,y) - plane

Fig. 3 Non-dimensional shear stress $\tau_{\theta z}$ versus ρ

Fig. 4 Non-dimensional shear stress $\tau_{\theta z}$ versus θ for Mg

Fig. 5 Non-dimensional shear stress τ_{rz} versus θ for Mg

Fig. 6 The ratio of shear stress $t_{\theta z}$ to shear stress for isotropic bodies

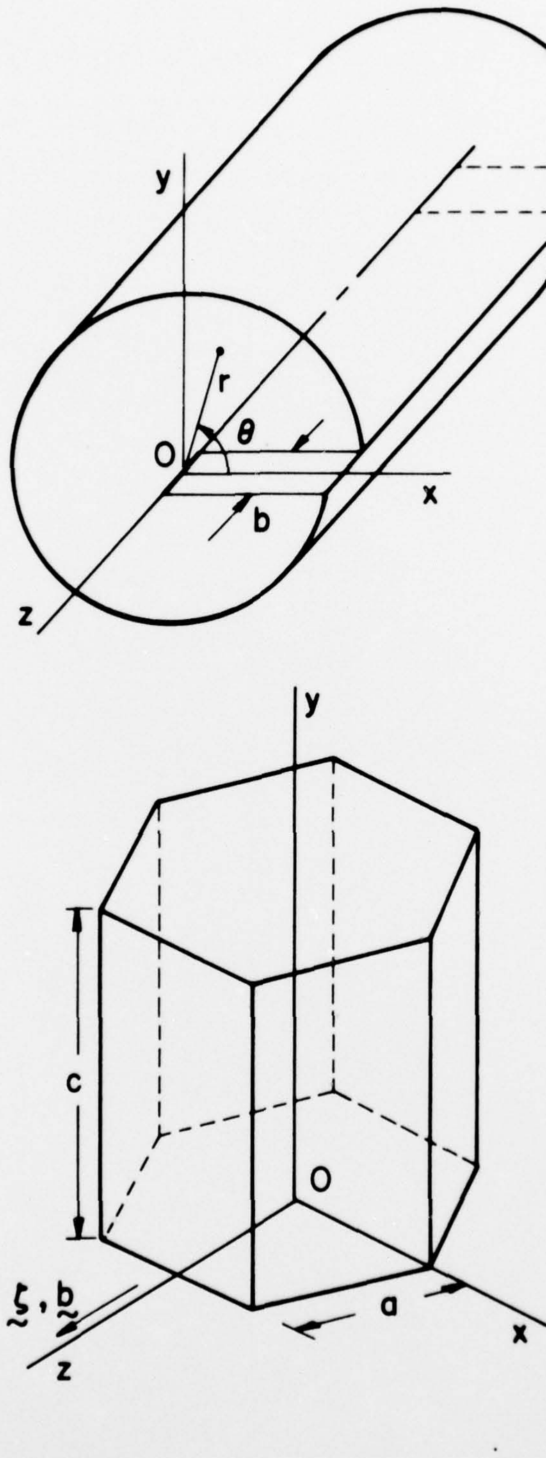


FIGURE 1

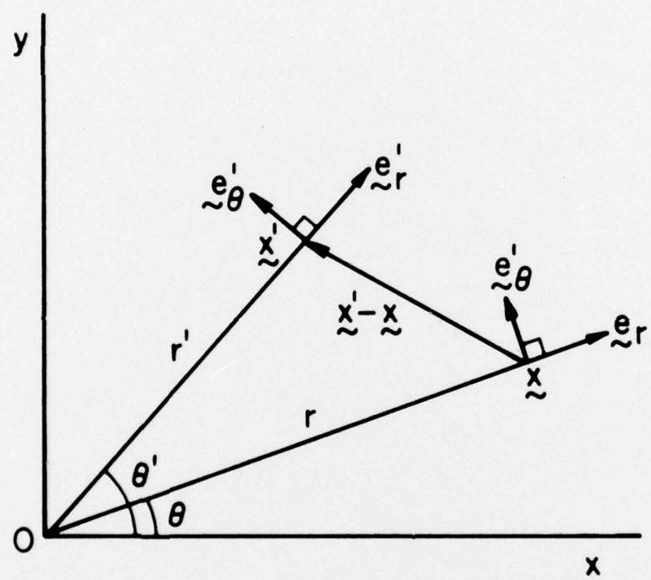
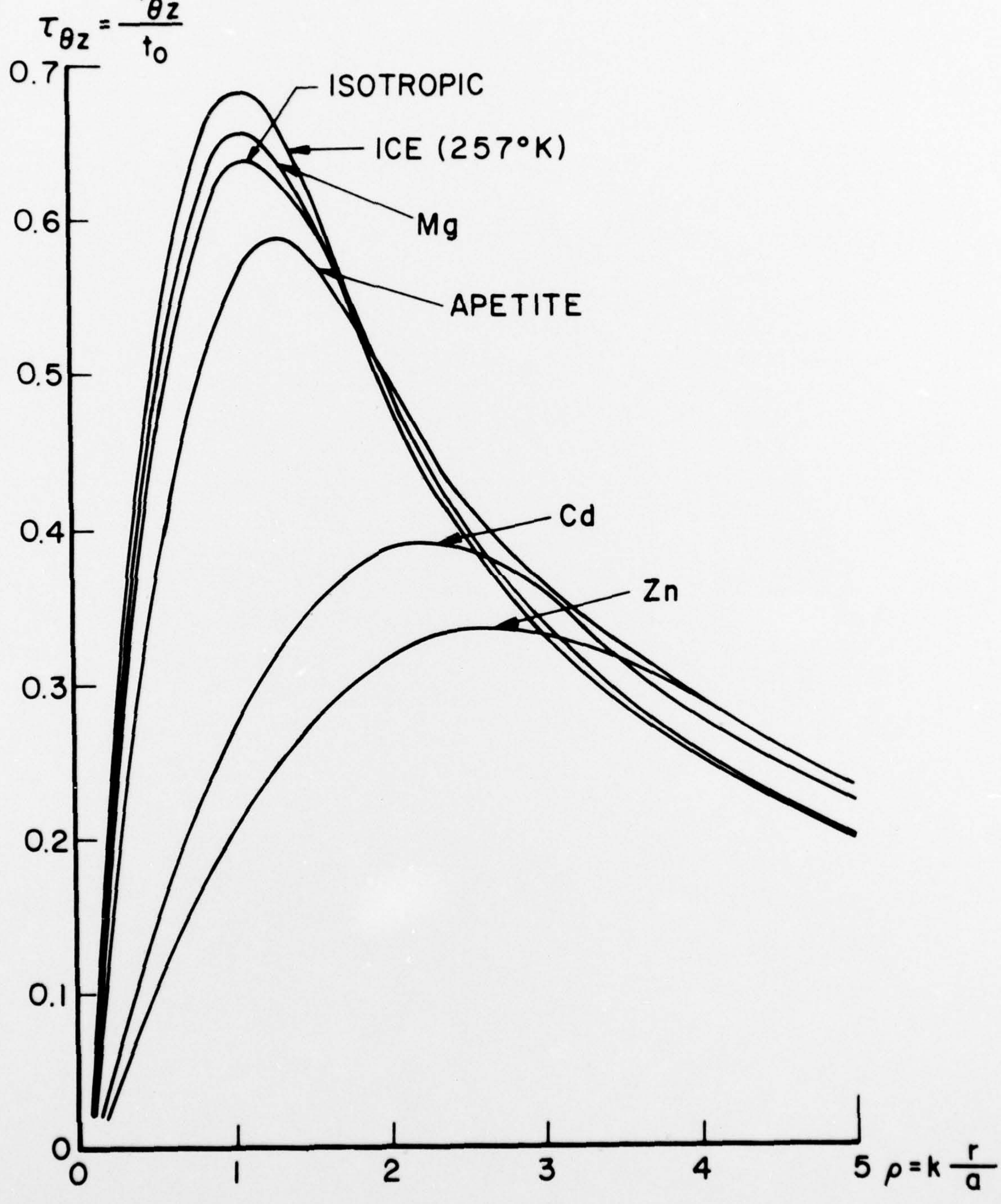

y
$\underset{\sim}{e}'_\theta$
$\underset{\sim}{e}'_r$
$\underset{\sim}{x}'$
$\underset{\sim}{e}'_\theta$
$\underset{\sim}{x}' - \underset{\sim}{x}$
r'
$\underset{\sim}{e}_r$
$\underset{\sim}{x}$
r
θ'
θ
O
x

FIGURE 2



$\tau_{\theta z} = \frac{t_{\theta z}}{t_0}$
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
ISOTROPIC
ICE (257°K)
Mg
APETITE
Cd
Zn
0
1
2
3
4
5
$\rho = k\frac{r}{a}$

FIGURE 3

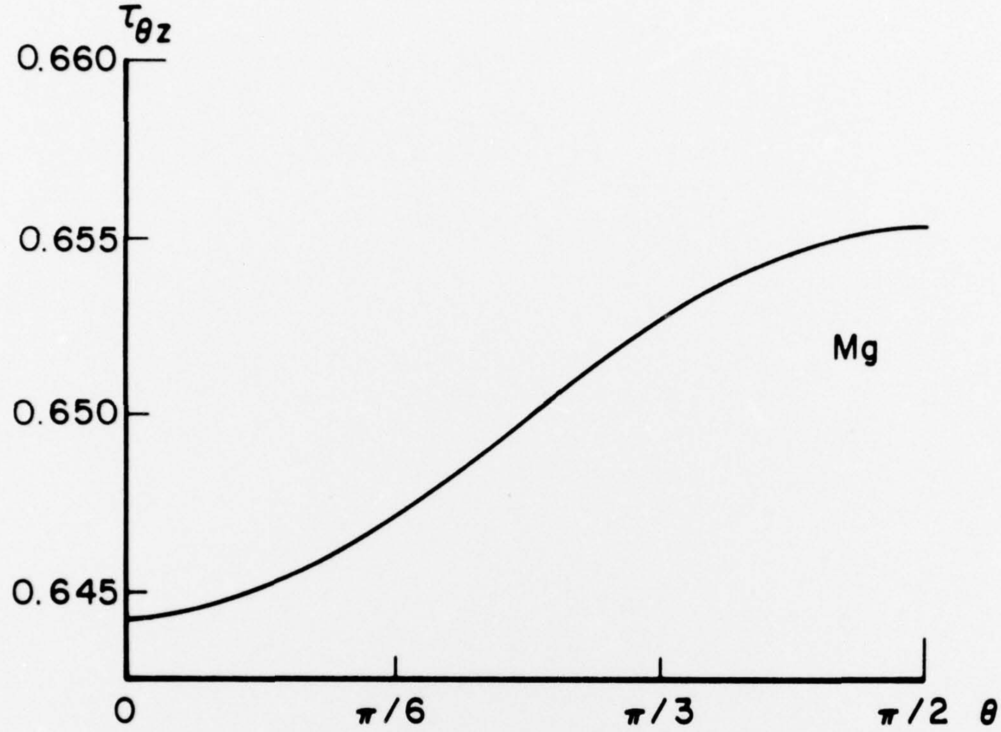


FIGURE 4

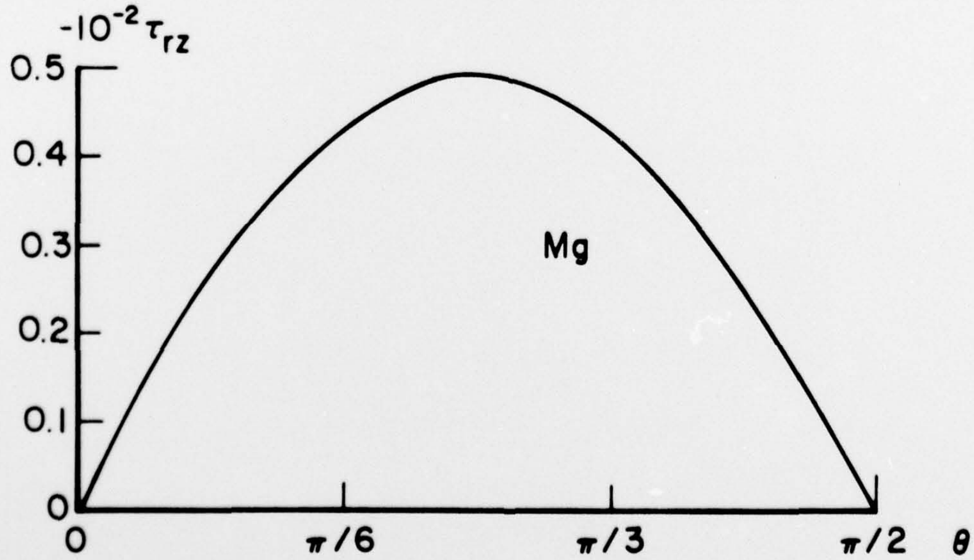
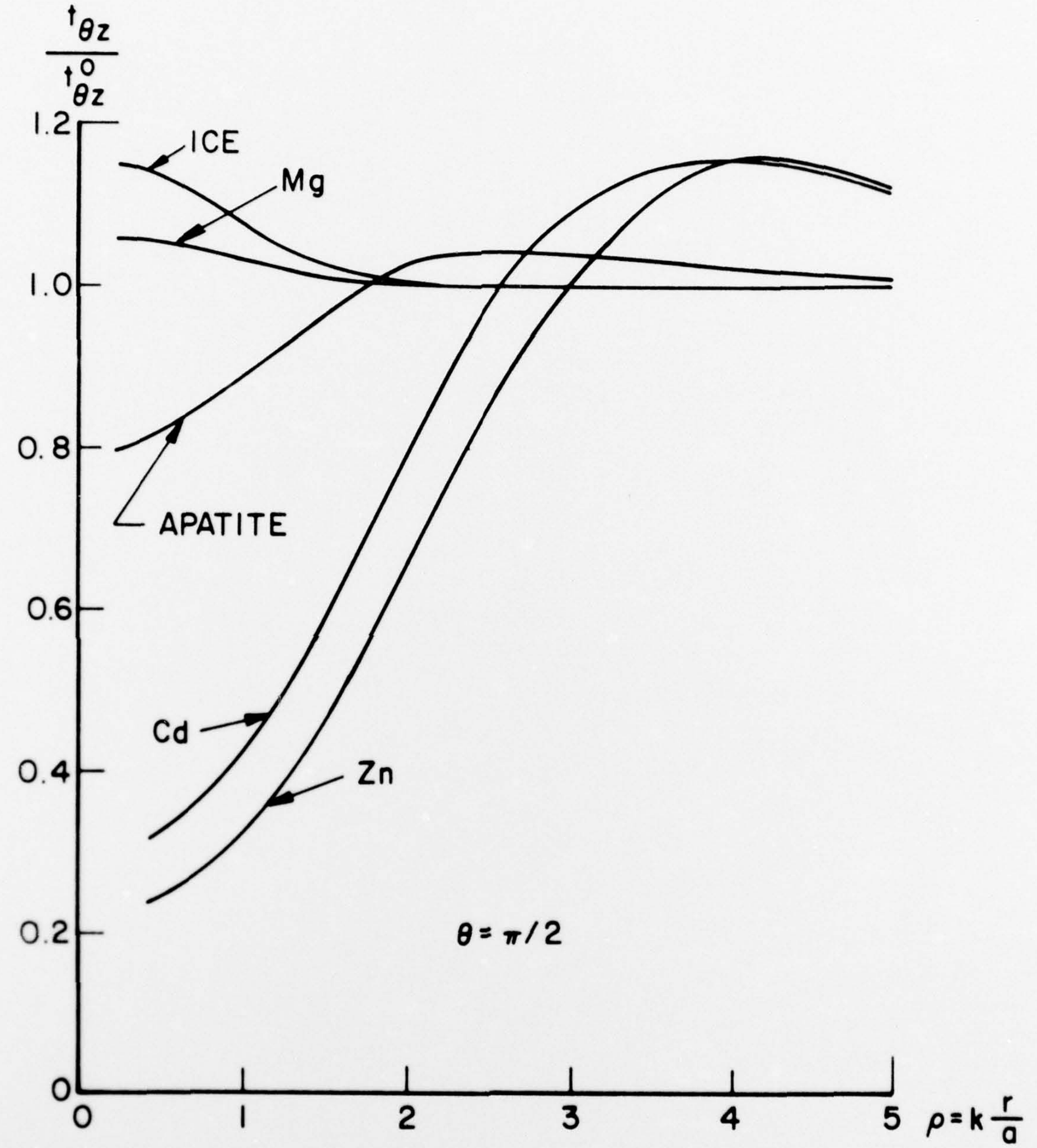


FIGURE 5



$\frac{t_{\theta z}}{t^{o}_{\theta z}}$
1.2
1.0
0.8
0.6
0.4
0.2
0
ICE
Mg
APATITE
Cd
Zn
$\theta = \pi/2$
0
1
2
3
4
5
$\rho = k\frac{r}{a}$

FIGURE 6

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The solution is given for the problem of screw dislocation in hexagonal crystals with long range interatomic interactions. The field equations of nonlocal elastic solids are employed to determine the anti-plane shear stresses and the elastic energy for a screw dislocation in the basal plane. Interestingly enough, none of the classical stress and energy singularities are present in the nonlocal solutions. Maximum shear stresses are calculated for several hexagonal crystals and compared with the isotropic materials. Theoretical → over

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19. shear stress to initiate a dislocation with a Burger's vector of one atomic distance is calculated and found to be in the acceptable range known from the lattice dynamic calculations.

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