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The screw dislocation problem in incompressible finite elastostatics: a discussion of nonlinear effects

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Abstract. The jump conditions arising in the formulation of dislocation problems in finite elastostatics are discussed and a full field solution of the anti-plane shear type is given for the screw dislocation problem. The solution is valid for the *most general* homogeneous isotropic incompressible nonlinear elastic solid. The level of nonlinearity is defined for this solution and compared to "dislocation core" estimates in materials science.

1. Introduction

Full field solutions for both screw and edge dislocations are well known in linearized elastostatics (e.g., Hirth and Lothe [1]). The displacement gradients arising in these grow unboundedly as the dislocation line is approached, in contradiction to the assumption of infinitesimal deformations.

It is often desired to establish the extent to which the solution of the linearized problem provides a good approximation to that of the fully nonlinear elastostatics problem. So far this has been attempted by requiring the norm of the *infinitesimal* strain tensor field to be less than a given positive number, small compared to unity, and identifying the domain in the body where this condition holds. This approach of using linear solutions to establish the extent of nonlinear zones is justified *only* in the absence of a solution to the fully nonlinear problem, for lack of alternatives. A number of studies attempt to produce improved estimates of nonlinearity present in the deformation fields due to dislocations. Some of them, making use of second order elasticity theory are reviewed by Teodosiu [2]. On the other hand, Seeger and Wesolowski [3] consider a screw dislocation in a compressible material and give approximate results concerning small displacements superposed on a large deformation, for a particular material.

Other investigations employ a type of theory where the stress deformation relations are nonlinear, but the displacement gradients are still assumed small, as in the deformation theory of plasticity.

In particular Kachanov, [4] solves the screw dislocation problem in an infinite medium, while Champion and Atkinson [5] consider such a dislocation in a half-space and its interaction with the boundary.

Kachanov demonstrates that the displacement field which is the solution of the linearized problem also satisfies the problem posed in terms of displacements for a "physically nonlinear" elasticity theory. However, in both Kachanov [4] and Champion and Atkinson [5] the unbounded displacement gradients arising still contradict the kinematic assumptions and the question of validity of these solutions still remains.

In the present work (Section 2) we review some preliminaries from the equilibrium theory of finite anti-plane shear for incompressible hyperelastic isotropic bodies. In Section 3 we discuss the formulation of the jump-conditions appropriate to the general dislocation problem in finite elastostatics. Here we adopt the approach proposed by Teodosiu [2] for the displacement jump conditions. To complete the formulation we propose certain additional conditions on the tractions, arising from basic equilibrium considerations. From these we derive some results pertaining to the smoothness of the deformation and stress fields, which are analogous to the ones arising in the infinitesimal theory of Somigliana dislocations, as discussed in Teodosiu [2].

The problem of an infinite straight screw dislocation is posed in Section 4, in the context of the previous section. Here we consider a finite deformation of anti-plane shear type. This choice restricts the applicability of the results to large deformation of *incompressible* materials, since the corresponding equilibrium equations for compressible materials are not in general satisfied. We provide a full field solution for arbitrary incompressible isotropic materials. The corresponding displacement field is shown to coincide with the one predicted in the infinitesimal theory. However, the stress field depends strongly on the particular choice of constitutive law and it exhibits strong nonlinearities which are not evident in any of the studies where infinitesimal deformations are assumed (e.g. [4] and [5]).

In Section 5 we consider the stored strain energy associated with the fields obtained in Section 4, and compare it with expressions derived from the linear theory. The stored energy is found to depend on the choice of the particular elastic potential (strain energy density) function adopted in the constitutive law and is given by an integral which is improper if the dislocation line is included in the region of integration. A specific choice of the constitutive law, however, gives rise to *bounded stored energy* in contrast to the linear theory.

This particular constitutive model exhibits bounded shear stresses at any amount of shear. By a suitable choice of certain parameters one can adjust the maximal stress to correspond to the amplitude of stress assumed in the Peierls model of a dislocation (Hirth and Lothe [1]). It is interesting to note that the resulting stored energy expression from finite elasticity theory comes remarkably close to that of the Peierls energy.

On the other hand, a measure of nonlinearity based on a comparison of energies stored in a given region is shown to be insensitive to certain types of nonlinearity and thus inadequate. For a certain constitutive law the stored energy expression coincides with the one from the linear theory, hence the fact that there is significant nonlinearity in the stresses is not apparent in such an approach.

To overcome such difficulties, we adopt a *quantitative* measure of nonlinearity based on the stress field, following the approach of Knowles and Rosakis [6] who used a similar measure for crack problems in anti-plane shear. By requiring this measure to be greater than a given error tolerance, we identify the region where the discrepancy between the nonlinear and linear solutions is larger than this value. This allows one to study the effect of parameters of constitutive nonlinearity on the extent of the nonlinear zone for the screw dislocation. In conclusion we compare the results to estimates of the core region obtained by semidiscrete and other numerical methods employing atomistic considerations.

2. Finite anti-plane shear

Let the cylindrical region R be occupied by a homogeneous, isotropic, elastic body in the unstressed state, which is chosen to be the reference configuration. A deformation

$$\boldsymbol{y} = \boldsymbol{y}(\boldsymbol{x}) = \boldsymbol{x} + \boldsymbol{u}(\boldsymbol{x}), \quad \boldsymbol{x} \in R, \tag{2.1}$$

maps a material point with position vector $\boldsymbol{x}$ on to a point $\boldsymbol{y}$ in R^*, which is the region occupied by the body in the deformed configuration. Accordingly, $\boldsymbol{u}(\boldsymbol{x})$ is the displacement of point $\boldsymbol{x}$. Let

$$\boldsymbol{F}(\boldsymbol{x}) = \nabla \boldsymbol{y}(\boldsymbol{x}), \quad \boldsymbol{x} \in R \tag{2.2}$$

be the deformation gradient at $\boldsymbol{x}$, and

$$J = \det \boldsymbol{F} > 0, \quad \boldsymbol{G} = \boldsymbol{F}\boldsymbol{F}^T \quad \text{on} \quad R \tag{2.3}$$

be the Jacobian determinant and the left Cauchy–Green tensor, respectively.

The Piola stress $\boldsymbol{\sigma}$, associated with force per unit undeformed area, and the Cauchy stress $\boldsymbol{\tau}$, associated with force per unit deformed area, are related by[1]

$$\boldsymbol{\sigma} = J\boldsymbol{\tau}\boldsymbol{F}^{-1}, \quad \boldsymbol{\tau} = \frac{1}{J}\boldsymbol{\sigma}\boldsymbol{F}^{T} \tag{2.4}$$

with the understanding that $\boldsymbol{\tau}$ is defined on R^*, whereas $\boldsymbol{\sigma}$ is defined on R. The equilibrium equations can be written in two forms, provided that body forces vanish:

$$\begin{aligned} \nabla \cdot \boldsymbol{\sigma} &= \mathbf{0} \quad \text{on} \quad R, \quad \text{or} \\ \nabla \cdot \boldsymbol{\tau} &= \mathbf{0} \quad \text{on} \quad R^* \quad \text{and} \\ \boldsymbol{\tau} &= \boldsymbol{\tau}^T \quad \text{on} \quad R^*. \end{aligned} \tag{2.5}$$

We choose a right handed, Cartesian coordinate system common to both deformed and undeformed configurations, such that a point $\boldsymbol{x}$ has coordinates x_1, x_2, x_3. The x_3 axis is chosen parallel to the generators of the cylindrical region R.

An *anti-plane shear* deformation has the component form

$$y_\alpha = x_\alpha, \quad y_3 = x_3 + u(x_1, x_2), \tag{2.6}$$

and u is called the out of plane displacement and can be thought of as a function defined on an arbitrary plane cross section Π of R. From (2.2), (2.3), (2.6) the matrices of components of $\boldsymbol{F}$ and $\boldsymbol{G}$ are given by

$$[F_{ij}] = [y_{i,j}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ u_{,1} & u_{,2} & 1 \end{bmatrix},$$

$$\text{on} \quad R \tag{2.7}$$

$$[G_{ij}] = \begin{bmatrix} 1 & 0 & u_{,1} \\ 0 & 1 & u_{,2} \\ u_{,1} & u_{,2} & 1 + |\nabla u|^2 \end{bmatrix}, \quad |\nabla u|^2 = u_{,\alpha}u_{,\alpha}.$$

[1] Boldface letters indicate vectors or tensors of rank two. Superscripts -1, T, $-T$ denote the inversion, transposition, and inversion of the transpose of a rank-two tensor, respectively. Latin subscribed indices have the range 1,2,3. Greek indices have the range 1,2. Summation convention is adopted unless otherwise specified.

It is important to note that (2.7) and the first of (2.3) yield that

$$J \equiv \det \boldsymbol{F} = 1 \quad \text{on} \quad R. \tag{2.8}$$

The above signifies that *every* anti-plane shear deformation is locally volume preserving. Incompressible materials can only sustain locally volume preserving deformations which satisfy condition (2.8).

For an elastic material the mechanical response is governed by the elastic potential, or strain energy density function $W = W(\boldsymbol{F})$. In case the material is isotropic the elastic potential depends on the deformation gradient $\boldsymbol{F}$ only through the three fundamental scalar invariants of the left Cauchy–Green Tensor $\boldsymbol{G} = \boldsymbol{F}\boldsymbol{F}^T$, which are given by

$$I_1(\boldsymbol{G}) = \operatorname{tr}\boldsymbol{G}, \quad I_2(\boldsymbol{G}) = \tfrac{1}{2}[(\operatorname{tr}\boldsymbol{G})^2 - \operatorname{tr}(\boldsymbol{G}^2)], \quad I_3(\boldsymbol{G}) = \det \boldsymbol{G} = J^2. \tag{2.9}$$

Incompressibility dictates that for every deformation $I_3(\boldsymbol{G}) \equiv 1$; thus for incompressible materials

$$W(\boldsymbol{F}) = W(I_1(\boldsymbol{F}\boldsymbol{F}^T), I_2(\boldsymbol{F}\boldsymbol{F}^T)). \tag{2.10}$$

The component version of the stress deformation relations for an incompressible material is

$$\sigma_{ij} = \frac{\partial W(\boldsymbol{F})}{\partial F_{ij}} - pF_{ji}^{-1}. \tag{2.11}$$

where $p = p(\boldsymbol{x})$ on R is an arbitrary scalar pressure field which is undetermined by the constitutive law and whose presence eliminates overdetermination arising from the incompressibility constraint (2.8). In view of (2.10), for an isotropic material (2.11) becomes

$$\boldsymbol{\sigma} = 2\left[\frac{\partial W}{\partial I_1}\boldsymbol{F} + \frac{\partial W}{\partial I_2}(I_1\mathbf{1} - \boldsymbol{G})\boldsymbol{F}\right] - p\boldsymbol{F}^{-T}. \tag{2.12}$$

By (2.4) the corresponding expression for the Cauchy stress is

$$\boldsymbol{\tau} = 2\left[\frac{\partial W}{\partial I_1}\boldsymbol{G} + \frac{\partial W}{\partial I_2}(I_1\mathbf{1} - \boldsymbol{G})\boldsymbol{G}\right] - p\mathbf{1}, \tag{2.13}$$

where **1** in (2.12), (2.13), stands for the idem tensor (with components δ_{ij}, the Kronecker delta). For anti-plane shear (2.4) and (2.7) yield

$$I_1(\boldsymbol{G}) = I_2(\boldsymbol{G}) = 3 + |\nabla u|^2. \tag{2.14}$$

Substituting (2.7) into (2.12), (2.13) we obtain the components of $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$:

$$\begin{aligned}
\sigma_{\alpha\beta} &= \left[2\frac{\partial W}{\partial I_1} + 2(2 + |\nabla u|^2)\frac{\partial W}{\partial I_2} - p\right]\delta_{\alpha\beta} - 2\frac{\partial W}{\partial I_2}u_{,\alpha}u_{,\beta},\\
\sigma_{\alpha 3} &= \left[-2\frac{\partial W}{\partial I_2} + p\right]u_{,\alpha}, \quad \sigma_{3\alpha} = 2\left(\frac{\partial W}{\partial I_1} + \frac{\partial W}{\partial I_2}\right)u_{,\alpha},\\
\sigma_{33} &= 2\frac{\partial W}{\partial I_1} + 4\frac{\partial W}{\partial I_2} - p, \qquad (2.15)\\
\tau_{\beta\alpha} &= \tau_{\alpha\beta} = \sigma_{\alpha\beta}, \quad \tau_{\alpha 3} = \tau_{3\alpha} = \sigma_{3\alpha},\\
\tau_{33} &= 2(1 + |\nabla u|^2)\frac{\partial W}{\partial I_1} + 2(2 + |\nabla u|^2)\frac{\partial W}{\partial I_2} - p.
\end{aligned}$$

Having (2.14) in mind one observes that with the possible exception of p, all other quantities in the right-hand sides of (2.15) depend on (x_1, x_2) only. For convenience we state here in advance that p can be shown to depend on x_3 only in case of x_3-dependent tractions on ∂R (Knowles [7] p. 405). Thus for our purposes $p = p(x_1, x_2)$, and the same is true for the stresses $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$. From this fact and (2.5), (2.15) it follows that the equilibrium equations in terms of displacements reduce to a system of three quasilinear partial differential equations (Knowles [8]) for the two unknown functions $u(x_1, x_2)$ and $p(x_1, x_2)$, valid on the cross section Π of the cylindrical region R for which $x_3 = 0$:

$$\left[p - 2\left(\frac{\partial W}{\partial I_1} + (2 + |\nabla u|^2)\frac{\partial W}{\partial I_2}\right)\right]_{,\alpha} + \left(2\frac{\partial W}{\partial I_2}u_{,\alpha}, u_{,\beta}\right)_{,\beta} = 0 \quad \text{on} \quad \Pi, \tag{2.16}$$

$$\left[2\left(\frac{\partial W}{\partial I_1} + \frac{\partial W}{\partial I_2}\right)u_{,\beta}\right]_{,\beta} = 0 \quad \text{on} \quad \Pi, \tag{2.17}$$

where

$$\frac{\partial W}{\partial I_\alpha} = \frac{\partial W}{\partial I_\alpha}(3 + |\nabla u|^2, 3 + |\nabla u|^2).$$

An important sub-class of incompressible isotropic materials is the one for which the elastic potential depends only on the first invariant of $\boldsymbol{G}$; the so-called Generalized Neo-Hookean Materials:

$$W = W(I_1). \tag{2.18}$$

For such materials the system (2.16), (2.17) reduces to

$$(2W'(3 + |\nabla u|^2)u_{,\beta})_{,\beta} = 0 \quad \text{on} \quad \Pi, \tag{2.19}$$

where a prime denotes differentiation with respect to the argument. A particular member of the above subclass is the neo-Hookean solid whose elastic potential is given by

$$W(I_1) = \frac{\mu}{2}(I_1 - 3), \tag{2.20}$$

where μ is the shear modulus for *infinitesimal* deformations. Note that for this particular material the displacement equations of equilibrium reduce to

$$\nabla^2 u = 0 \quad \text{on} \quad \Pi, \tag{2.21}$$

which is precisely the form of the equation of anti-plane shear for *infinitesimal* deformations. Thus for anti-plane shear problems with displacement boundary conditions, a solution of the linearized problem also satisfies the corresponding nonlinear one for the neo-Hookean material. However, a nonlinearity is exhibited in the Cauchy stresses for the neo-Hookean material, as will be shown subsequently in relation to the screw dislocation.

In the event that u takes the form

$$u(x_1, x_2) = k_\alpha x_\alpha \tag{2.22}$$

where k_α are the components of a constant vector $\boldsymbol{k}$, the deformation is termed *simple shear*. Letting

$$\tau = (\tau_{3\alpha}\tau_{3\alpha})^{1/2} = (\sigma_{3\alpha}\sigma_{3\alpha})^{1/2}, \quad k = |\nabla u| = (k_\alpha k_\alpha)^{1/2} \tag{2.23}$$

be the *resultant shear stress* and *amount of shear* respectively, (2.15) furnishes the so-called shear-response function:

$$\tau = \tau(k) = 2\left(\frac{\partial W}{\partial I_1} + \frac{\partial W}{\partial I_2}\right) k, \quad I_\alpha = 3 + k^2, \; -\infty < k < \infty. \tag{2.24}$$

Note that the shear modulus of the material at *infinitesimal* deformations is given by

$$\mu = 2\left(\frac{\partial W}{\partial I_1} + \frac{\partial W}{\partial I_2}\right)_{I_\alpha = 3}. \tag{2.25}$$

We will only consider here materials for which

$$\mu > 0, \quad \frac{d\tau}{dk} > 0, \quad -\infty < k < \infty; \tag{2.26}$$

i.e. materials having positive shear modulus at infinitesimal deformations and such that the slope of the shear response curve (the tangent shear modulus) is positive at any amount of shear.

These restrictions assure that the displacement equations of equilibrium (2.16) (2.17) are *elliptic* for every solution u,p and at every point in Π, as is pointed out by Knowles [7].

3. Formulation of the screw dislocation problem

In this section we attempt to model an infinite, straight dislocation in a crystal. To that effect, consider a half plane, called the *cut surface*, separating two adjacent planes of atoms. The straight line bounding the cut surface is called the *dislocation line*. A dislocation is a deformation such that any two atoms whose projections onto the cut surface are separated by a fixed vector in the *undislocated* configuration become nearest neighbors in the dislocated configuration of the crystal. Hence their projections onto the cut surface coincide in the dislocated configuration. The associated vector difference of the projections of these atoms in the *undislocated* configuration is called the *true Burger's vector*, and is a constant, often chosen equal to a

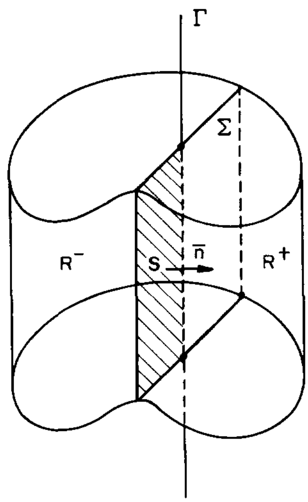

Fig. 1. Cylindrical region R, showing dislocation line Γ and cut surface S.

crystallographic lattice vector.[2] On the other hand the jump in *displacement* of the two atoms whose projections *coincide* in the *undislocated* configuration is called the *apparent Burger's vector* and in general is a function of position on the cut surface.

We consider a hyperelastic incompressible[3] body, isotropic, homogeneous and occupying a cylindrical (not necessarily circular) region R in the reference configuration. We let Γ be a straight line parallel to the generators of the lateral surface and lying in the interior or R. Given a half-plane with Γ as its boundary we let S be the intersection of its interior and R. Γ and S are the material dislocation line and material dislocation surface, respectively. The region R' consists of all points in R exterior to Γ and S. Let Σ be the plane containing S and R^+, R^- be such that $R^+ \cap R^- = \emptyset$, $R^+ \cup R^- = R' - \Sigma$. We choose $\bar{\boldsymbol{n}}$ to be the unit normal to S pointing into R^+ (see Fig. 1).

For present purposes a dislocation is a deformation $\hat{\boldsymbol{y}}$ which maps R on to a region R_* and has the following properties:

A. The mapping $\hat{\boldsymbol{y}}$ is one-to-one on R' and the associated displacement field $\boldsymbol{u}$, given by (2.1), is twice continuously differentiable on R', and there is

[2] Thus the length of the Burger's vector is of the same order as one interatomic distance, and is thus usually assumed small compared to some characteristic length of the cross-section of R.

[3] The discussion in this section up to equation (3.10) also holds for compressible bodies with only slight modifications.

a pressure field p, continuously differentiable on R' so that $\boldsymbol{u}$, p satisfy (2.1) through (2.5) and (2.8), (2.11). The deformation is thus locally volume preserving and equilibrated.

B. Let $\boldsymbol{b}$ be a given constant vector such that $\boldsymbol{b} \cdot \bar{\boldsymbol{n}} = 0$ and let

$$S' = \{\boldsymbol{x}/\boldsymbol{x} \in S, \boldsymbol{x} + \boldsymbol{b} \in S\}.$$

Then the limits

$$\begin{aligned} \hat{\boldsymbol{y}}^+(\boldsymbol{x}) &= \lim_{\boldsymbol{x}^+ \to \boldsymbol{x}} \hat{\boldsymbol{y}}(\boldsymbol{x}^+), && \boldsymbol{x} \in S', \quad \boldsymbol{x}^+ \in R^+ \\ \hat{\boldsymbol{y}}^-(\boldsymbol{x} + \boldsymbol{b}) &= \lim_{\boldsymbol{x}^- \to \boldsymbol{x}} \hat{\boldsymbol{y}}(\boldsymbol{x}^- + \boldsymbol{b}), && \boldsymbol{x} \in S', \quad \boldsymbol{x}^- \in R^- \end{aligned} \tag{3.1}$$

and the limits $\overset{+}{\boldsymbol{F}}$, $\overset{-}{\boldsymbol{F}}$, p^+, p^-, similarly defined on S', exist for every $\boldsymbol{x} \in S'$ and are continuous in $\boldsymbol{x}$ on S'.

C. There is a surface S_* associated with the deformed configuration of the body as follows:

$$\hat{\boldsymbol{y}}^+(\boldsymbol{x}) = \hat{\boldsymbol{y}}^-(\boldsymbol{x} + \boldsymbol{b}) \in S_*, \quad \forall\, \boldsymbol{x} \in S'. \tag{3.2}$$

D. Also,

$$[\boldsymbol{\tau}^+(\boldsymbol{y}) - \boldsymbol{\tau}^-(\boldsymbol{y})]\boldsymbol{n}(\boldsymbol{y}) = 0, \quad \forall\, \boldsymbol{y} \in S_*, \tag{3.3}$$

where

$$\left.\begin{aligned} \boldsymbol{\tau}^+(\boldsymbol{y}) &= \boldsymbol{\sigma}^+(\boldsymbol{x})\overset{+}{\boldsymbol{F}}{}^{-T}(\boldsymbol{x}), && \boldsymbol{y} = \hat{\boldsymbol{y}}^+(\boldsymbol{x}), \\ \boldsymbol{\tau}^-(\boldsymbol{y}) &= \boldsymbol{\sigma}^-(\boldsymbol{x} + \boldsymbol{b})\overset{-}{\boldsymbol{F}}{}^{-T}(\boldsymbol{x} + \boldsymbol{b}), && \boldsymbol{y} = \hat{\boldsymbol{y}}^-(\boldsymbol{x} + \boldsymbol{b}) \end{aligned}\right\} \quad \forall\, \boldsymbol{x} \in S' \tag{3.4}$$

and $\sigma^\pm$ are related to $\overset{+}{\boldsymbol{F}}$, $\overset{-}{\boldsymbol{F}} p^\pm$ via (2.11), whereas $\boldsymbol{n}(\boldsymbol{y})$ is the unit normal to S_* at $\boldsymbol{y}$.

In the above, the surface $S' \subset S$ is chosen to contain all points with position vector $\boldsymbol{x}$, on the cut surface, such that the point with position vector $\boldsymbol{x} + \boldsymbol{b}$ also belongs to the cut surface. This is necessary in order to state the jump condition (3.2), which is interpreted as follows: Choose points $\boldsymbol{x}$, $\boldsymbol{x} + \boldsymbol{b} \in S'$. Then material points in a small neighborhood of $\boldsymbol{x}$ in R^+ and in a small neighborhood of $\boldsymbol{x} + \boldsymbol{b}$ in R^- will have deformation images both lying in a small neighborhood of a point in the "deformed" surface S_*. On the other hand (3.3) represents the requirement that the tractions be continuous across the "deformed image" S_* of the cut surface. This is shown by choosing a suitably small sphere, centered at a point $\boldsymbol{y} \in S_*$ and containing portions of the deformed images of both R^+ and R^-, and applying balance of Cauchy tractions on its boundary, having assumed property (3.1).

One can recast requirement (D) in terms of nominal (Piola) stresses, thus making it appropriate for a referential formulation: Letting $\boldsymbol{m}_1$, $\boldsymbol{m}_2$ be unit vectors forming an orthonormal triplet with $\bar{\boldsymbol{n}}$, having in mind that S is a planar surface, one deduces from (3.2) that

$$[\overset{+}{\boldsymbol{F}}(\boldsymbol{x}) - \overset{-}{\boldsymbol{F}}(\boldsymbol{x} + \boldsymbol{b})]\boldsymbol{m}_\alpha = \boldsymbol{0}, \quad \forall\, \boldsymbol{x} \in S'. \tag{3.5}$$

Thus by a standard formula and (3.5), it follows that

$$\boldsymbol{n}(\hat{\boldsymbol{y}}^+(\boldsymbol{x})) = \frac{1}{j(\boldsymbol{x})}\overset{+}{\boldsymbol{F}}{}^{-T}(\boldsymbol{x})\bar{\boldsymbol{n}} = \boldsymbol{n}(\hat{\boldsymbol{y}}^-(\boldsymbol{x} + \boldsymbol{b})) = \frac{1}{j(\boldsymbol{x})}\overset{-}{\boldsymbol{F}}{}^{-T}(\boldsymbol{x} + \boldsymbol{b})\bar{\boldsymbol{n}} \tag{3.6}$$

where

$$j(\boldsymbol{x}) = |\overset{+}{\boldsymbol{F}}(\boldsymbol{x})\boldsymbol{m}_1 \wedge \overset{+}{\boldsymbol{F}}(\boldsymbol{x})\boldsymbol{m}_2| = |\overset{-}{\boldsymbol{F}}(\boldsymbol{x} + \boldsymbol{b})\boldsymbol{m}_1 \wedge \overset{-}{\boldsymbol{F}}(\boldsymbol{x} + \boldsymbol{b})\boldsymbol{m}_2|.$$

The symbol "$\wedge$" stands for the cross-product of two vectors. In view of (3.4), (3.6) and (3.3) yields

$$[\boldsymbol{\sigma}^+(\boldsymbol{x}) - \boldsymbol{\sigma}^-(\boldsymbol{x} + \boldsymbol{b})]\bar{\boldsymbol{n}} = \boldsymbol{0} \quad \forall\, \boldsymbol{x} \in S'. \tag{3.7}$$

The vector $\boldsymbol{b}$ is the *true Burger's vector* of the dislocation. Note that (3.2) can be rewritten as follows by using (2.1):

$$\boldsymbol{u}^+(\boldsymbol{x}) - \boldsymbol{u}^-(\boldsymbol{x} + \boldsymbol{b}) = \boldsymbol{b} \quad \text{on} \quad S'. \tag{3.8}$$

On the other hand the *apparent Burger's vector* $\hat{\boldsymbol{b}}(\boldsymbol{x})$ is defined by

$$\hat{\boldsymbol{b}}(\boldsymbol{x}) = \boldsymbol{u}^+(\boldsymbol{x} + \boldsymbol{b}) - \boldsymbol{u}^-(\boldsymbol{x} + \boldsymbol{b}), \quad \boldsymbol{x} \in S', \tag{3.9}$$

and in general is not constant on S', while it depends on the true Burger's vector through the deformation as shown by Teodosiu [2] who uses the equivalent of property (3.2) to characterize a dislocation.

The various types of dislocations arise from different choices of the direction of $\boldsymbol{b}$ in relation to that of ξ, the unit vector along the dislocation line Γ. Choosing $\boldsymbol{b}$ normal to ξ corresponds to an *edge dislocation*, whereas $\boldsymbol{b}$ parallel to ξ corresponds to a *screw dislocation*. For the remainder of the present work we confine attention to the latter type. We choose a Cartesian Coordinate frame with base vectors $\boldsymbol{e}_1$, $\boldsymbol{e}_2 = \bar{\boldsymbol{n}}$, $\boldsymbol{e}_3 = \xi$ and such that Γ passes through the origin. The material cut surface S is the part of the (x_1, x_3) half plane interior to R with x_1 positive, Γ being the x_3 axis, and $b = |\boldsymbol{b}|$, $\boldsymbol{b} = b\boldsymbol{e}_3$.

Inspection of (3.8) shows that points on either side of S undergo relative displacement in the x_3 direction or

$$\left.\begin{aligned} u_3^+(x_1, 0, x_3) - u_3^-(x_1, 0, x_3 + b) &= b \\ u_\alpha^+(x_1, 0, x_3) - u_\alpha^-(x_1, 0, x_3 + b) &= 0 \end{aligned}\right\}, \quad x_1 > 0. \tag{3.10}$$

Thus there is no jump in the in-plane displacement components in the sense of (3.10). Motivated by the above, we assume at this point that the deformation is of anti-plane shear type, and investigate the consequences of (2.6) on (3.3), (3.8). Accordingly, we assume that there are scalar fields $u(x_1, x_2)$, $p(x_1, x_2)$ defined on the cross-section Π' of R' for which $x_3 = 0$. (Letting Π be the cross section of R, we delete from it the origin and positive x_1 axis to obtain Π'.) The fields u,p are to conform to the smoothness assumptions of property (A) and satisfy the equilibrium equations (2.16) (2.17) on Π'. In view of property (B), (2.6) dictates that

$$u_3^\pm(x_1, 0, x_3) = u_3^\pm(x_1, 0, x_3 + b) = u^\pm(x_1, 0), \quad x_1 > 0. \tag{3.11}$$

Hence (3.8), (3.9) both reduce to a jump condition for u:

$$u^+(x_1, 0) - u^-(x_1, 0) = b, \quad x_1 > 0, \tag{3.12}$$

whence the true and apparent Burger's vectors necessarily coincide.[4] Note that by virtue of (2.15) all fields become independent of x_3. Also it is clear from (2.6) that an anti-plane shear deformation maps R' onto a cylindrical region of the same cross-section, thus the material cut surface S and the

[4] The true and apparent Burger's vectors necessarily coincide whenever the limiting values of the displacements at either side of the cut S are independent of position on the cut. Roughly speaking this means that each of the "faces" of the cut suffers a rigid translation, in the fashion of a dislocation as described originally by Volterra.

corresponding spatial one S_* have the same projection on the positive x_1 axis and their unit normals coincide with the unit vector $\boldsymbol{e}_2$. Consequently (3.3), (3.7) reduce to

$$\left.\begin{aligned} \tau_{i2}^{+}(x_1, 0) - \tau_{i2}^{-}(x_1, 0) &= 0, \\ \text{or} \quad \sigma_{i2}^{+}(x_1, 0) - \sigma_{i2}^{-}(x_1, 0) &= 0 \end{aligned}\right\}, \quad x_1 > 0. \tag{3.13}$$

On the other hand the specialization of the jump conditions (3.5) for anti-plane shear, implies

$$u_{,1}^{+}(x_1, 0) - u_{,1}^{-}(x_1, 0) = 0 \tag{3.14}$$

whereas $u_{,2}$ in general can jump. The jump conditions (3.13), (3.14) arise in the theory of equilibrium shocks in anti-plane shear, discussed by Knowles [9]. These are weak solutions of the equations (2.16), (2.17), such that the surfaces (having the x_3-axis as generator) across which u and the tractions are continuous, whereas p and ∇u suffer discontinuities, leading to jump conditions identical in form to (3.13), (3.14). It is stated in Knowles [9] that for materials obeying (2.18), and having positive infinitesimal shear modulus, the discontinuity in ∇u vanishes, provided the slope of the shear response curve is always positive i.e., whenever (2.26) holds. One can show that the same holds true in case of a general isotropic material. In order to apply this result to the present situation (where the displacement itself is discontinuous) we need to modify the argument presented in Knowles [9]. We choose a point $(\mathring{x}_1, 0, 0) \in \Pi \cap S$ and let $D_\varrho \subset \Pi$ be the open disc of radius ϱ centered at it with $0 < \varrho < \mathring{x}_1$. Also $D_\varrho^{\pm} = D_\varrho \cap R^{\pm}$.

We define $\hat{u}(x_1, x_2)$, $\hat{p}(x_1, x_2)$ on $D_\varrho^{\pm}$ as follows:

$$\left.\begin{aligned} \hat{u} &= u && \text{on} \quad D_\varrho^{+}, \\ \hat{u} &= u + b && \text{on} \quad D_\varrho^{-}, \\ \hat{p} &= p && \text{on} \quad D_\varrho^{\pm}. \end{aligned}\right\}. \tag{3.15}$$

We note that by (3.15)

$$\nabla \hat{u} = \nabla u, \quad \hat{\boldsymbol{\tau}} = \boldsymbol{\tau}, \quad \hat{\boldsymbol{\sigma}} = \boldsymbol{\sigma} \quad \text{on} \quad D_\varrho^{\pm}, \tag{3.16}$$

where $\hat{\boldsymbol{\sigma}}$, $\hat{\boldsymbol{\tau}}$ are related to $\hat{u}$, $\hat{p}$ by (2.15). Hence by (3.15)

$$\hat{u}^{+}(x_1, 0) - \hat{u}^{-}(x_1, 0) = 0, \quad \mathring{x}_1 - \varrho < x_1 < \mathring{x} + \varrho,$$

whereas $\hat{\sigma}$, $\hat{\tau}$, $\nabla\hat{u}$ satisfy (3.13), (3.14) on the same interval. Hence $\hat{u}$ qualifies as a weak solution of (2.16) (2.17) on D_ϱ as defined in Section 6 of Knowles [11]. Having already assumed (2.26) we conclude from (3.16) that

$$\nabla u^+ - \nabla u^- = \mathbf{0} \Rightarrow \overset{+}{\sigma} = \sigma^- \overset{+}{\tau} = \tau^- \quad \text{on} \quad D_\varrho \cap S. \tag{3.17}$$

Thus $\nabla\hat{u}$ can be extended by continuity to the projection of S on Π, making $\hat{u}$ continuously differentiable on D_ϱ and twice continuously differentiable of $D_\varrho^\pm$. On the other hand, ellipticity is precisely the requirement that the second partial derivatives of $\hat{u}$ be continuous across $D_\varrho \cap S$ provided it has the smoothness properties just mentioned.[5] Similarly, $\hat{p}$ will be continuously differentiable on D_ϱ. In a view of (3.15), we arrive at the following conclusion. If there is an anti-plane shear deformation conforming to properties (A) through (D), with out-of-plane displacement satisfying (3.12), for an incompressible, isotropic, homogeneous body whose shear response function satisfies (2.26), then there are scalar, vector, tensor fields, p, $\boldsymbol{g}$, $\boldsymbol{\sigma}$, *continuously differentiable on* $R - \Gamma$, such that $\boldsymbol{\sigma}$, p satisfy (2.11) on R and

$$\boldsymbol{g} = \nabla u \quad \text{on} \quad R', \tag{3.18}$$

whereas $\boldsymbol{\sigma}$, p, u are related through (3.18), (2.5) on R'.

Properties (A) through (D) seem a natural way to characterize the finite deformation associated with straight dislocations in elastic bodies. One observes, however, that relation (3.18) differs from the corresponding one arising in *linearized elastostatics*. Nonetheless it is seen that if one adopts the assumption that the norm of the displacement gradient be small compared to unity, property (A) allows one to write

$$\boldsymbol{u}^-(\boldsymbol{x} + \boldsymbol{b}) = \boldsymbol{u}^-(\boldsymbol{x}) + (\nabla\boldsymbol{u}^-)\boldsymbol{b} + o(|\boldsymbol{b}|) \quad \text{as} \quad |\boldsymbol{b}| \to 0. \tag{3.19}$$

Given, that $\|\nabla u\| \ll 1$ and that $|\boldsymbol{b}|$ is usually chosen to be much less than a characteristic length of the region R one sees that the second term in the right-hand side of (3.19) can be dropped, yielding for the purposes of linear elasticity:

$$\mathring{\boldsymbol{u}}^-(\boldsymbol{x}) - \mathring{\boldsymbol{u}}^+(\boldsymbol{x}) = \boldsymbol{b} \quad \text{on} \quad S \tag{3.20}$$

[5] For a definition of ellipticity of the displacement equations of equilibrium in elastostatics see Zee and Sternberg [10]. Note that $\hat{u}$, $\hat{p}$ quality as a relaxed solution of the equilibrium equations at the point $\hat{\boldsymbol{x}}$ in the terminology of [10].

in place of (3.8) and (3.9). Similarly, one obtains for the linearized stress field $\mathring{\boldsymbol{t}}$

$$(\mathring{\boldsymbol{t}}^{+}(\boldsymbol{x}) - \mathring{\boldsymbol{t}}^{-}(\boldsymbol{x}))\bar{\boldsymbol{n}} = 0 \quad \text{on} \quad S. \tag{3.21}$$

Expressions (3.20) (3.21) are the ones commonly used as jump conditions for the so-called dislocation of Somigliana type in the linear theory, as pointed out by Teodosiu [2].

4. Screw dislocation in a circular cylinder

We now apply the results of the previous discussion to a particular problem, namely a screw dislocation in a circular cylinder, with the dislocation line at the axis and vanishing traction on the lateral surface. We introduce polar coordinates (r, θ) for the (x_1, x_2) plane so that

$$x_1 = r\cos\theta, \quad x_2 = r\sin\theta, \quad 0 \leqslant r \leqslant a, \quad 0 \leqslant \theta < 2\pi$$

and let $\Pi = \{(r, \theta)/0 < r \leqslant a,\ 0 \leqslant \theta < 2\pi\}$ be the cross-section of R with radius $a > 0$ and the origin deleted, whereas $\Pi' = \{(r, \theta)/0 < r < a,\ 0 < \theta < 2\pi\}$ is the cross-section of R' with the dislocation line and cut deleted (Fig. 2). We assume R to be occupied by an incompressible homogeneous, isotropic, elastic material in the reference configuration,

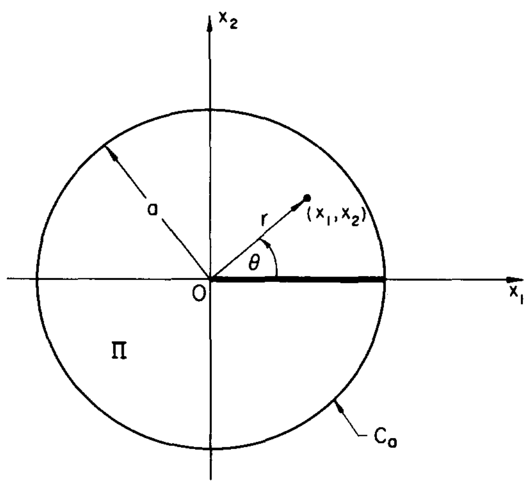

Fig. 2. Cross section Π of cylinder with dislocation.

characterized by an elastic potential $W(I_1, I_2)$ conforming to the ellipticity restriction (2.26). We seek an out-of-plane displacement field u, twice continuously differentiable and bounded on Π', whose gradient is continuously differentiable on Π by extension, and a pressure field p, continuously differentiable on Π, such that the equilibrium equations (2.16), (2.17) are satisfied on Π. Also, u is subject to the jump condition

$$u^+(x_1, 0) - u^-(x_1, 0) = b, \quad 0 < x_1 < a, \quad b = \text{const.} > 0. \tag{4.1}$$

On the other hand the circle $r = a$, denoted by C_a, is to be traction free:

$$\tau_{i\alpha}(x_1, x_2)n_\alpha(x_1, x_2) = 0, \quad r = \sqrt{x_\alpha x_\alpha} = a, \tag{4.2}$$

where $n_\alpha(x_1, x_2) = x_\alpha/a$ are the components of the unit outward normal to C_a.

Note that the following two relations are equivalent to (4.2):

$$\left.\begin{aligned} &\frac{\partial u}{\partial n} = u_{,\alpha}n_\alpha = 0 && \text{on} \quad C_a, \\ &2\frac{\partial W}{\partial I_1} + 2(2 + |\nabla u|^2)\frac{\partial W}{\partial I_2} - p = 0 && \text{on} \quad C_a. \end{aligned}\right\} \tag{4.3}$$

We begin by specializing the problem (2.16), (2.17), (4.1), (4.3) to the Neo-Hookean material, obeying (2.20). Equations (2.16), (2.17) reduce to

$$\nabla^2 u = 0, \quad p = \text{const.} \quad \text{on} \quad \Pi'. \tag{4.4}$$

Note that the first of (4.4) and (4.2) together with (4.1) constitute the equivalent problem for *linearized* elastostatics, the solution of which is standard (see, e.g., Hirth and Lothe [1]). In terms of polar coordinates,

$$u = -\frac{b\theta}{2\pi} \quad \text{on} \quad \Pi' \tag{4.5}$$

satisfies (4.4), (4.1) and the first of (4.3). Also, setting $p = \mu$ on Π satisfies the second of (4.3), thus (4.2) holds as well. We denote by $\mathring{\tau}$ the stress tensor field on Π for the linearized problem. For the screw dislocation

$$\left.\begin{aligned} &\mathring{\tau}_{3\alpha} = \mathring{\tau}_{\alpha 3} = \mu u_{,\alpha} = \frac{\mu b}{2\pi}\frac{\varepsilon_{\beta\alpha}x_\beta}{r^2} && \text{on} \quad \Pi, \\ &\mathring{\tau}_{\alpha\beta} = \mathring{\tau}_{33} = 0 && \text{on} \quad \Pi, \end{aligned}\right. \tag{4.6}$$

where $\varepsilon_{11} = \varepsilon_{22} = 0$, $\varepsilon_{12} = -\varepsilon_{21} = 1$ are the components of the two-dimensional alternator. As was just mentioned, the displacement field for the Neo-Hookean material (for finite deformations) is also given by (4.5). However the Cauchy stress field differs from the linearized one as shown by (2.15):

$$\left.\begin{aligned} \tau_{i\alpha} &= \tau_{\alpha i} = \mathring{\tau}_{i\alpha}, \\ \tau_{33} &= \mu|\nabla u|^2 = \frac{\mu b^2}{4\pi^2}\frac{1}{r^2} \end{aligned}\right\} \quad \text{on} \quad \Pi. \tag{4.7}$$

It becomes apparent from (4.7), (2.23) that although the resultant shear stress depends linearly on the amount of shear, τ_{33} depends on its square, thus its effect is of *second order* with respect to the displacement gradient. Indeed, in the linearized case (4.6), $\mathring{\tau}_{33}$ vanishes. In the Neo-Hookean case, τ_{33}, becomes the dominant stress component as the dislocation line is approached ($r \to 0$), whereas for large enough distance r the shear stresses $\tau_{3\alpha}$ dominate and the Cauchy stress field approaches the linearized one.

We now consider the equations (2.16), (2.17) for an arbitrary choice of the potential $W(I_1, I_2)$. First, observing that the pressure does not appear in (2.17), we let

$$M(\mathrm{R}) = 2\left(\frac{\partial W}{\partial I_1} + \frac{\partial W}{\partial I_2}\right)_{I_\alpha = 3+\mathrm{R}}, \quad 0 \leqslant \mathrm{R} < \infty. \tag{4.8}$$

On letting

$$\mathrm{R} = |\nabla u|^2, \quad \mathrm{R}_{,\beta} = 2u_{,\beta\alpha}u_{,\beta} \quad \text{on} \quad \Pi,$$

(2.17) becomes

$$M(|\nabla u|^2)u_{,\beta\beta} + 2M'(|\nabla u|^2)u_{,\alpha}u_{,\alpha\beta}u_{,\beta} = 0 \quad \text{on} \quad \Pi. \tag{4.9}$$

One clearly expects different solutions u of (4.9) for different choices of W and thus M. Although this possibility is by no means ruled out, it suffices for the present purposes to verify by direct calculation that u given by (4.5), satisfies

$$u_{,\beta\beta} = 0, \quad u_{,\alpha}u_{,\alpha\beta}u_{,\beta} = 0 \quad \text{on} \quad \Pi', \tag{4.10}$$

thus it is a solution of (4.9) for every choice of M continuously differentiable. In fact, Knowles [11] shows that the only choices of u satisfying (4.10) – and thus (4.9) for every smooth M – are the following:

$$u = c_1\theta + c_2, \quad c_1, c_2 = \text{const.}, \quad u = k_\alpha x_\alpha, \quad k_\alpha = \text{const.}$$

We note that for a suitable choice of the constants, c_1, c_2, the first of these yields (4.5), whereas the second corresponds to simple shear.

As is shown in Knowles [11], if u satisfies (4.10) then one can choose p so that (2.16) is also satisfied. For the remainder of this section u will be given by (4.5) which is known to satisfy (2.17) for every choice of W (twice continuously differentiable with respect to $I_\alpha, I_\alpha \geqslant 3$), and also (4.1) and the first of (4.3). It remains to find p such that (2.16) and the second of (4.3) hold in order to arrive at the solution. To that effect let

$$\omega_\alpha(\mathrm{R}) = \left.\frac{\partial W}{\partial I_\alpha}\right|_{I_\alpha = 3+\mathrm{R}}, \quad 0 \leqslant \mathrm{R} < \infty,$$

$$\mathrm{R} = |\nabla u|^2 = \frac{b^2}{4\pi^2 r^2} \quad \text{on} \quad \Pi.$$

Then, by (4.10), (2.16) becomes

$$\{p - 2[\omega_1(\mathrm{R}) + (2 + \mathrm{R})\omega_2(\mathrm{R})]\}_{,\alpha} + 2\omega_2(\mathrm{R})\mathrm{R}_{,\alpha} = 0 \quad \text{on} \quad \Pi. \tag{4.11}$$

Letting

$$\Omega(\mathrm{R}) = \int_0^{\mathrm{R}} \omega_2(\varrho)\, \mathrm{d}\varrho,$$

one sees that this reduces to

$$\{p - 2[\omega_1(\mathrm{R}) + (2 + \mathrm{R})\omega_2(\mathrm{R}) - \Omega(\mathrm{R})]\}_{,\alpha} = 0 \quad \text{on} \quad \Pi.$$

We thus let

$$P(\mathrm{R}) = 2[\omega_1(\mathrm{R}) + (2 + \mathrm{R})\omega_2(\mathrm{R}) - \Omega(\mathrm{R})], \quad 0 \leqslant \mathrm{R} < \infty,$$

$$p(x_1, x_2) = P(|\nabla u(x_1, x_2)|^2) + d \quad \text{on} \quad \Pi, \quad d = \text{const.} \tag{4.12}$$

The constant d is determined by invoking the second of (4.3), which together with (4.12) reduce to

$$d = \Omega\left(\frac{b^2}{4\pi^2 a^2}\right),$$

and the pressure is determined:

$$p = 2\frac{\partial W}{\partial I_1} + 2(2 + |\nabla u|^2)\frac{\partial W}{\partial I_2} + 2\int_{(b^2/4\pi^2 r^2)}^{(b^2/4\pi^2 a^2)} \frac{\partial W}{\partial I_2}(3 + \varrho, 3 + \varrho)\,\mathrm{d}\varrho, \tag{4.13}$$

where $u = -b\theta/(2\pi)$, $|\nabla u|^2 = b^2/(4\pi^2 r^2)$, on Π'. The fields u, p given by (4.5), (4.13) provide the solution of (2.16), (2.17), (4.1), (4.2). The corresponding Cauchy stress field components arise from (2.15), (4.5), (4.13):

$$\tau_{\alpha\beta} = \left[2\int_{(b/2\pi a)^2}^{(b/2\pi r)^2} \frac{\partial W}{\partial I_2}(3 + \varrho, 3 + \varrho)\,\mathrm{d}\varrho\right]\delta_{\alpha\beta} - 2\frac{\partial W}{\partial I_2}\left(\delta_{\alpha\beta} - \frac{x_\alpha x_\beta}{r^2}\right)\frac{b^2}{4\pi^2 r^2},$$

$$\tau_{\alpha 3} = \tau_{3\alpha} = 2\left(\frac{\partial W}{\partial I_1} + \frac{\partial W}{\partial I_2}\right)\frac{b\varepsilon_{\beta\alpha}x_\beta}{2\pi r^2}, \tag{4.14}$$

$$\tau_{33} = 2\frac{\partial W}{\partial I_1}\frac{b^2}{4\pi^2 r^2} + 2\int_{(b/2\pi a)^2}^{(b/2\pi r)^2} \frac{\partial W}{\partial I_2}(3 + \varrho, 3 + \varrho)\,\mathrm{d}\varrho,$$

where

$$\frac{\partial W}{\partial I_\alpha} = \frac{\partial W}{\partial I_\alpha}\left(3 + \frac{b^2}{4\pi^2 r^2}, 3 + \frac{b^2}{4\pi^2 r^2}\right), \quad 0 < r \leqslant a.$$

An example is furnished by the Mooney-Rivlin material, characterized by

$$W = \frac{(\mu - B)}{2}(I_1 - 3) + \frac{B}{2}(I_2 - 3), \quad I_\alpha \geqslant 3, \tag{4.15}$$

μ, B const., $\mu \geqslant B > 0$. The restrictions imposed on μ, B ensure ellipticity (2.26). (4.14) becomes

$$\left.\begin{aligned} \tau_{\alpha\beta} &= B\frac{b^2}{4\pi^2}\left(\frac{x_\alpha x_\beta}{r^4} - \frac{\delta_{\alpha\beta}}{a^2}\right),\\ \tau_{\alpha 3} &= \tau_{3\alpha} = \frac{\mu b \varepsilon_{\beta\alpha} x_\beta}{2\pi r^2},\\ \tau_{33} &= \frac{b^2}{4\pi^2}\left(\frac{\mu}{r^2} - \frac{B}{a^2}\right) \end{aligned}\right\} \quad 0 < r \leqslant a. \tag{4.16}$$

On the other hand, setting $B = 0$, $\mu > 0$ in (4.16) one recovers the Neo-Hookean case (4.7) as expected from (4.15). In (4.16) a strong nonlinearity is exhibited *near* the dislocation line in $\tau_{\alpha\beta}$, and τ_{33} since

$$\tau_{\alpha\beta} = O(r^{-2}), \quad \tau_{33} = O(r^{-2}), \quad \tau_{\alpha 3} = O(r^{-1}) \quad \text{as} \quad r \to 0, \tag{4.17}$$

whereas in the Neo-Hookean case $\tau_{\alpha\beta}$ vanishes.

For a generalized Neo-Hookean material characterized by $W = W(I_1)$, (4.14) specializes to

$$\left.\begin{aligned} \tau_{\alpha\beta} &= \tau_{\beta\alpha} = 0,\\ \tau_{\alpha 3} &= \tau_{3\alpha} = W'\left(3 + \frac{b^2}{4\pi^2 r^2}\right)\frac{b}{2\pi r^2}\varepsilon_{\beta\alpha}x_\beta,\\ \tau_{33} &= 2W'\left(3 + \frac{b^2}{4\pi^2 r^2}\right)\frac{b^2}{4\pi^2 r^2} \end{aligned}\right\} \quad 0 < r \leqslant a. \tag{4.18}$$

Note that the stress field in this case does not depend on the radius of the cylinder. This is clear from the fact that the constant d in (4.12) vanishes for generalized Neo-Hookean materials.

In order to make a quantitative statement regarding the effect of the nonlinearity in the stress field it is instructive to consider the following important subclass of the Generalized Neo-Hookean materials. These are characterized by an elastic potential function of the form

$$W(I_1) = \frac{\mu}{2c}\left\{\left[1 + \frac{c}{n}(I_1 - 3)\right]^n - 1\right\}, \quad I_1 \geqslant 3, \tag{4.19}$$

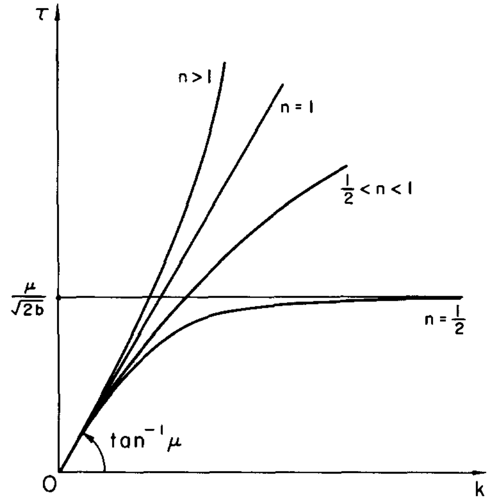

Fig. 3. Shear response curves for generalized neo-Hookean power law materials.

where μ, n, c are material constants. These materials are known as Power Law materials. The infinitesimal shear modulus μ and the constant c are restricted here to be positive. The parameter n plays the role of a "hardening exponent". From (4.18), (2.24) the shear response function becomes

$$\tau(k) = \mu\left[1 + \frac{c}{n}k^2\right]^{n-1} k, \quad -\infty < k < \infty. \tag{4.20}$$

In view of the restrictions on μ, c, the ellipticity condition (2.26) becomes equivalent to $n \geqslant 1/2$. As is noted in Knowles [7], the case $n = 1/2$ gives rise to a bounded shear stress; $\tau \to \mu/\sqrt{2c}$ as $k \to \infty$, whereas for $n > 1/2$, $\tau \to \infty$ as $k \to \infty$. Characteristic shapes of shear response curves for various values of n are shown in Fig. 3. In view of (4.19) the Cauchy stress components are obtained from (4.14):

$$\left.\begin{aligned} \tau_{\alpha\beta} &= \tau_{\beta\alpha} = 0, \\ \tau_{3\alpha} &= \tau_{\alpha 3} = \mu\left[1 + \frac{cb^2}{4\pi^2 n r^2}\right]^{n-1} \frac{b}{2\pi}\frac{\varepsilon_{\beta\alpha}x_\beta}{r^2}, \\ \tau_{33} &= \mu\left[1 + \frac{cb^2}{4\pi^2 n r^2}\right]^{n-1} \frac{b^2}{4\pi^2 r^2} \end{aligned}\right\} \quad 0 < r \leqslant a. \tag{4.21}$$

Apart from the problem for the cylinder of bounded cross section, it is interesting to consider the following alternative. Let the region R be the whole space, so that Π' consists of all points in the (x_1, x_2) plane exterior to the positive x_1-axis and the origin. Instead of (4.3) we require that

$$\tau = o(1) \quad \text{as} \quad r \to \infty. \tag{4.22}$$

We also require the elastic potential to be such that in the absence of pressure the stresses vanish at the undeformed state $(I_1, I_2) = (3, 3)$. It is easy to verify that the stress field for this situation and for a general material $W(I_1, I_2)$ is obtained by taking the limit as $a \to \infty$ in the expressions (4.14). It suffices to note that $I_\alpha \to 3$ as $r \to \infty$ and thus the condition on the stresses, (4.22), is indeed satisfied.

The specialization (4.18) of (4.14) appropriate to Generalized Neo-Hookean materials is, as mentioned, independent of the radius a. Furthermore the stress field automatically satisfies the condition (4.22) at infinity. Moreover, all circular cylinders centered at the dislocation line (x_3-axis) are traction free. For these materials, letting (4.18) be valid for $a \leqslant r < \infty$ $(a > 0)$ provides the stress field for the exterior problem where R is the region exterior to the cylinder of radius a with vanishing fractions and the stress is subject to (4.22). Similarly if R is the region between the cylindrical traction free surfaces $r = a_1$ and $r = a_2$ $(a_2 > a_1 > 0)$, (4.18) is again appropriate for $a_1 \leqslant r \leqslant a_2$.

5. Scale of the nonlinear effect (estimates of the dislocation core region)

The use of nonlinear elasticity theory in the analysis of the screw dislocation problem considered here shows that considerable nonlinear effects will predominate in the vicinity of the dislocation line. The large displacement gradients predicted as the dislocation line is approached clearly demonstrate the inadequacy of the linearized elasticity theory, as well as of any "small strain," "physically nonlinear" theory, in describing the deformation field accurately. In addition and as is evident by equations (4.14), (4.17) and (4.18), a strong nonlinearity in the resulting stress field is demonstrated by the existence of the highly singular stress components $\tau_{\alpha\beta}$ and τ_{33}, an effect which is *entirely absent* when the linear theory or the "physically nonlinear" theories [4] are used.

Insofar as we know, there are no rigorous analytical estimates available of the extent of the nonlinearities in a dislocation problem. Moreover, even a precise version of the question seems to be lacking. In this section, we formulate and answer such a question for two particular screw dislocation problems. The first problem corresponds to a screw dislocation in an unbounded domain occupied by a generalized Neo-Hookean solid ($W = W(I_1)$) with the stress components required to approach zero away from the dislocation line. The second problem corresponds to a screw dislocation in an unbounded domain occupied by a Neo-Hookean solid ($W = \mu/2(I_1 - 3)$) with the deformation approaching a prescribed simple shear away from the dislocation line. For the above problems two measures of nonlinearity of the solution are discussed. The first is based on the calculation of energy stored in the region between two circular cylindrical surfaces centered at the dislocation line. The second is based on an appropriate generalization of the stress nonlinearity measure introduced by Knowles and Rosakis [6] for the description of nonlinear effects in a mode III crack problem. Finally the sensitivity of the two nonlinear measures is discussed and their results are compared to the estimates of dislocation "core"-size predictions based on numerical semi-discrete atomistic calculations.

5.1. Energy calculations. The screw dislocation in a generalized Neo-Hookean solid with stresses vanishing at infinity

We now apply the results of Section 4 to the particular problem of a screw dislocation in an unbounded domain occupied by a solid belonging to an important subclass of generalized Neo-Hookean solids, namely the power law material. For this problem the stress field tends to vanish away from the dislocation line. Our goal is the calculation of the strain energy per unit dislocation line length stored in the material occupying a region P bounded by two cylindrical surfaces of radii ϱ and R, respectively, where $0 < \varrho < R < \infty$. The energy per unit length $E(R, \varrho; n)$ is obtained by integration of the strain energy density $W(I_1)$ for a power law material (4.19) over the cross-section of the cylindrical region P, for different values of the hardening exponent n:

$$E(R, \varrho; n) = \frac{\mu}{2c} \int_o^{2\pi} \int_\varrho^R \left\{ \left[1 + \frac{c}{n} |\nabla u|^2 \right]^n - 1 \right\} r \mathrm{d}\, r \mathrm{d}\theta, \tag{5.1.1}$$

where according to the second of (4.13), $|\nabla u|^2 = b^2/(4\pi^2 r^2)$, $r > 0$.

Closed-form expressions for $E(R, \varrho; n)$ can be obtained for particular representative values of n. Characteristic shapes of shear response curves for power hardening solids corresponding to different values of n are shown in Fig. 2.

For n integer, $n > 1$, equation (5.1.1) gives

$$E(R, \varrho; n) = -\frac{\mu b^2}{8\pi n}\sum_{k=1}^{n-1}\frac{k}{n-k}\left[\left(1+\frac{cb^2}{4\pi^2 nR^2}\right)^{n-k} - \left(1+\frac{cb^2}{4\pi^2 n\varrho^2}\right)^{n-k}\right] + \frac{\mu b^2}{4\pi}\ln\frac{R}{\varrho}, \quad 0 < \varrho < R < \infty. \tag{5.1.2}$$

For $n = 2$ the above expression becomes

$$E(R, \varrho; 2) = \frac{\mu b^4 c}{128\pi^3}\left[\frac{1}{\varrho^2} - \frac{1}{R^2}\right] + \frac{\mu b^2}{4\pi}\ln\frac{R}{\varrho}, \quad 0 < \varrho < R < \infty. \tag{5.1.3}$$

As is evident from equations (5.1.2) and (5.1.3), the energy per unit length ofr $n > 1$ differs from the one predicted by the linearized elasticity theory through terms of order $b^2(b/\varrho)^{2(n-1)}$ as the dislocation line is approached ($\varrho \to 0$). On the other hand for $n = 1$ (Neo-Hookean solid) (5.1) gives:

$$E(R, \varrho; 1) = \frac{\mu b^2}{4\pi}\ln\frac{R}{\varrho}, \quad 0 < \varrho < R < \infty. \tag{5.1.4}$$

For this case the expression for the energy per unit dislocation line length, is *identical* to the analogous expression predicted by the linearized elasticity theory. As already discussed in Section 4, the stress field due to the screw dislocation in a Neo-Hookean solid, is the same as the one predicted by linear elasticity with the exception of the axial normal stress $\tau_{33} = (\mu b^2)/(2\pi r^2)$, which provides the only manifestation of *substantial* nonlinear effect at the vicinity of the dislocation line (core-region). The existence of a strong nonlinear effect in this case is not reflected in the calculation of the energy per unit length. This clearly demonstrates that the energy is *not* a very sensitive measure of nonlinearities. As a result, attempts to calculate the extent of the dislocation core region by comparison of energies evaluated by means of linear and nonlinear theories are expected to underestimate the region of dominance of core nonlinearities. For example, if such a comparison is carried out for the Neo-Hookean solid, the predicted nonlinear region would be of zero radius, a result which is clearly incorrect in view of the large displacement gradients and the non-linearities present through the axial normal stress τ_{33}. The above observations are also related to the use of numerical, discrete or semi-discrete atomistic models for the calculation of dislocation core regions. In such calculations the numerical estimates of energy based on atomistic models are compared to the energy predicted by linear elasticity theory. The extent of the region of nonlinearity is then defined as the distance from the dislocation line for which the two energy predictions differ by a fixed percentage. Such techniques have been extensively reviewed by Hirth and Lothe [1] and by Teodosiu [2]. As pointed out by Teodosiu, atomistic calculations give core regions of radius of the order of one Burger's vector, with displacement gradients as high as 30% there. On the other hand the *linear* elastic solution matches the atomic displacements only at larger distances of the order of 10–15 b (Teodosiu [2]).

For $n = 1/2$, the strain energy per unit dislocation length becomes

$$E(R, \varrho; 1/2) = \frac{\pi\mu}{2c}\left[R^2\left(1 + \frac{cb^2}{2\pi^2 R^2}\right)^{1/2} - \varrho^2\left(1 + \frac{cb^2}{2\pi^2\varrho^2}\right)^{1/2}\right]$$

$$- \frac{\pi\mu}{2c}[R^2 - \varrho^2]$$

$$+ \frac{\mu b^2}{8\pi}\ln\left[\frac{R^2\left[1 + \frac{cb^2}{4\pi^2 R^2} + \left(1 + \frac{cb^2}{2\pi^2 R^2}\right)^{1/2}\right]}{\varrho^2\left[1 + \frac{cb^2}{4\pi^2\varrho^2} + \left(1 + \frac{cb^2}{2\pi^2\varrho^2}\right)^{1/2}\right]}\right],$$

$$0 < \varrho < R < \infty. \tag{5.1.5}$$

For $n = 1/2$, the stress field (4.21) becomes

$$\left.\begin{aligned} \tau_{\alpha\beta} &= \tau_{\beta\alpha} = 0, \\ \tau_{\alpha 3} &= \tau_{3\alpha} = \frac{\mu b}{2\pi}\left[1 + \frac{cb^2}{2\pi^2 r^2}\right]^{-1/2}\frac{\varepsilon_{\beta\alpha}x_\beta}{r^2}, \\ \tau_{33} &= \frac{\mu b^2}{4\pi^2}\left[1 + \frac{cb^2}{2\pi^2 r^2}\right]^{-1/2}\frac{1}{r^2} \end{aligned}\right\} \quad (0 < r < \infty); \tag{5.1.6}$$

expressing (5.1.6) in terms of polar coordinates one sees that the assymptotic behavior of the shear stress components $\tau_{\alpha 3}$ as $r \to 0$ is given by

$$\left.\begin{aligned} \tau_{13} &\sim -(\mu/\sqrt{2c})\sin\theta, \\ \tau_{23} &\sim (\mu/\sqrt{2c})\cos\theta \end{aligned}\right\} \quad \text{as} \quad r \to 0. \tag{5.1.7}$$

(5.1.7) shows that for $n = 1/2$ the shear stress components $\tau_{\alpha 3}$ *are bounded* as $r \to 0$ with the maximum amplitude of $\mu/\sqrt{2c}$, which, as expected, corresponds to the assymptotic value of the stress in the shear response curve as $k \to \infty$.

In addition (5.1.5) shows that the limit of the energy as $\varrho \to 0$ exists and is given by

$$E(R, 0; \tfrac{1}{2}) = \lim_{\varrho \to 0} E(R, \varrho; \tfrac{1}{2}) = \frac{\pi\mu}{2c}\left[R^2\left(1 + \frac{cb^2}{2\pi^2 R^2}\right)^{1/2} - R^2\right]$$
$$+ \frac{\mu b^2}{4\pi} \ln\left\{\frac{2\pi R}{\sqrt{cb}}\left[1 + \frac{cb^2}{4\pi^2 R^2} + \left(1 + \frac{cb^2}{2\pi^2 R^2}\right)^{1/2}\right]^{1/2}\right\},$$
$$R > 0. \tag{5.1.8}$$

It is crucial to note that for $n > 1/2$, the integral (5.1.1) does not exist for $\varrho = 0$. The case $n = 1/2$ is exceptional in the sense that it is the only one, among those admitted by the ellipticity restriction (2.26), which gives rise to finite strain energy stored in a region containing the dislocation line.

For $R \gg \sqrt{(c/2)}\, b/\pi$ equation (5.1.8) can be expressed as

$$E(R, 0; \tfrac{1}{2}) = \frac{\mu b^2}{4\pi}(\tfrac{1}{2} + \ln 2) + \frac{\mu b^2}{4\pi} \ln\left(\sqrt{\frac{2}{c}}\frac{\pi R}{b}\right)$$
$$+ O\left(\left(\sqrt{\frac{2}{c}}\frac{\pi R}{b}\right)^{-2}\right) \quad \text{as} \quad \sqrt{\frac{2}{c}}\frac{\pi R}{b} \to \infty. \tag{5.1.9}$$

Expression (5.1.9) bears an interesting similarity to the analogous expression for the energy per unit dislocation line length calculated on the basis of the approximate simple model suggested by Peierls (Hirth and Lothe [1], p. 218). The Peierls model attempts to take into account the lattice periodicity at the vicinity of a dislocation in a crystalline solid.

As the dislocation line is approached, the stress according to Peierls remains bounded with a maximum amplitude of $\mu b/2\pi d$ at $r = 0$ (d is the interatomic spacing of the crystal). The energy per unit dislocation line also remains bounded as $\varrho \to 0$ and is given by Hirth and Lothe [1]:

$$E_{\text{PEIERLS}} = \frac{\mu b^2}{4\pi} + \frac{\mu b^2}{4\pi} \ln \frac{R}{d}. \tag{5.1.10}$$

In the absence of rigorous nonlinear treatments of the dislocation problem, the Peierls model has been very successful in providing some early answers to a number of important materials science questions that could not be addressed by means of the classical linear elasticity theory. Although no *direct* analogy can be drawn between our treatment and this model, we feel that it is instructive to demonstrate the similarity in the resulting energy expressions. If, for the sake of comparison only, the amplitude of the stresses predicted by Peierls, $\mu b/2\pi d$, is set equal to the amplitude of the stresses, $\mu/\sqrt{2c}$, predicted in (5.1.7), for $n = 1/2$, then $c = 2\pi^2 d/b$ and expression (5.1.9) for the energy per unit dislocation line can be written as

$$E = (1.2)\frac{\mu b^2}{4\pi} + \frac{\mu b^2}{4\pi}\ln\frac{R}{d}. \tag{5.1.11}$$

Given the differences between the two treatments, expressions (5.1.10) and (5.1.11) are in excellent agreement. This is largely due to the fact that both approaches adopt constitutive models with bounded shear stresses.

Following the approach outlined by Hirth and Lothe [1] (page 232) an estimate of the size of the core region ϱ_c can be obtained if either of (5.1.10) or (5.1.11) is equated to

$$\frac{\mu b^2}{4\pi}\ln\frac{R}{\varrho_c}.$$

The estimate of ϱ_c thus obtained is given by

$$\varrho_c = \frac{b\sqrt{2c}}{2\pi e^{1.2}} = \frac{d}{e^{1.2}}. \tag{5.1.12}$$

The above estimate is in very good agreement with the one presented by Peierls as well as with the results of atomistic calculations described in Teodosiu [2]. Thus for $\varrho_c < \varrho < R$ the energy calculated in terms of the nonlinear and linear models are in good agreement. On the other hand, as will be demonstrated in the next section, this estimate *gravely underestimates* the region of dominance of nonlinear effects at the vicinity of the dislocation line.

5.2. Dislocation in a Neo-Hookean solid subjected to simple shear at infinity

Here the problem of a screw dislocation in an unbounded domain, occupied by a Neo-Hookean solid, with the deformation approaching simple shear at infinity will be addressed. Although this problem was not considered earlier its solution can easily be constructed by making use of results presented in Section 2. For the neo-Hookean case, the dislocation problem stated above specializes exactly (and not merely by linearization) in view of (2.21) to

$$\begin{aligned} u_{,\alpha\alpha} &= 0 \quad \text{on} \quad R, \\ u^+(x_1, 0) - u^-(x_1, 0) &= b, \quad 0 < x_1 < \infty, \\ u(x_1, x_2) &\sim \boldsymbol{k} \cdot \boldsymbol{x} \quad \text{as} \quad x_1^2 + x_2^2 \to \infty, \end{aligned} \tag{5.2.1}$$

where $\boldsymbol{k} = k_1 \boldsymbol{e}_1 + k_2 \boldsymbol{e}_2$, is the amount of shear at infinity.

It should be noted here that although the boundary value problem (5.2.1) is a linear one, the nonlinear effect is demonstrated through the existence of the axial stress τ_{33} given by

$$\tau_{33} = \mu |\nabla u|^2.$$

The solution of (5.2.1) is the same as the one of the linearized case and is given by

$$u = -\frac{b\theta}{2\pi} + r(k_1 \cos\theta + k_2 \sin\theta) = -\frac{b\theta}{2\pi} + k_\alpha x_\alpha,$$

$$\forall\, r > 0,\ 0 < \theta < 2\pi. \tag{5.2.2}$$

The corresponding stress field is given by

$$\left.\begin{aligned} \tau_{\alpha\beta} &= \tau_{\beta\alpha} = \mathring{\tau}_{\alpha\beta} = 0, \\ \tau_{\alpha 3} &= \tau_{3\alpha} = \mathring{\tau}_{3\alpha} = \frac{\mu b}{2\pi} \frac{\varepsilon_{\beta\alpha} x_\beta}{r^2} + \mu k_\alpha, \\ \tau_{33} &= \mu \left[k_\alpha k_\alpha + \frac{b}{\pi r^2} \varepsilon_{\alpha\beta} k_\alpha x_\beta + \frac{b^2}{4\pi^2 r^2} \right] \end{aligned}\right\} \forall\, r > 0,\ 0 < \theta < 2\pi, \tag{5.2.3}$$

where $r^2 = x_1^2 + x_2^2$ and $\mathring{\tau}_{ij}$ are the stress components for the solution of the linearized problem. The strain energy per unit dislocation line length stored by the material bounded by two cylindrical surfaces of radii ϱ and R, respectively, where $0 < \varrho < R < \infty$ is given by means of (5.1.1), (5.2.2) for $n = 1$ as

$$E'(R, \varrho; 1) = \frac{\mu}{2} \int_o^{2\pi} \int_o^R |\nabla u|^2 \, r \mathrm{d}r d\theta, \quad 0 < \varrho < R < \infty, \tag{5.2.4}$$

where

$$|\nabla u|^2 = k_\alpha k_\alpha + \frac{b}{\pi r^2} \varepsilon_{\alpha\beta} k_\alpha x_\beta + \frac{b^2}{4\pi^2 r^2}.$$

Thus (5.2.4) becomes

$$E'(R, \varrho; 1) = \mu\pi k_\alpha k_\alpha (R^2 - r^2) + \frac{\mu b^2}{4\pi} \ln \frac{R}{r}, \quad 0 < \varrho < R < \infty. \tag{5.2.5}$$

$E'(R, \varrho; 1)$ is the same as in the linearized case and does not reflect the strong nonlinear effect clearly exhibited by the existence of a non-zero axial tension τ_{33}. As a matter of fact, the dependence of τ_{33} on k_α indicates that, in addition to the region near the dislocation line, nonlinear effects may dominate through the entire domain for certain values of the amount of shear k_α prescribed at infinity. This behavior will be discussed in detail in the following section.

5.3. A stress nonlinearity measure

As demonstrated in Section 5.1, the strain energy per unit length calculated by means of fully nonlinear continuum models, or computed on the basis of the discrete atomistic models of dislocations in crystals, may be insensitive to certain strong nonlinear effects present at the vicinity of the dislocation line. A more appropriate estimate of the extent of nonlinearities should be based on some measure of the difference of the stress field predicted by the fully nonlinear theory presented above and the corresponding linearized stress field. Indeed the ratio $\|\boldsymbol{\tau} - \mathring{\boldsymbol{\tau}}\| / \|\mathring{\boldsymbol{\tau}}\|$ seems to provide a natural measure of the size of the local nonlinear effect. The reason for this choice is the following: For all problems considered in the present work the displacement fields *happen* to coincide for both the nonlinear and linearized problems. As a result, nonlinear effects assert themselves only through the stress fields. In the above ratio $\boldsymbol{\tau}$ is the Cauchy stress tensor obtained by means of the nonlinear analysis while $\mathring{\boldsymbol{\tau}}$ is the equivalent quantity obtained for the same problem by means of the linearized theory. The proposed measure is a generalization of the ratio used by Knowles and Rosakis [6], for the study of nonlinear effects in the case of a mode-III crack in a neo-Hookean solid. Indeed for a neo-Hookean solid undergoing an antiplane shear deformation the above ratio reduces to $\tau_{33}/\|\mathring{\tau}\|$ which is proportional to the ratio used in Knowles and Rosakis [6].

If ξ is a given constant representing a specific error tolerance, $0 < \xi < 1$, the elastic field at a given point will be said to be *approximately linear at level* ξ if $\|\tau - \mathring{\tau}\|/\|\mathring{\tau}\| < \xi$ at that point. Accordingly, we define the *ξ-level nonlinear zone* N_ξ as the set of all points (x_1, x_2) such that,

$$\frac{\|\tau(x_1, x_2) - \mathring{\tau}(x_1, x_2)\|}{\|\mathring{\tau}(x_1, x_2)\|} \geqslant \xi, \tag{5.3.1}$$

where $\|\tau\| = \sqrt{\tau_{ij}\tau_{ij}}$.

For a generalized neo-Hookean solid undergoing an antiplane shear deformation the components of the stress field are given by

$$\begin{aligned} \tau_{\alpha\beta} &= \tau_{\beta\alpha} = 0, \\ \tau_{3\alpha} &= \tau_{\alpha 3} = 2W'(I_1)u_{,\alpha}, \\ \tau_{33} &= 2W'(I_1)|\nabla u|^2, \end{aligned} \tag{5.3.2}$$

while the corresponding components computed on the basis of the linear theory are

$$\begin{aligned} \mathring{\tau}_{\alpha\beta} &= \mathring{\tau}_{\beta\alpha} = 0, \\ \mathring{\tau}_{3\alpha} &= \mathring{\tau}_{\alpha 3} = \mu u_{,\alpha}, \\ \mathring{\tau}_{33} &= 0. \end{aligned} \tag{5.3.3}$$

Thus from (5.3.1), (5.3.2), and (5.3.3) we conclude that the ξ-level nonlinear zone is the set of points for which

$$\frac{[(W'(I_1))^2|\nabla u|^2 + 2(2W'(I_1) - \mu)^2]^{1/2}}{\sqrt{2}\mu} \geqslant \xi. \tag{5.3.4}$$

For the particular case of a screw dislocation in an infinite domain occupied by a power law material, with the stresses vanishing at infinity,

$$2W'(I_1) = \mu\left[1 + \frac{c}{n}|\nabla u|^2\right]^{n-1}, \quad |\nabla u|^2 = \frac{b^2}{4\pi^2 r^2},$$

and the above becomes

$$\hat{\xi}\left(\frac{r}{b}, n, c\right) \equiv \left[\left(1 + \frac{cb^2}{4\pi^2 nr^2}\right)^{2n-2}\left(\frac{b^2}{8\pi r^2} + 1\right) - 2\left(1 + \frac{cb^2}{4\pi^2 nr^2}\right)^{n-1} + 1\right]^{1/2} \geqslant \xi. \tag{5.3.5}$$

Note that the boundary of N_ξ is a circle centered at the origin whose radius will, in general, depend on ξ, b, n, and c. For the case of a neo-Hookean solid, ($n = 1$), (5.3.5) becomes independent of c and is given by

$$\hat{\xi}\left(\frac{r}{b}, 1, c\right) = \left(\frac{b^2}{8\pi^2 r^2}\right)^{1/2} \geqslant \xi.$$

The above shows that the radius r_ξ of the ξ-level nonlinear zone is equal to

$$r_\xi = \frac{b}{2\sqrt{2}\pi\xi}. \tag{5.3.6}$$

For $\xi = 1\%$, (5.3.6) gives $r_\xi = 11.5b$. This value is consistent with the distance from the dislocation line for which atomistic calculations are in good agreement with the linearized elasticity solution (Teodosiu [2]). For $n \neq 1$, r_ξ depends on the choice of c and n. Fig. 4 and Fig. 5 show $\hat{\xi}(r/b, n, c)$, the left hand side of (5.25), plotted versus r/b for various values of n. In Fig. 4, c is taken to be 20 whereas in fig. 5, c is 100. Given a value

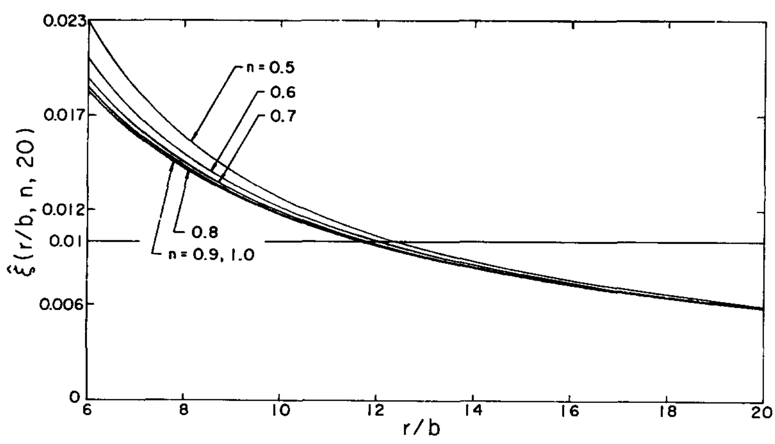

Fig. 4(a). Nonlinear stress measure $\hat{\xi}(r/b, n, 20)$ versus normalized radius r/b for various values of hardening exponent n ($n = 0.5, 0.6, 0.7, 0.8, 0.9, 1.0$).

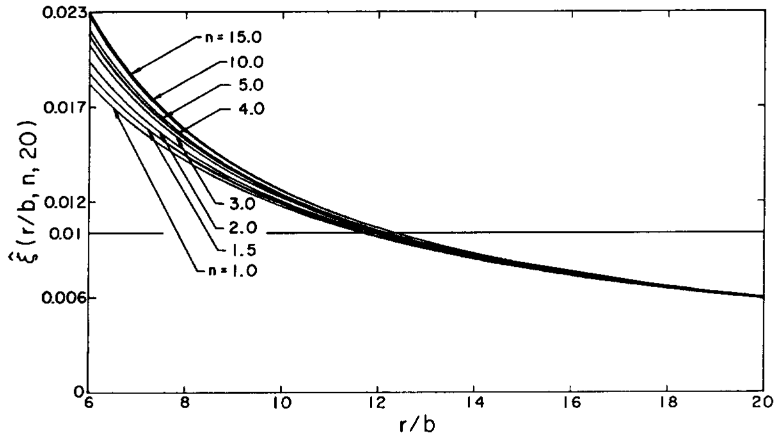

Fig. 4(b). Nonlinear stress measure $\xi(r/b,\ n,\ 20)$ versus normalized radius r/b for various values of hardening exponent n (n = 1.0, 1.5, 2.0, 3.0, 4.0, 5.0, 10.0, 15.0).

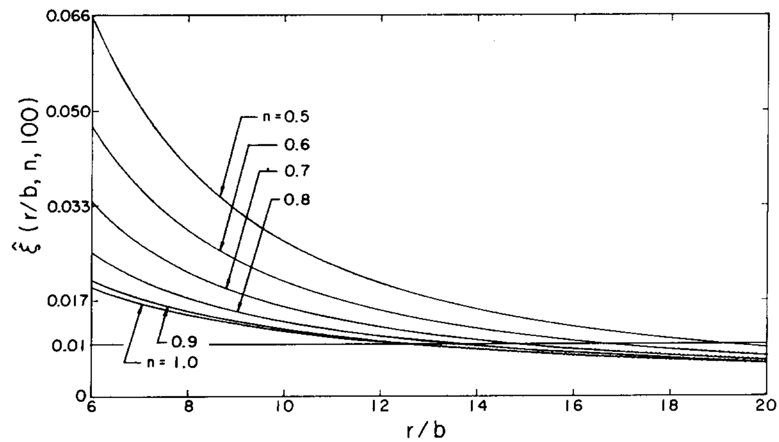

Fig. 5(a). Nonlinear stress measure $\xi(r/b,\ n,\ 100)$ versus normalized radius r/b for various values of hardening exponent n (n = 0.5, 0.6, 0.7, 0.8, 0.9, 1.0).

of ξ (say $\xi = 1\%$, as indicated by the horizontal dotted line) the radius r_ξ of the nonlinear zone can easily be calculated from these figures. The sensitivity of the radius of the nonlinear zone to c is shown in Figs. 6(a, b) where r_ξ, ($\xi = 1\%$) is plotted versus c for a variety of values of n. In Fig. 6(a), n was taken to be 0.5, 0.6, 0.7, 0.8, 0.9, and 1, whereas in Fig. 6(b), n was 1, 1.5, 2, 3, 4, 5, 10, 15. The results indicate that for $c < 10$ the radius of the nonlinear zone is insensitive to the choice of n. It is also evident from Fig. 6(a, b) that $n = 1/2$ always results in the largest predictions of r_ξ for given c.

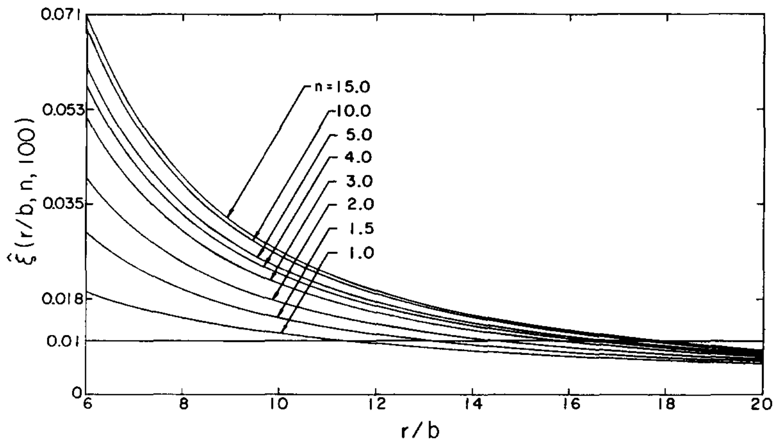

Fig. 5(b). Nonlinear stress measure $\xi(r/b, n, 100)$ versus normalized radius r/b for various values of hardening exponent n (n = 1.0, 1.5, 2.0, 3.0, 4.0, 5.0, 10.0, 15.0).

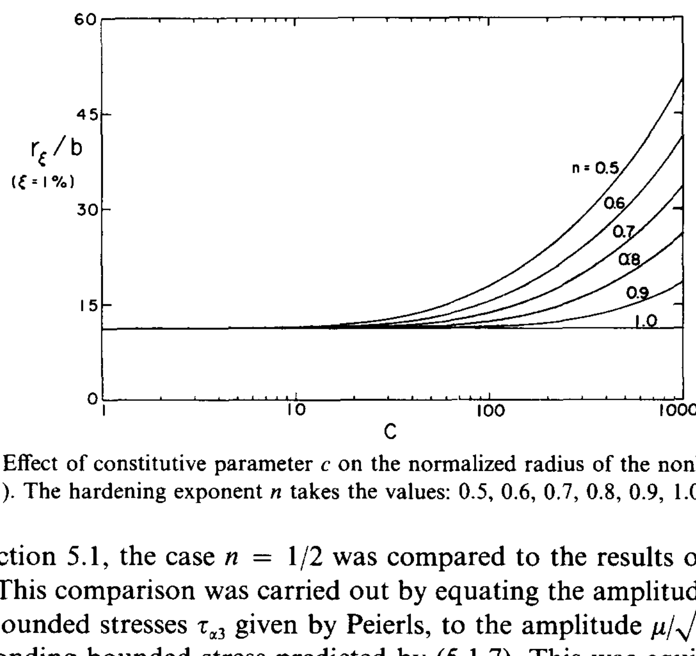

Fig. 6(a). Effect of constitutive parameter c on the normalized radius of the nonlinear zone (ξ = 0.01). The hardening exponent n takes the values: 0.5, 0.6, 0.7, 0.8, 0.9, 1.0.

In Section 5.1, the case $n = 1/2$ was compared to the results of Peierls' model. This comparison was carried out by equating the amplitude $\mu b/2\pi d$ of the bounded stresses $\tau_{\alpha 3}$ given by Peierls, to the amplitude $\mu/\sqrt{2c}$ of the corresponding bounded stress predicted by (5.1.7). This was equivalent to setting $c = 2\pi^2 d/b \simeq 20$.

It is interesting to note here that for $n = 1/2$ and $c = 20$ as above, Fig. 4(a) predicts a value of $r_\xi \simeq 12.4b$. This value, is an order of magnitude *larger* than the estimate of non-linear zone side predicted in (5.1.12) by means of an energy argument for the same problem. This disagreement is by

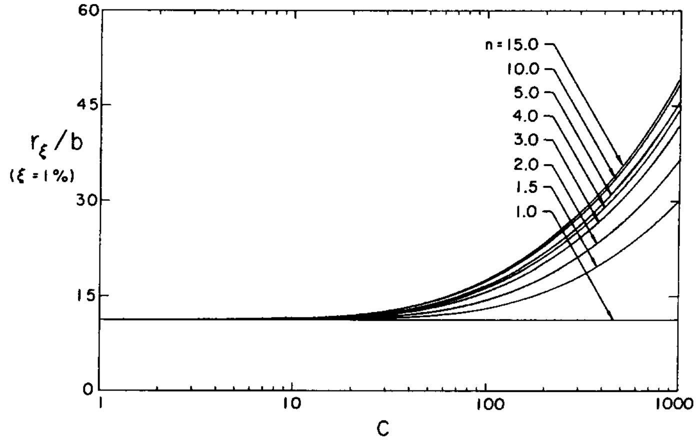

Fig. 6(b). Effect of constitutive parameter c on the normalized radius of the nonlinear zone ($\xi = 0.01$). The hardening exponent n takes the values: 1.0, 1.5, 2.0, 3.0, 4.0, 5.0, 10.0, 15.0.

no means unexpected since, as discussed in Section 5.1, energy is *not a very sensitive measure* of nonlinearities. Indeed the estimate $r_\xi \simeq 12.4b$ is in good agreement with the atomistic calculations referred above (Teodosiu [2]).

The nonlinear stress measure (5.3.4) can also be applied to the study of the more complex problem of a dislocation in an unbounded domain occupied by a neo-Hookean solid with the deformation approaching simple shear at infinity. In this case, and as demonstrated by equation (5.2.3) the resulting nonlinearity will also depend on the amount of shear k_α and will not necessarily be confined to the region surrounding the dislocation line.

For a neo-Hookean solid $W'(I_1) = \mu$ and (5.3.4) reduces to

$$\frac{1}{\sqrt{2}}|\nabla u| \geqslant \xi.$$

Use of (5.2.2) reduces the above to

$$\frac{1}{\sqrt{2}}\left[k_\alpha k_\alpha + \frac{b}{\pi r^2}\varepsilon_{\alpha\beta}k_\alpha x_\beta + \frac{b^2}{4\pi^2 r^2}\right]^{1/2} \geqslant \xi. \tag{5.3.7}$$

Equation (5.3.7) can also be expressed as

$$\left(x_1 - \frac{bk_2}{2\pi(k^2 - 2\xi^2)}\right)^2 + \left(x_2 + \frac{bk_1}{2\pi^2(k^2 - 2\xi^2)}\right)^2 \geqslant \frac{\xi^2 b^2}{2\pi^2(k^2 - 2\xi^2)^2}, \tag{5.3.8}$$

where $k^2 = k_\alpha k_\alpha$, $\xi > 0$, $k_\alpha > 0$.

We call the nonlinear effect *contained* at level ξ if N_ξ is bounded and contains the dislocation line. Otherwise we say that N_ξ is *uncontained*. In particular if the *complement* of N_ξ is bounded, then N_ξ will be called *enveloping*.

For $k_\alpha = 0$, (5.3.8) reduces to (5.3.6) and the nonlinear effect is contained for every ξ level: The boundary of the nonlinear zone is a circle centered at the origin of radius $r_\xi = b/2\sqrt{2}\pi\xi$. A schematic of the nonlinear zone for $k_\alpha = 0$ is shown in Fig. 7a.

For $0 < k < \sqrt{2}\xi$, the nonlinear zone is *contained and is composed of the boundary and the interior of a circle of* radius $b\xi/\sqrt{2}\pi(2\xi^2 - k^2)$ centered at $x_1 = bk_2/2\pi(k^2 - 2\xi^2)$, $x_2 = -bk_1/2\pi(k^2 - 2\xi^2)$. This circle contains the origin for every $k < \sqrt{2}\xi$ (see Fig. 7(b)). As $k \to \sqrt{2}\xi$ the radius of the circle increases and its center recedes to infinity.

For $k = \sqrt{2}\xi$ the circle degenerates to a straight line with intercepts $x_1 = b/4\pi k_2$ and $x_2 = -b/4\pi k_1$ (see Fig. 7(c)), and the nonlinear zone, which is *uncontained*, occupies the half plane defined by

$$\frac{b^2}{4\pi^2} - \frac{b}{\pi}(k_2 x_1 - k_1 x_2) \geqslant 0.$$

For $k > \sqrt{2}\xi$ the nonlinear zone N_ξ becomes *enveloping*. It then occupies the *exterior and boundary* of a circle of radius $b\xi/\sqrt{2}\pi(k^2 - 2\xi^2)$ centered at $x_1 = bk_2/2\pi(k^2 - 2\xi^2)$, $x_2 = -bk_1/2\pi(k^2 - 2\xi^2)$ which does not contain the origin for every $k > \sqrt{2}\xi$ (see Fig. 7(d)).

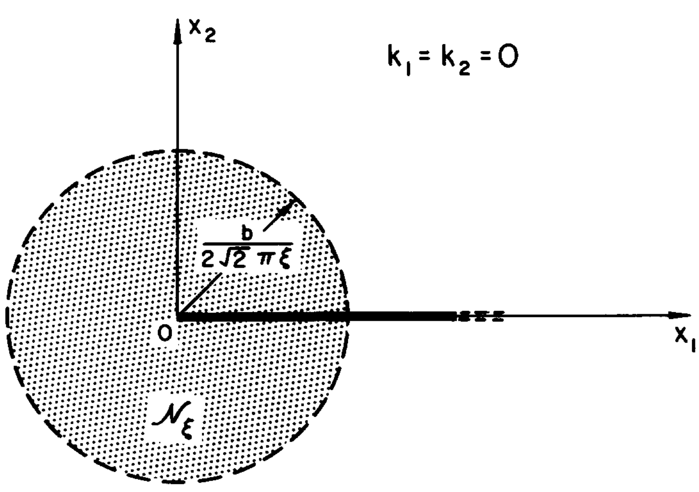

Fig. 7(a). ξ-level nonlinear zone N_ξ (shaded), $k_\alpha = 0$.

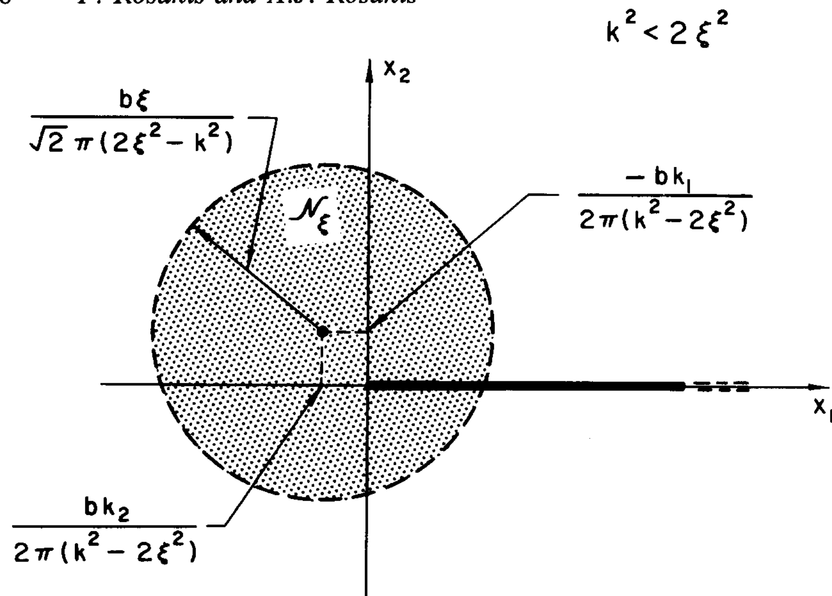

Fig. 7(b). ξ-level nonlinear zone N_ξ (shaded), $0 < k < \sqrt{2}\xi$.

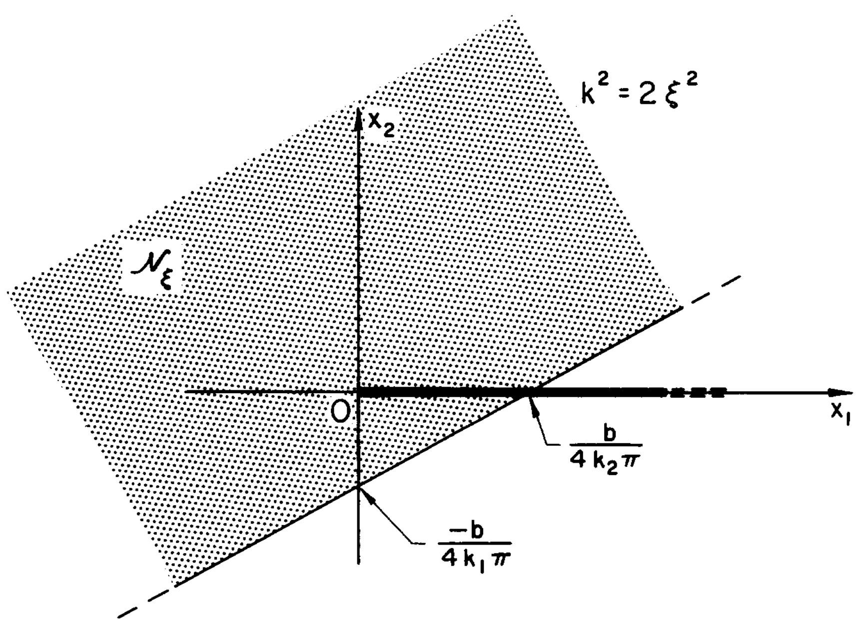

Fig. 7(c). ξ-level nonlinear zone N_ξ (shaded), $k = \sqrt{2}\xi$.

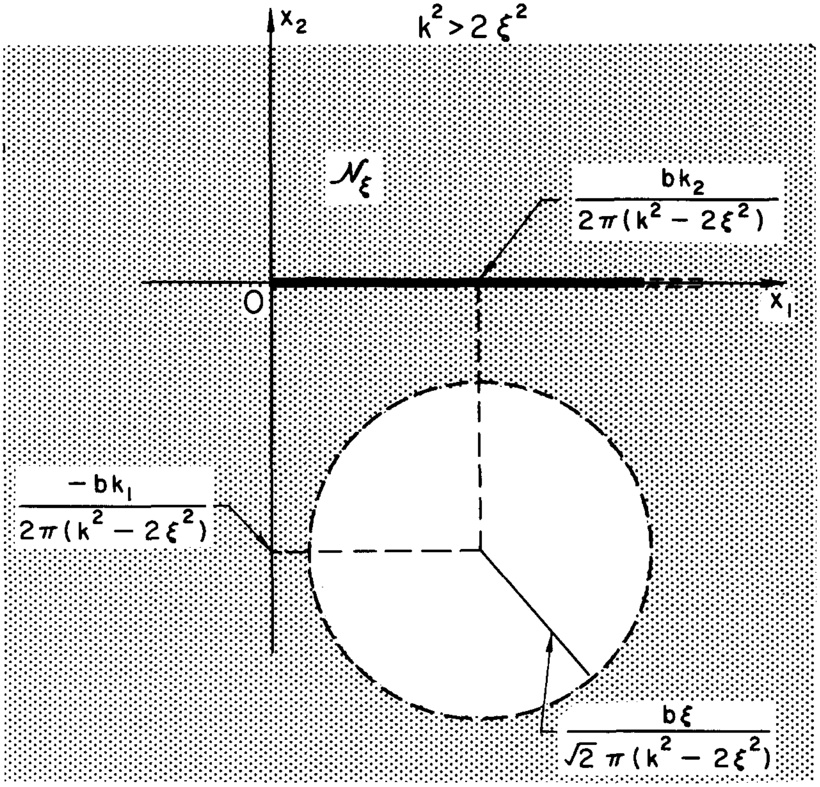

Fig. 7(d). ξ-level nonlinear zone N_ξ (shaded), $k > \sqrt{2}\xi$.

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