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Twist disclination in the field theory of elastoplasticity

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Abstract

In this paper we study the twist disclination within the elastoplastic defect theory. Using the stress function method, we found exact analytical solutions for all characteristic fields of a straight twist disclination in an infinitely extended linear isotropic medium. The elastic stress, elastic strain and displacement have no singularities at the disclination line. We found modified stress functions for the twist disclination. In addition, we calculate the disclination density, effective Frank vector, disclination torsion and effective Burgers vector of a straight twist disclination. By means of gauge theory of defects we decompose the elastic distortion into the translational and rotational gauge fields of the straight twist disclination.

1. Introduction

Disclinations are very important and interesting lattice defects. They may be defects in warped and twisted materials. Disclinations have been investigated in the context of applications to liquid crystals as twisting discontinuities [1, 2], Abrikosov lattices formed by magnetic flux lines in the mixed state of type-II superconductors [3], polymers formed by chain kinking and twisting of molecules [4], Bloch wall lattices [5, 6], biological structures [7], amorphous bodies [8] and rotation plastic deformations [9, 10]. Because disclinations cause strong elastic distortions and lattice bending it seems that very strong distortions are necessary in order to realize disclinations in crystals.

A disclination is characterized by a closure failure of the rotation for a closed circuit round the disclination line. There are wedge and twist disclinations. If the Frank angle (rotation failure) of the disclination is a symmetry angle of the lattice, then the disclination is called a perfect disclination. Such disclinations have been introduced by Anthony [11] and deWit [12, 13]. In the case of a twist disclination the rotation axis is perpendicular to the disclination line. The smallest value of the Frank vector is $\pi/2$ in a cubic lattice and $\pi/3$ in a

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hexagonal lattice. If the Frank angle is not a symmetry angle of the lattice, the disclination is called a partial disclination. They play an important role, e.g., in building of twin boundaries (see, e.g., [14]). Disclinations correspond, in general, to Volterra's distortions of the second kind (see also [15]). Thus, these defects are of rotational type. They are different from the so-called Frank's (spin) disclinations which are elementary defects in liquid crystals (see [1]).

The traditional description of elastic fields produced by defects (e.g. dislocations, disclinations and cracks) is based on the classical theory of linear elasticity. However, classical elasticity breaks down near the defect line and leads to singularities. This is unfortunate since the defect core is a very important region in the theory of defects. Of course, such singularities are unphysical and an improved model of defects should eliminate them.

On the other hand, there are other non-standard continuum models of defects, e.g., the nonlocal continuum model [16–21], the strain gradient elasticity [22–28] and the field theory of elastoplasticity which has been developed from the gauge theory of defects [29–34]. All these theories are successfully applied to the description of screw and edge dislocations. In this context the stresses have no singularities at the dislocation line. In addition, the dislocation core arises naturally. In particular, the field theory of elastoplasticity is a gauge theory of defects in which the defects cause plasticity. The corresponding gauge fields may be identified with the plastic distortion. With the help of this theory the elastic and plastic part of the total distortion can be calculated. The total distortion is defined in terms of a displacement and consists of the elastic and plastic parts. In the case of dislocations (see, e.g., [33]) the elastic distortion is continuous even in the dislocation core and the plastic part becomes discontinuous. But in the case of disclinations the situation is less completely worked out. The stresses of straight wedge and twist disclinations have been calculated by Povstenko [20] in the framework of Eringen's nonlocal elasticity and by Gutkin and Aifantis [26–28] with the help of strain gradient elasticity. However, no rotation and displacement vectors, no bend–twist and no disclination and dislocation density tensors were obtained in their works. In a recent paper [34] the wedge disclination has been investigated in the field theory of elastoplasticity. It was possible to calculate all characteristic field quantities. It has been seen that the disclination core may be defined quite naturally in this framework.

In this paper we want to extend our study for a straight twist disclination. We use the field theory of elastoplasticity to find nonsingular solutions for the stress and strain fields and the rotation and displacement fields. In addition, we investigate the relation to gauge theory of defects. We use the stress function method and hope to close the gap between the nonlocal and strain gradient results for the case of a straight twist disclination. In this framework we want to work out all geometric quantities of a twist disclination.

2. Basic equations

In this section we apply the field theory of elastoplasticity to the case of a straight twist disclination. In elastoplasticity the elastic distortion is given by [29–32]

$$\beta_{ij} = \partial_j u_i + \tilde{\beta}_{ij}. \tag{2.1}$$

It is an additive decomposition of the elastic distortion into compatible and purely incompatible distortion. This decomposition can be justified with the help of the gauge theory of defects [29]. The displacement field u_i gives rise to a compatible distortion and the tensor $\tilde{\beta}_{ij}$ is the proper incompatible part of the elastic distortion.

The Burgers vector b_i is defined with the help of the distortion tensor

$$b_i = \oint_\gamma \beta_{ij}\,\mathrm{d}x_j, \tag{2.2}$$

where γ denotes the Burgers circuit. In elastoplasticity the linear elastic strain tensor is given by means of the incompatible distortion tensor (2.1) according to

$$E_{ij} \equiv \beta_{(ij)} = \tfrac{1}{2}(\partial_i u_j + \partial_j u_i + \tilde{\beta}_{ij} + \tilde{\beta}_{ji}), \qquad E_{ij} = E_{ji}. \tag{2.3}$$

The force stress is the response quantity to elastic strain and is given by the (generalized) Hooke's law for an isotropic medium:

$$\sigma_{ij} = 2\mu\left(E_{ij} + \frac{\nu}{1-2\nu}\delta_{ij}E_{kk}\right), \qquad \sigma_{ij} = \sigma_{ji}, \tag{2.4}$$

where μ, ν are shear modulus and Poisson's ratio, respectively. The force stress satisfies the force equilibrium condition

$$\partial_j \sigma_{ij} = 0. \tag{2.5}$$

The inverse of Hooke's law reads

$$E_{ij} = \frac{1}{2\mu}\left(\sigma_{ij} - \frac{\nu}{1+\nu}\delta_{ij}\sigma_{kk}\right). \tag{2.6}$$

In the conventional disclination theory [11–13, 35] the torsion tensor (linear version of Cartan's torsion) is defined by

$$\alpha_{ij} := \epsilon_{jkl}(\partial_k \beta_{il} + \epsilon_{ilm}\varphi^*_{mk}) = \epsilon_{jkl}(\partial_k \tilde{\beta}_{il} + \epsilon_{ilm}\varphi^*_{mk}). \tag{2.7}$$

Anthony called it the disclination torsion (see [11]). On the other hand, it is sometimes called the dislocation density in the theory of disclinations (see, e.g., [12, 13, 35]). φ^*_{ij} was introduced by Mura [35] as 'plastic rotation' and deWit [12, 13, 36] called this quantity the 'disclination loop density'. The field $\tilde{\beta}_{ij}$ may be identified with deWit's 'dislocation loop density'. For a dislocation it yields $\varphi^*_{ij} = 0$ and then (2.7) has the shape of a proper dislocation density. Using the elastic bend–twist tensor (see, e.g., [37])

$$k_{ij} = \partial_j \omega_i - \varphi^*_{ij}, \tag{2.8}$$

with the rotation vector

$$\omega_i = -\tfrac{1}{2}\epsilon_{ijk}\beta_{jk}, \tag{2.9}$$

equation (2.7) can be rewritten according to (see also [11, 36, 37])

$$\alpha_{ij} = \epsilon_{jkl}(\partial_k E_{il} + \epsilon_{iml}k_{mk}) = \epsilon_{jkl}\partial_k E_{il} + \delta_{ij}k_{ll} - k_{ji}. \tag{2.10}$$

The index i indicates the direction of the Burgers vector, j the dislocation line direction. Thus, the diagonal components of α_{ij} represent screw dislocations, the off-diagonal components edge dislocations.

The so-called disclination density tensor of a discrete disclination is defined by [11–13, 35–37]

$$\Theta_{ij} := \epsilon_{jmn}\partial_m k_{in} = -\epsilon_{jmn}\partial_m \varphi^*_{in}. \tag{2.11}$$

The index i indicates the direction of the Frank vector, j the disclination line direction. Thus, the diagonal components of Θ_{ij} represent wedge disclinations, the off-diagonal components twist disclinations. The Frank vector Ω_i is defined with the help of the elastic bend–twist tensor

$$\Omega_i = \oint_\gamma k_{ij}\,\mathrm{d}x_j. \tag{2.12}$$

Consequently, the dislocation density and the disclination density satisfy the following compatibility equations (first and second Bianchi identities):

$$\partial_j \alpha_{ij} - \epsilon_{ikl}\Theta_{kl} = 0, \tag{2.13}$$

$$\partial_j \Theta_{ij} = 0. \tag{2.14}$$

On the other hand, the theory of defects (dislocations and disclinations) can be considered as a gauge model of defects in solids [38, 39]. The gauge group is the group $ISO(3) = T(3) \otimes SO(3)$ ($T(3)$ is the three-dimensional translational group, $SO(3)$ is the three-dimensional rotational group and $\otimes$ denotes the semi-direct product). In this framework, we are able to decompose the incompatible distortion (2.1). That is, the incompatible distortion takes the (linearized) form [38–41]

$$\tilde{\beta}_{ij} = \phi_{ij} + \epsilon_{ikl} W_{kj} x_l, \tag{2.15}$$

where ϕ_{ij} and W_{ij} are the translational and rotational gauge fields, respectively. More precisely, ϕ_{ij} is the translational part of the generalized affine connection [42, 43] and W_{ij} the rotational connection (see also [44]). The torsion and the disclination density tensor are defined by

$$\alpha_{ij} = \epsilon_{jkl} \partial_k \phi_{il} + \epsilon_{ikl} \Theta_{kj} x_l, \tag{2.16}$$

$$\Theta_{ij} = \epsilon_{jmn} \partial_m W_{in}. \tag{2.17}$$

The disclination density tensor (2.17) is the linearized Riemann–Cartan curvature tensor or equivalently the corresponding Einstein tensor. It can be seen that a non-vanishing disclination tensor (2.17) gives a contribution to the torsion tensor (2.16). This piece may be called the disclination torsion. Therefore, the torsion (2.16) has a contribution from both the translational sector (=dislocations) and the rotational sector (=dislocations). Of course, in the case of dislocations (teleparallelism), $\Theta_{ij} = 0$, the disclination torsion is zero and only the first piece in (2.16), which is the proper dislocation density tensor, gives a non-vanishing contribution. If we compare equation (2.11) with (2.17), we may identify (see also [40])

$$W_{ij} \equiv -\varphi^*_{ij}. \tag{2.18}$$

Using equations (2.15), (2.17) and (2.18), one is able to prove the equivalence between (2.10) and (2.16).

The basic equation for the force stress in an isotropic medium is the following inhomogeneous Helmholtz equation [32]:

$$(1 - \kappa^{-2}\Delta)\sigma_{ij} = \overset{\circ}{\sigma}_{ij}, \qquad \kappa^2 = \frac{2\mu}{a_1}, \tag{2.19}$$

where $\overset{\circ}{\sigma}_{ij}$ is the stress tensor obtained for the same traction boundary-value problem within the theory of classical elasticity. It is important to note that (2.19) agrees with the field equation for the stress field in Eringen's nonlocal elasticity [16, 17] and in gradient elasticity [24]. The factor κ^{-1} has the physical dimension of a length and it defines, therefore, an internal characteristic length. If we consider the two-dimensional problem and use the Green function of the two-dimensional Helmholtz equation, we may solve the field equation for every component of the stress field (2.19) with the help of the convolution integral

$$\sigma_{ij}(r) = \int_V \alpha(r - r')\overset{\circ}{\sigma}_{ij}(r')\,\mathrm{d}v(r'), \tag{2.20}$$

with the two-dimensional Green function

$$\alpha(r - r') = \frac{\kappa^2}{2\pi} K_0(\kappa(r - r')), \tag{2.21}$$

with $r = \sqrt{x^2 + y^2}$. Here K_n is the modified Bessel function of the second kind and $n = 0, 1, \ldots$ denotes the order of this function. Thus,

$$(1 - \kappa^{-2}\Delta)\alpha(r) = \delta(r), \tag{2.22}$$

where $\delta(r) := \delta(x)\delta(y)$ denotes the two-dimensional Dirac delta function. In this way, we deduce Eringen's so-called nonlocal constitutive relation for a linear homogeneous, isotropic solid with Green function (2.21) as nonlocal kernel. This kernel (2.21) has its maximum at $r = r'$ and describes the nonlocal interaction. Its two-dimensional volume integral is

$$\int_V \alpha(r - r')\, \mathrm{d}v(r) = 1, \tag{2.23}$$

and is the normalization condition for the nonlocal kernel. In the classical limit ($\kappa^{-1} \to 0$), it becomes the Dirac delta function

$$\lim_{\kappa^{-1}\to 0} \alpha(r - r') = \delta(r - r'). \tag{2.24}$$

Note that Eringen [16–19] found the two-dimensional kernel (2.21) by giving the best match with the Born–von Kármán model of the atomic lattice dynamics and the atomistic dispersion curves. He used the choice $e_0 = 0.39$ for the length

$$\kappa^{-1} = e_0 a, \tag{2.25}$$

where a is an internal length (e.g. the atomic lattice parameter) and e_0 is a material constant.

Using the inverse of the generalized Hooke's law (2.6) and (2.19), we obtain an inhomogeneous Helmholtz equation for every component of the strain tensor (see [32]):

$$(1 - \kappa^{-2}\Delta)E_{ij} = \overset{\circ}{E}_{ij}, \tag{2.26}$$

where $\overset{\circ}{E}_{ij}$ is the classical strain tensor. Equation (2.26) is similar to the equation for the strain in gradient theory used by Gutkin and Aifantis [22–24] if we identify κ^{-2} with the gradient coefficient (see, e.g., equation (4) in [24]). Since the strain tensor fulfils an inhomogeneous Helmholtz equation, we may rewrite (2.26) as a nonlocal relation for the strain:

$$E_{ij}(r) = \int_V \alpha(r - r')\overset{\circ}{E}_{ij}(r')\, \mathrm{d}v(r'), \tag{2.27}$$

which is similar to the nonlocal relation for the stress (2.19). Thus, field theory of elastoplasticity may be considered as a nonlocal theory for the stress as well as the strain tensor. In contrast to Eringen in the nonlocal theory where only the stress tensor has a nonlocal form, we assume that the stress and strain fields at infinity should have the same form for both the classical and elastoplastic field theory.

3. Classical solution

In this section we present the 'classical' stress field for a straight twist disclination in an infinitely extended isotropic body with the help of the stress function method. We assume that the disclination line is along the z-axis and the Frank vector has the following form: $\boldsymbol{\Omega} \equiv (0, \Omega, 0)$. In contrast to the case for a wedge disclination or screw and edge dislocations, the situation is not really a two-dimensional problem for the twist disclination. In the case of a straight twist disclination the three-dimensional space may be considered as a product of the two-dimensional xy-plane and the independent one-dimensional z-line [13]. In this situation the z-axis plays a peculiar role.

The classical solution for the elastic stress fields was originally given by deWit [13]:

$$\overset{\circ}{\sigma}_{xx} = -\frac{\mu\Omega}{2\pi(1-\nu)}\frac{zy(y^2 + 3x^2)}{r^4}, \tag{3.1}$$

$$\overset{\circ}{\sigma}_{yy} = -\frac{\mu\Omega}{2\pi(1-\nu)}\frac{zy(y^2 - x^2)}{r^4}, \tag{3.2}$$

$$\overset{\circ}{\sigma}_{xy} = \frac{\mu\Omega}{2\pi(1-\nu)}\frac{zx(x^2 - y^2)}{r^4}, \tag{3.3}$$

$$\overset{\circ}{\sigma}_{zz} = -\frac{\mu\Omega\nu}{\pi(1-\nu)}\frac{zy}{r^2}, \tag{3.4}$$

$$\overset{\circ}{\sigma}_{zx} = \frac{\mu\Omega}{2\pi(1-\nu)}\frac{xy}{r^2}, \tag{3.5}$$

$$\overset{\circ}{\sigma}_{zy} = -\frac{\mu\Omega}{2\pi(1-\nu)}\left\{(1-2\nu)\ln r + \frac{x^2}{r^2}\right\}. \tag{3.6}$$

Obviously, the expressions (3.1)–(3.4) contain the classical singularity $\sim r^{-1}$ and a logarithmic singularity $\sim \ln r$ in (3.6). Thus, the classical elastic stress is infinite at the disclination line. The reason is that the classical theory of elasticity breaks down in the disclination core with the result that in the defect core region classical elasticity fails to apply. Usually, the radius of this region is estimated by means of atomic models. Due to the unphysical singularities it is erroneous to argue that the stress has a maximum/minimum value at the defect line.

For the situation of the strain condition, $\overset{\circ}{E}_{zz} = 0$, equations (3.1)–(3.6) can be calculated by using the so-called stress function method in the following form:

$$\overset{\circ}{\sigma}_{ij} = \begin{pmatrix} \partial^2_{yy}\overset{\circ}{f} & -\partial^2_{xy}\overset{\circ}{f} & -\partial_y\overset{\circ}{F} \\ -\partial^2_{xy}\overset{\circ}{f} & \partial^2_{xx}\overset{\circ}{f} & \partial_x\overset{\circ}{F} + \partial_z\overset{\circ}{g} \\ -\partial_y\overset{\circ}{F} & \partial_x\overset{\circ}{F} + \partial_z\overset{\circ}{g} & \overset{\circ}{p} \end{pmatrix}. \tag{3.7}$$

The stress is given in terms of the stress functions $\overset{\circ}{f}$, $\overset{\circ}{F}$, $\overset{\circ}{g}$ and $\overset{\circ}{p}$. In order to satisfy the force equilibrium the stress $\overset{\circ}{\sigma}_{zz}$ has to fulfil the condition

$$\overset{\circ}{p} = \nu\Delta\overset{\circ}{f} = -\partial_y\overset{\circ}{g}, \tag{3.8}$$

where $\Delta \equiv \partial^2_{xx} + \partial^2_{yy}$ denotes the two-dimensional Laplacian. The 'classical' stress functions for the stress fields (3.7) are

$$\overset{\circ}{f} = -\frac{\mu\Omega}{2\pi(1-\nu)}zy\ln r, \tag{3.9}$$

$$\overset{\circ}{F} = -\frac{\mu\Omega}{2\pi(1-\nu)}x\ln r, \tag{3.10}$$

$$\overset{\circ}{g} = \frac{\mu\Omega\nu}{\pi(1-\nu)}z\ln r. \tag{3.11}$$

They satisfy the following two-dimensional differential equations:

$$\Delta\Delta\overset{\circ}{f} = -\frac{2\mu\Omega z}{(1-\nu)}\partial_y\delta(r), \tag{3.12}$$

$$\Delta\Delta\overset{\circ}{F} = -\frac{2\mu\Omega}{(1-\nu)}\partial_x\delta(r), \tag{3.13}$$

$$\Delta\overset{\circ}{g} = \frac{2\mu\Omega\nu z}{(1-\nu)}\delta(r). \tag{3.14}$$

Thus, $\overset{\circ}{f}$ and $\overset{\circ}{F}$ are biharmonic stress functions and $\overset{\circ}{g}$ is a harmonic one. We see that $\overset{\circ}{F}$ is an Airy stress function, $\overset{\circ}{f}$ is an Airy stress function multiplied by z and on the other hand $\overset{\circ}{g}$ is a Prandtl stress function multiplied by z (up to constant pre-factors).

For convenience we give the classical elastic strain of the straight twist disclination (see [13])

$$\overset{\circ}{E}_{xx} = -\frac{\Omega}{4\pi(1-\nu)}\frac{zy}{r^2}\left\{(1-2\nu) + \frac{2x^2}{r^2}\right\}, \tag{3.15}$$

$$\overset{\circ}{E}_{yy} = -\frac{\Omega}{4\pi(1-\nu)}\frac{zy}{r^2}\left\{(1-2\nu) - \frac{2x^2}{r^2}\right\}, \tag{3.16}$$

$$\overset{\circ}{E}_{xy} = \frac{\Omega}{4\pi(1-\nu)}\frac{zx}{r^2}\left\{1 - \frac{2y^2}{r^2}\right\}, \tag{3.17}$$

$$\overset{\circ}{E}_{zx} = \frac{\Omega}{4\pi(1-\nu)}\frac{xy}{r^2}, \tag{3.18}$$

$$\overset{\circ}{E}_{zy} = -\frac{\Omega}{4\pi(1-\nu)}\left\{(1-2\nu)\ln r + \frac{x^2}{r^2}\right\}, \tag{3.19}$$

which contains the 'classical' singularities at $r = 0$.

4. Nonsingular solution

In this section we want to consider the twist disclination in the elastoplastic field theory to find modified solutions without the 'classical' singularities. The modified solutions are used to estimate the extent of disclination core, thus providing information which cannot be obtained by using classical elasticity theory.

We make for the modified stress field an ansatz in terms of unknown stress functions which has the same form as the classical stress field (3.7):

$$\sigma_{ij} = \begin{pmatrix} \partial^2_{yy} f & -\partial^2_{xy} f & -\partial_y F \\ -\partial^2_{xy} f & \partial^2_{xx} f & \partial_x F + \partial_z g \\ -\partial_y F & \partial_x F + \partial_z g & p \end{pmatrix}, \tag{4.1}$$

with the relation

$$p = \nu\Delta f = -\partial_y g. \tag{4.2}$$

Substituting (4.1) and (3.7) into (2.19) we obtain three inhomogeneous Helmholtz equations for the unknown stress functions:

$$(1-\kappa^{-2}\Delta)f = -\frac{\mu\Omega}{2\pi(1-\nu)}zy\ln r, \tag{4.3}$$

$$(1-\kappa^{-2}\Delta)F = -\frac{\mu\Omega}{2\pi(1-\nu)}x\ln r, \tag{4.4}$$

$$(1-\kappa^{-2}\Delta)g = \frac{\mu\Omega\nu}{\pi(1-\nu)}z\ln r. \tag{4.5}$$

The inhomogeneous parts of (4.3)–(4.5) are the classical stress functions. Using the same procedure as in the case of a straight edge dislocation (see [32]) in order to solve the inhomogeneous Helmholtz equations, we can find the solutions of (4.3)–(4.5). The solutions for the modified stress functions of a straight twist disclination are given by

$$f = -\frac{\mu\Omega}{2\pi(1-\nu)}zy\left\{\ln r + \frac{2}{\kappa^2 r^2}(1-\kappa r K_1(\kappa r))\right\}, \tag{4.6}$$

$$F = -\frac{\mu\Omega}{2\pi(1-\nu)}x\left\{\ln r + \frac{2}{\kappa^2 r^2}(1-\kappa r K_1(\kappa r))\right\}, \tag{4.7}$$

$$g = \frac{\mu\Omega\nu}{\pi(1-\nu)}z\{\ln r + K_0(\kappa r)\}, \tag{4.8}$$

where the first pieces are the classical stress functions (3.9)–(3.11).

By means of equation (4.1) and the stress functions (4.6)–(4.8), we are able to calculate the modified stress of a straight twist disclination. So we find for the elastic stress in Cartesian coordinates

$$\sigma_{xx} = -\frac{\mu\Omega}{2\pi(1-\nu)}\frac{zy}{r^4}\bigg\{(y^2+3x^2)+\frac{4}{\kappa^2r^2}(y^2-3x^2) - 2y^2\kappa r K_1(\kappa r) - 2(y^2-3x^2)K_2(\kappa r)\bigg\}, \quad (4.9)$$

$$\sigma_{yy} = -\frac{\mu\Omega}{2\pi(1-\nu)}\frac{zy}{r^4}\bigg\{(y^2-x^2)-\frac{4}{\kappa^2r^2}(y^2-3x^2) - 2x^2\kappa r K_1(\kappa r) + 2(y^2-3x^2)K_2(\kappa r)\bigg\}, \quad (4.10)$$

$$\sigma_{xy} = \frac{\mu\Omega}{2\pi(1-\nu)}\frac{zx}{r^4}\bigg\{(x^2-y^2)-\frac{4}{\kappa^2r^2}(x^2-3y^2) - 2y^2\kappa r K_1(\kappa r) + 2(x^2-3y^2)K_2(\kappa r)\bigg\}, \quad (4.11)$$

$$\sigma_{zz} = -\frac{\mu\Omega\nu}{\pi(1-\nu)}\frac{zy}{r^2}\{1-\kappa r K_1(\kappa r)\}, \quad (4.12)$$

$$\sigma_{zx} = \frac{\mu\Omega}{2\pi(1-\nu)}\frac{xy}{r^2}\bigg\{1-\frac{2}{\kappa^2r^2}(2-\kappa^2r^2K_2(\kappa r))\bigg\}, \quad (4.13)$$

$$\sigma_{zy} = -\frac{\mu\Omega}{2\pi(1-\nu)}\bigg\{(1-2\nu)(\ln r + K_0(\kappa r)) + \frac{x^2}{r^2} - \frac{(x^2-y^2)}{\kappa^2r^4}(2-\kappa^2r^2K_2(\kappa r))\bigg\}. \quad (4.14)$$

These stresses are plotted in figure 1. If we identify $\kappa \equiv 1/\sqrt{c}$ (c is the gradient coefficient used by Gutkin and Aifantis), the components of the stress (4.9)–(4.14) are in agreement with the stress field obtained by Gutkin and Aifantis [27, 28] in the framework of strain gradient elasticity by using the Fourier transform method. It is interesting to note that the stresses (4.9)–(4.12) caused by the straight twist disclination with the Frank vector $\mathbf{\Omega} \equiv (0, \Omega, 0)$ coincide with the stresses due to the straight edge dislocation with the Burgers vector $\boldsymbol{b} \equiv (b, 0, 0)$ replacing Ωz by b (compare with equations (3.15)–(3.18) in [32]). The trace of the stress tensor $\sigma_{kk} = \sigma_{xx} + \sigma_{yy} + \sigma_{zz}$ produced by the twist disclination in an isotropic medium is

$$\sigma_{kk} = -\frac{\mu\Omega(1+\nu)}{\pi(1-\nu)}\frac{zy}{r^2}\{1-\kappa r K_1(\kappa r)\}. \quad (4.15)$$

We may now discuss some details of the stresses near the disclination core region in the xy-plane. The stresses (4.9)–(4.12) vanish at the disclination line instead of being singular as predicted by classical elasticity. Every component of (4.9)–(4.12) has a maximum and a minimum near the disclination line. Because the extreme values are of opposite sign a zero point must be at the defect line. In addition, the stress (4.14) has a maximum value at the disclination line. The extreme values may serve as a measure of critical stress level at which fracture or failure can occur. Contrary to the case for classical elasticity, stresses (4.9)–(4.14) are finite at the defect line. Therefore, the stress fields have no artificial singularities at the core and the maximum stress occurs at a short distance away from the disclination line (see figure 1). In fact, when $r \to 0$, we have

$$K_0(\kappa r) \to -\left[\gamma + \ln\frac{\kappa r}{2}\right], \qquad K_1(\kappa r) \to \frac{1}{\kappa r}, \qquad K_2(\kappa r) \to -\frac{1}{2} + \frac{2}{(\kappa r)^2},$$

and thus $\sigma_{ij} \to 0$. Here γ denotes the Euler constant. It can be seen that the stresses have the following extreme values in the xy-plane: $|\sigma_{xx}(0,y)| \simeq 0.546\kappa\frac{\mu\Omega z}{2\pi(1-\nu)}$ at $|y| \simeq 0.996\kappa^{-1}$, $|\sigma_{yy}(0,y)| \simeq 0.260\kappa\frac{\mu\Omega z}{2\pi(1-\nu)}$ at $|y| \simeq 1.494\kappa^{-1}$, $|\sigma_{xy}(x,0)| \simeq 0.260\kappa\frac{\mu\Omega z}{2\pi(1-\nu)}$ at

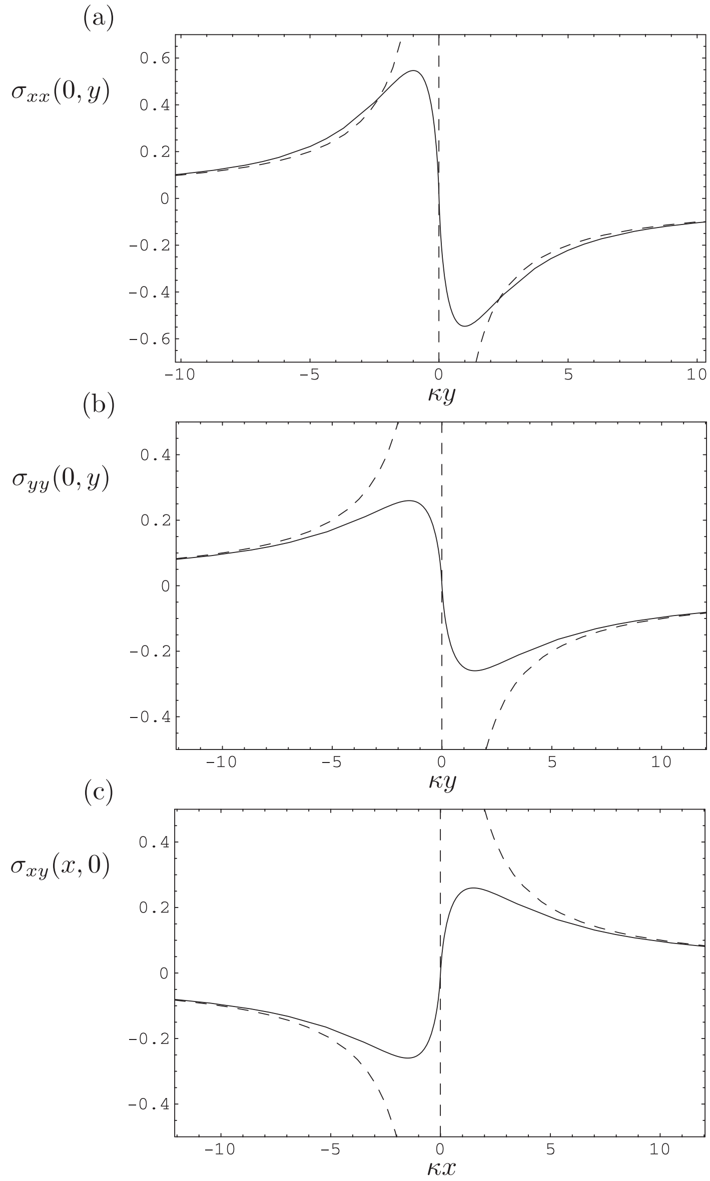


Figure 1. The stress components of a twist disclination near the disclination line: (a) $\sigma_{xx}(0, y)$, (b) $\sigma_{yy}(0, y)$, (c) $\sigma_{xy}(x, 0)$ are given in units of $\mu\Omega z\kappa/[2\pi(1-\nu)]$, (d) $\sigma_{zz}(0, y)$ is given in units of $\mu\Omega\nu\kappa/[\pi(1-\nu)]$ and (e) $\sigma_{zy}(x, 0)$ is given in units of $\mu\Omega/[2\pi(1-\nu)]$. The dashed curves represent the classical stress components.

$|x| \simeq 1.494\kappa^{-1}$, $|\sigma_{zz}(0, y)| \simeq 0.399\kappa\frac{\mu\Omega\nu z}{\pi(1-\nu)}$ at $|y| \simeq 1.114\kappa^{-1}$ and $|\sigma_{kk}(0, y)| \simeq 0.399\kappa\frac{\mu\Omega(1+\nu)z}{\pi(1-\nu)}$ at $|y| \simeq 1.114\kappa^{-1}$. The stresses σ_{xx}, σ_{yy} and σ_{xy} are modified near the disclination core ($0 \leqslant r \leqslant 12\kappa^{-1}$). The stress σ_{zz} and the trace σ_{kk} are modified in the region $0 \leqslant r \leqslant 6\kappa^{-1}$. Far from the disclination line ($r \gg 12\kappa^{-1}$) the modified and the classical solutions of the stress of a twist disclination coincide. In addition, it can be seen that at $z = 0$ the stresses (4.9)–(4.12) are zero. The stress σ_{zy} has at $r = 0$ the maximum value:

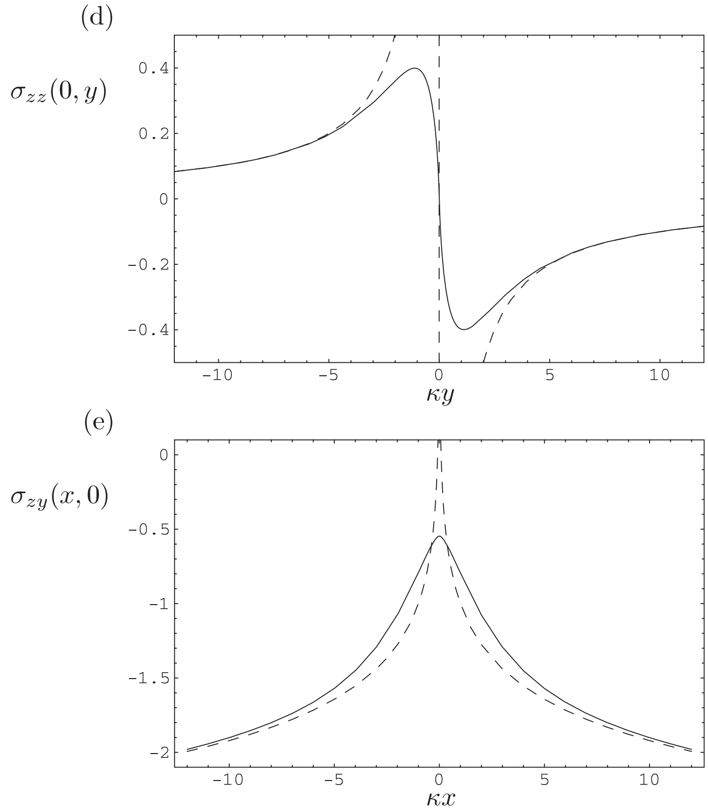


Figure 1. (Continued.)

$\sigma_{zy}(0) \simeq \frac{\mu\Omega}{2\pi(1-\nu)}[(1-2\nu)(\gamma + \ln\frac{\kappa}{2}) - \frac{1}{2}]$ and with $\nu = 0.3$: $\sigma_{zy}(x,0) \simeq \frac{\mu\Omega}{2\pi(1-\nu)}[0.4\ln\kappa - 0.546]$ (see figure 1(e) where a constant term proportional to $\ln\kappa$ is dropped out). Consequently, one can equate the maximum shear stresses to the cohesive shear stresses to obtain conditions to produce a disclination of single atomic distance.

Due to the two-dimensional symmetry it is convenient to express the stresses in cylindrical coordinates. The stress tensor has the following form in cylindrical coordinates:

$$\sigma_{rr} = -\frac{\mu\Omega}{2\pi(1-\nu)}\frac{z\sin\varphi}{r}\left\{1 - \frac{4}{\kappa^2 r^2} + 2K_2(\kappa r)\right\}, \tag{4.16}$$

$$\sigma_{r\varphi} = \frac{\mu\Omega}{2\pi(1-\nu)}\frac{z\cos\varphi}{r}\left\{1 - \frac{4}{\kappa^2 r^2} + 2K_2(\kappa r)\right\}, \tag{4.17}$$

$$\sigma_{\varphi\varphi} = -\frac{\mu\Omega}{2\pi(1-\nu)}\frac{z\sin\varphi}{r}\left\{1 + \frac{4}{\kappa^2 r^2} - 2K_2(\kappa r) - 2\kappa r K_1(\kappa r)\right\}, \tag{4.18}$$

$$\sigma_{zz} = -\frac{\mu\Omega\nu}{\pi(1-\nu)}\frac{z\sin\varphi}{r}\{1 - \kappa r K_1(\kappa r)\}, \tag{4.19}$$

$$\sigma_{zr} = -\frac{\mu\Omega}{2\pi(1-\nu)}\sin\varphi\left\{(1-2\nu)(\ln r + K_0(\kappa r)) + \frac{2}{\kappa^2 r^2} - K_2(\kappa r)\right\}, \tag{4.20}$$

$$\sigma_{z\varphi} = -\frac{\mu\Omega}{2\pi(1-\nu)}\cos\varphi\left\{(1-2\nu)(\ln r + K_0(\kappa r)) + 1 - \frac{2}{\kappa^2 r^2} + K_2(\kappa r)\right\}. \tag{4.21}$$

The fields (4.16)–(4.21) agree with the expressions given by Povstenko [20] in the framework of nonlocal elasticity if we use the identification $\kappa \equiv 1/(\tau l)$. He used the two-dimensional nonlocal kernel (2.21) which is Green function of the two-dimensional Helmholtz equation. Again, if one replaces Ωz by b, the stresses (4.16)–(4.21) agree with the stresses of an edge dislocation in cylindrical coordinates (compare with equations (3.27)–(3.30) in [32]). The stresses (4.16)–(4.21) coincide with the classical ones far from the disclination core. The stresses (4.16)–(4.19) are zero at the disclination line. In principle we may discuss the extreme values of (4.16)–(4.21) in the xy-plane. For example, the stresses (4.16) and (4.18) have the extreme values $|\sigma_{rr}| \simeq 0.260\kappa \frac{\mu\Omega z \sin\varphi}{2\pi(1-\nu)}$ at $r \simeq 1.494\kappa^{-1}$ and $|\sigma_{\varphi\varphi}| \simeq 0.547\kappa \frac{\mu\Omega z \sin\varphi}{2\pi(1-\nu)}$ at $r \simeq 0.996\kappa^{-1}$. The stresses (4.20) and (4.21) have the following values at $r = 0$: $\sigma_{zr}(0) \simeq \frac{\mu\Omega \sin\varphi}{2\pi(1-\nu)}[(1-2\nu)(\gamma + \ln\frac{\kappa}{2}) - \frac{1}{2}]$ and $\sigma_{z\varphi}(0) \simeq \frac{\mu\Omega \cos\varphi}{2\pi(1-\nu)}[(1-2\nu)(\gamma + \ln\frac{\kappa}{2}) - \frac{1}{2}]$.

The elastic strain is given in terms of stress functions:

$$E_{ij} = \frac{1}{2\mu}\begin{pmatrix} \partial^2_{yy} f - \nu\Delta f & -\partial^2_{xy} f & -\partial_y F \\ -\partial^2_{xy} f & \partial^2_{xx} f - \nu\Delta f & \partial_x F + \partial_z g \\ -\partial_y F & \partial_x F + \partial_z g & 0 \end{pmatrix}. \tag{4.22}$$

For the elastic strain of a twist disclination we find

$$E_{xx} = -\frac{\Omega}{4\pi(1-\nu)}\frac{zy}{r^2}\bigg\{(1-2\nu) + \frac{2x^2}{r^2} + \frac{4}{\kappa^2 r^4}(y^2 - 3x^2) - 2\left(\frac{y^2}{r^2} - \nu\right)\kappa r K_1(\kappa r) - \frac{2}{r^2}(y^2 - 3x^2)K_2(\kappa r)\bigg\}, \tag{4.23}$$

$$E_{yy} = -\frac{\Omega}{4\pi(1-\nu)}\frac{zy}{r^2}\bigg\{(1-2\nu) - \frac{2x^2}{r^2} - \frac{4}{\kappa^2 r^4}(y^2 - 3x^2) - 2\left(\frac{x^2}{r^2} - \nu\right)\kappa r K_1(\kappa r) + \frac{2}{r^2}(y^2 - 3x^2)K_2(\kappa r)\bigg\}, \tag{4.24}$$

$$E_{xy} = \frac{\Omega}{4\pi(1-\nu)}\frac{zx}{r^2}\bigg\{1 - \frac{2y^2}{r^2} - \frac{4}{\kappa^2 r^4}(x^2 - 3y^2) - \frac{2y^2}{r^2}\kappa r K_1(\kappa r) + \frac{2}{r^2}(x^2 - 3y^2)K_2(\kappa r)\bigg\}, \tag{4.25}$$

$$E_{zx} = \frac{\Omega}{4\pi(1-\nu)}\frac{xy}{r^2}\bigg\{1 - \frac{2}{\kappa^2 r^2}(2 - \kappa^2 r^2 K_2(\kappa r))\bigg\}, \tag{4.26}$$

$$E_{zy} = -\frac{\Omega}{4\pi(1-\nu)}\bigg\{(1-2\nu)(\ln r + K_0(\kappa r)) + \frac{x^2}{r^2} - \frac{(x^2 - y^2)}{\kappa^2 r^4}(2 - \kappa^2 r^2 K_2(\kappa r))\bigg\}. \tag{4.27}$$

The components of the strain tensor have in the xy-plane the following extreme values ($\nu = 0.3$): $|E_{xx}(0,y)| \simeq 0.308\kappa\frac{\Omega z}{4\pi(1-\nu)}$ at $|y| \simeq 0.922\kappa^{-1}$, $|E_{yy}(0,y)| \simeq 0.010\kappa\frac{\Omega z}{4\pi(1-\nu)}$ at $|y| \simeq 0.218\kappa^{-1}$, $|E_{yy}(0,y)| \simeq 0.054\kappa\frac{\Omega z}{4\pi(1-\nu)}$ at $|y| \simeq 4.130\kappa^{-1}$ and $|E_{xy}(x,0)| \simeq 0.260\kappa\frac{\Omega z}{4\pi(1-\nu)}$ at $|x| \simeq 1.494\kappa^{-1}$. It is interesting to note that $E_{yy}(0,y)$ is much smaller than $E_{xx}(0,y)$ within the core region. The strain E_{zy} has at $r = 0$ the value $E_{zy}(0) \simeq \frac{\mu\Omega}{4\pi(1-\nu)}[(1-2\nu)(\gamma + \ln\frac{\kappa}{2}) - \frac{1}{2}]$. The strain (4.23)–(4.27) coincides with the result given by Gutkin and Aifantis [26–28]. The dilatation E_{kk} reads

$$E_{kk} = -\frac{\Omega(1-2\nu)}{2\pi(1-\nu)}\frac{zy}{r^2}\{1 - \kappa r K_1(\kappa r)\}. \tag{4.28}$$

In the xy-plane it has the extremum $|E_{kk}(0,y)| \simeq 0.399\kappa\frac{\Omega(1-2\nu)z}{2\pi(1-\nu)}$ at $|y| \simeq 1.114\kappa^{-1}$. The elastic strain can be rewritten in cylindrical coordinates as follows:

$$E_{rr} = -\frac{\Omega}{4\pi(1-\nu)}\frac{z\sin\varphi}{r}\bigg\{(1-2\nu) - \frac{4}{\kappa^2 r^2} + 2K_2(\kappa r) + 2\nu K_1(\kappa r)\bigg\}, \tag{4.29}$$

$$E_{r\varphi} = \frac{\Omega}{4\pi(1-\nu)} \frac{z\cos\varphi}{r} \left\{1 - \frac{4}{\kappa^2 r^2} + 2K_2(\kappa r)\right\}, \tag{4.30}$$

$$E_{\varphi\varphi} = -\frac{\Omega}{4\pi(1-\nu)} \frac{z\sin\varphi}{r} \left\{(1-2\nu) + \frac{4}{\kappa^2 r^2} - 2K_2(\kappa r) - 2(1-\nu)\kappa r K_1(\kappa r)\right\}, \tag{4.31}$$

$$E_{zr} = -\frac{\Omega}{4\pi(1-\nu)} \sin\varphi \left\{(1-2\nu)(\ln r + K_0(\kappa r)) + \frac{2}{\kappa^2 r^2} - K_2(\kappa r)\right\}, \tag{4.32}$$

$$E_{z\varphi} = -\frac{\Omega}{4\pi(1-\nu)} \cos\varphi \left\{(1-2\nu)(\ln r + K_0(\kappa r)) + 1 - \frac{2}{\kappa^2 r^2} + K_2(\kappa r)\right\}. \tag{4.33}$$

The main feature of the solution given by (4.23)–(4.33) is the absence of any singularities near the disclination line. This solution coincides with the classical ones far from the disclination core.

Now we want to calculate the elastic bend–twist, torsion, disclination density and the rotation ($\omega_z \equiv -\beta_{[xy]}$ and $\omega_y \equiv \beta_{[xz]}$) of a twist disclination. They might be determined from the following conditions on the dislocation densities of the twist disclination:

$$\alpha_{xz} = -\frac{1-\nu}{2\mu} \partial_y \Delta f - \partial_x \omega_z, \tag{4.34}$$

$$\alpha_{yz} = \frac{1-\nu}{2\mu} \partial_x \Delta f - \partial_y \omega_z \equiv 0, \tag{4.35}$$

$$\alpha_{zz} = \frac{1}{2\mu} (\Delta F + \partial^2_{xz} g) - k_{zz} \equiv 0, \tag{4.36}$$

$$\alpha_{xx} = -\frac{1}{2\mu} (\partial^2_{yy} F - \partial^3_{zxy} f) - k_{xx} \equiv 0, \tag{4.37}$$

$$\alpha_{xy} = \frac{1}{2\mu} (\partial^2_{xy} F + \partial_z (\partial^2_{yy} f - \nu \Delta f)) - k_{yx} \equiv 0, \tag{4.38}$$

$$\alpha_{yx} = \frac{1}{2\mu} (\partial^2_{xy} F + \partial^2_{yz} g - \partial_z (\partial^2_{xx} f - \nu \Delta f)) - k_{xy} \equiv 0, \tag{4.39}$$

$$\alpha_{yy} = -\frac{1}{2\mu} (\partial^2_{xx} F + \partial^2_{xz} g + \partial^3_{zxy} f) - k_{yy} \equiv 0, \tag{4.40}$$

$$\alpha_{zx} = -\frac{1}{2\mu} \partial_z (\partial_x F + \partial_z g) - k_{xz} \equiv 0, \tag{4.41}$$

$$\alpha_{zy} = -\frac{1}{2\mu} \partial^2_{zy} F - k_{yz} \equiv 0, \tag{4.42}$$

$$\alpha_{jj} = 2k_{jj} \equiv 0. \tag{4.43}$$

The conditions (4.34)–(4.43) must be consistent with deWit's dislocation densities of a twist disclination. We will discuss this point in detail below. The equations (4.34) and (4.35) look like the conditions for the dislocation density of an edge dislocation (see [32]) such that the elastic bend–twists k_{zx} and k_{zy} are compatible. Equations (4.41) and (4.42) are trivially satisfied. From (4.34)–(4.40) we may determine the elastic bend–twist. So we find for the non-vanishing components of the elastic bend–twist tensor

$$k_{yx} = -\frac{\Omega}{2\pi} \frac{y}{r^2} \{1 - \kappa r K_1(\kappa r)\}, \tag{4.44}$$

$$k_{yy} = \frac{\Omega}{2\pi} \frac{x}{r^2} \{1 - \kappa r K_1(\kappa r)\}, \tag{4.45}$$

$$k_{zx} = \frac{\Omega z}{2\pi r^4} \{(x^2 - y^2)(1 - \kappa r K_1(\kappa r)) - \kappa^2 x^2 r^2 K_0(\kappa r)\}, \tag{4.46}$$

$$k_{zy} = \frac{\Omega z}{2\pi r^4} xy\{2(1 - \kappa r K_1(\kappa r)) - \kappa^2 r^2 K_0(\kappa r)\}, \tag{4.47}$$

$$k_{zz} = -\frac{\Omega}{2\pi}\frac{x}{r^2}\{1 - \kappa r K_1(\kappa r)\}. \tag{4.48}$$

The shape of (4.44) and (4.45) is analogous to the elastic bend–twist of a wedge disclination given in [34]. It can be seen that (4.46) and (4.47) are singular at the disclination line $r = 0$. If one replaces Ωz by b, equations (4.44) and (4.45) coincide with the elastic bend–twist of an edge dislocation (see [32, 33]). The component (4.48) has no singularity at the disclination line.

The elastic bend–twist tensor can be decomposed according to (2.8) into a gradient of the rotation vector and an incompatible part. We identify the incompatible part with the disclination loop density. It is analogous to the decomposition of the elastic distortion of a dislocation into a gradient of the displacement vector and an incompatible distortion (see [30–32]). We find for the non-vanishing components of the rotation vector

$$\omega_y = \frac{\Omega}{2\pi}\left\{\varphi(1 - \kappa r K_1(\kappa r)) + \frac{\pi}{2}\,\mathrm{sgn}(y)\kappa r K_1(\kappa r)\right\}, \tag{4.49}$$

$$\omega_z = -\frac{\Omega}{2\pi}\frac{zx}{r^2}\{1 - \kappa r K_1(\kappa r)\}. \tag{4.50}$$

Here we use a single-valued discontinuous form for φ (see [13, 22–24]). It is made unique by cutting the half-plane $y = 0$ at $x < 0$ and assuming φ to jump from π to $-\pi$ when crossing the cut. The far fields of the rotation vector (4.49) and (4.50) agree with deWit's expressions given in [13]. It yields $\mathrm{sgn}\, y = +1$ for $y > 0$ and $\mathrm{sgn}\, y = -1$ for $y < 0$. For $y \to +0$, the expression (4.49) is plotted in figure 2(a). It can be seen that the Bessel function terms which appear in (4.49) lead to a symmetric smoothing of the rotation vector profile, in contrast to the abrupt jump occurring in the classical solution. It is interesting to note that the size of such a transition zone is approximately $12/\kappa$ which gives the value $6/\kappa$ for the radius of the disclination core. The component (4.49) is discontinuous due to φ and (4.50) is continuous. The component (4.50) has in the xy-plane a maximum of $\omega_z(x, 0) \simeq 0.399\Omega\kappa z/[2\pi]$ at $x \simeq -1.114/\kappa$, a minimum of $\omega_z(x, 0) \simeq -0.399\Omega\kappa z/[2\pi]$ at $x \simeq 1.114/\kappa$ and no singularity at the disclination core (see figure 2(b)). It can be seen that k_{zx}, k_{zy} and k_{zz} are gradient terms of the rotation ω_z. In performing the differentiations of the rotation ω_y we obtain k_{yx} and k_{yy} plus excess terms which we identify as components of the disclination loop density. The non-vanishing components of the disclination loop density turn out to be

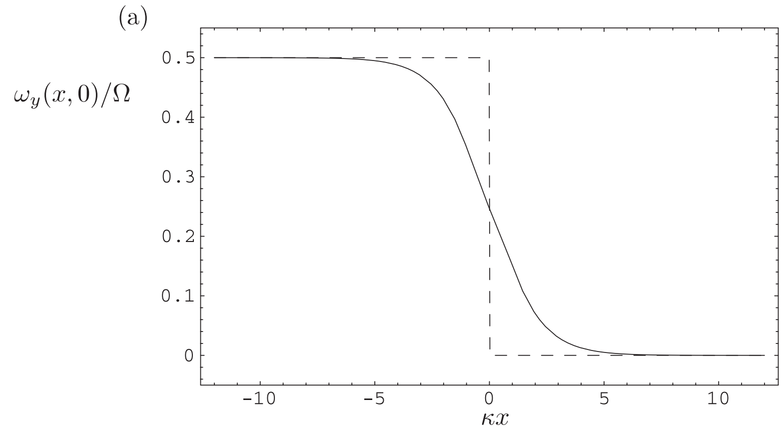
$$\varphi^*_{yx} = \frac{\Omega}{2\pi}\kappa^2 x K_0(\kappa r)\left(\varphi - \frac{\pi}{2}\,\mathrm{sgn}(y)\right), \tag{4.51}$$

$$\varphi^*_{yy} = \frac{\Omega}{2\pi}\left\{\kappa^2 y K_0(\kappa r)\left(\varphi - \frac{\pi}{2}\,\mathrm{sgn}(y)\right) + \pi\delta(y)(1 - \mathrm{sgn}(x)[1 - \kappa r K_1(\kappa r)])\right\}. \tag{4.52}$$

They contain the angle φ and the form is analogous to the plastic distortion of a dislocation (see [32]). Only the component φ^*_{yy} has a δ-singularity at $y = 0$ like the disclination loop density [13, 35] $\varphi^*_{yy} = (\Omega/2)\delta(y)(1 - \mathrm{sgn}(x))$.

Finally, we find for the elastic distortion of the straight twist disclination

$$\beta_{xx} = -\frac{\Omega}{4\pi(1-\nu)}\frac{zy}{r^2}\left\{(1 - 2\nu) + \frac{2x^2}{r^2} + \frac{4}{\kappa^2 r^4}(y^2 - 3x^2) - 2\left(\frac{y^2}{r^2} - \nu\right)\kappa r K_1(\kappa r) - \frac{2}{r^2}(y^2 - 3x^2)K_2(\kappa r)\right\}, \tag{4.53}$$



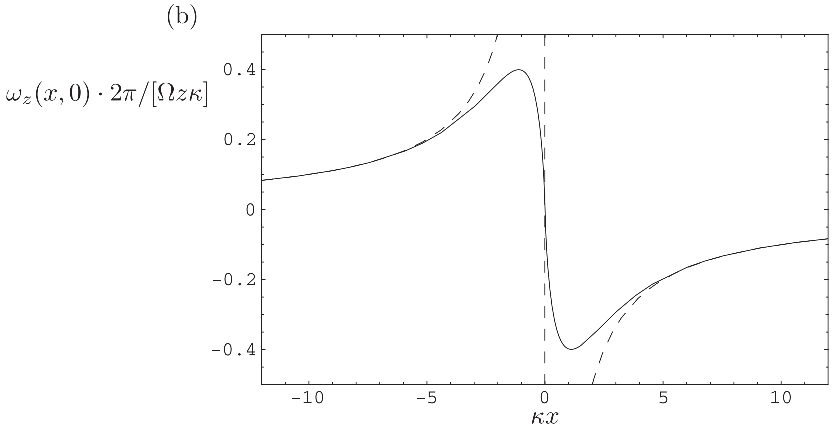


Figure 2. The rotation vector of a twist disclination: (a) $\omega_y(x, y \to +0)/\Omega$, (b) $\omega_z(x, 0)$, plotted in units of $\Omega z\kappa/[2\pi]$. The dashed curves represent the classical solution.

$$\beta_{xy} = \frac{\Omega}{4\pi(1-\nu)}\frac{zx}{r^2}\left\{(3-2\nu) - \frac{2y^2}{r^2} - \frac{4}{\kappa^2 r^4}(x^2-3y^2) - 2\left((1-\nu)+\frac{y^2}{r^2}\right)\kappa r K_1(\kappa r) + \frac{2}{r^2}(x^2-3y^2)K_2(\kappa r)\right\}, \tag{4.54}$$

$$\beta_{yx} = -\frac{\Omega}{4\pi(1-\nu)}\frac{zx}{r^2}\left\{(1-2\nu) + \frac{2y^2}{r^2} + \frac{4}{\kappa^2 r^4}(x^2-3y^2) - 2\left((1-\nu)-\frac{y^2}{r^2}\right)\kappa r K_1(\kappa r) - \frac{2}{r^2}(x^2-3y^2)K_2(\kappa r)\right\}, \tag{4.55}$$

$$\beta_{yy} = -\frac{\Omega}{4\pi(1-\nu)}\frac{zy}{r^2}\left\{(1-2\nu) - \frac{2x^2}{r^2} - \frac{4}{\kappa^2 r^4}(y^2-3x^2) - 2\left(\frac{x^2}{r^2}-\nu\right)\kappa r K_1(\kappa r) + \frac{2}{r^2}(y^2-3x^2)K_2(\kappa r)\right\}, \tag{4.56}$$

$$\beta_{zx} = \frac{\Omega}{4\pi(1-\nu)}\frac{xy}{r^2}\left\{1 - \frac{2}{\kappa^2 r^2}(2-\kappa^2 r^2 K_2(\kappa r))\right\} - \frac{\Omega}{2\pi}\left\{\varphi(1-\kappa r K_1(\kappa r)) + \frac{\pi}{2}\,\mathrm{sgn}(y)\kappa r K_1(\kappa r)\right\}, \tag{4.57}$$

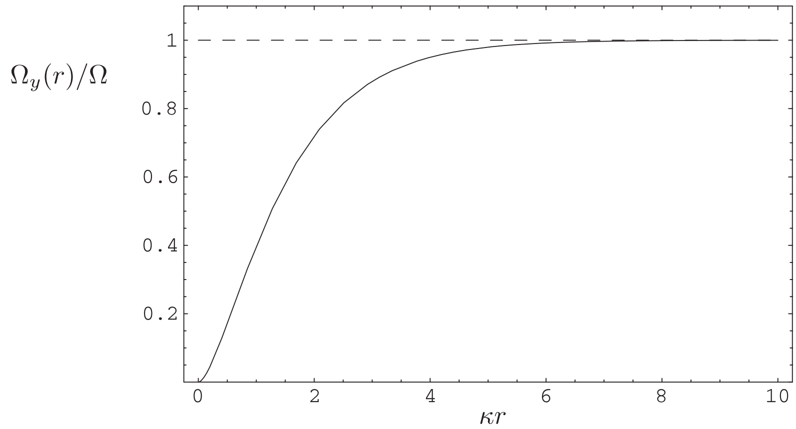


Figure 3. The effective Frank vector $\Omega_y(r)/\Omega$ (solid).

$$\beta_{xz} = \frac{\Omega}{4\pi(1-\nu)}\frac{xy}{r^2}\left\{1 - \frac{2}{\kappa^2 r^2}(2 - \kappa^2 r^2 K_2(\kappa r))\right\} + \frac{\Omega}{2\pi}\left\{\varphi(1 - \kappa r K_1(\kappa r)) + \frac{\pi}{2}\,\mathrm{sgn}(y)\kappa r K_1(\kappa r)\right\}, \quad (4.58)$$

$$\beta_{zy} = -\frac{\Omega}{4\pi(1-\nu)}\left\{(1-2\nu)(\ln r + K_0(\kappa r)) + \frac{x^2}{r^2} - \frac{(x^2 - y^2)}{\kappa^2 r^4}(2 - \kappa^2 r^2 K_2(\kappa r))\right\}, \quad (4.59)$$

$$\beta_{yz} = -\frac{\Omega}{4\pi(1-\nu)}\left\{(1-2\nu)(\ln r + K_0(\kappa r)) + \frac{x^2}{r^2} - \frac{(x^2 - y^2)}{\kappa^2 r^4}(2 - \kappa^2 r^2 K_2(\kappa r))\right\}. \quad (4.60)$$

Replacing Ωz by b, equations (4.53)–(4.56) are analogous to the elastic distortion of an edge dislocation (see [32]). The components of the elastic distortion (4.57) and (4.58) contain the angle φ in contrast to the dislocation case. But this is a typical property of a disclination.

With equation (2.12) we obtain for the effective Frank vector of the twist disclination

$$\Omega_y(r) = \oint_\gamma (k_{yx}\,\mathrm{d}x + k_{yy}\,\mathrm{d}y) = \Omega\{1 - \kappa r K_1(\kappa r)\}. \quad (4.61)$$

It differs appreciably from the constant value Ω in the region from $r = 0$ up to $r \simeq 6/\kappa$ (see figure 3). In fact, we find $\Omega_y(0) = 0$ and $\Omega_y(\infty) = \Omega$. Thus, this suggests taking $r_c \simeq 6/\kappa$ as the core radius of the disclination. The effective Frank vector $\Omega_y(r)$ of a straight twist disclination has the same form as the effective Frank vector $\Omega_z(r)$ of a straight wedge disclination which is given in [34].

In the case of a twist disclination we obtain the following disclination torsion:

$$\alpha_{xz} = \frac{\Omega\kappa^2}{2\pi} z K_0(\kappa r). \quad (4.62)$$

It looks like a dislocation density of a straight edge dislocation whose 'Burgers vector' Ωz depends on the position z. At the point $z = 0$ the dislocation density (4.62) is zero. The dislocation line of the edge dislocation coincides with the disclination line of the twist disclination. Therefore, this dislocation density implies a dislocation line with changing Burgers vector in agreement with deWit [13]. In the limit $1/\kappa \to 0$, deWit's classical expression $\alpha_{xz} = \Omega z \delta(r)$ is restored. Consequently, we found that the straight twist disclination contains a certain amount of dislocation density (see also [13]).

The elastic distortion gives rise to an effective Burgers vector

$$b_x(r) = \oint_\gamma (\beta_{xx}\,\mathrm{d}x + \beta_{xy}\,\mathrm{d}y) = \Omega z\{1 - \kappa r K_1(\kappa r)\}. \tag{4.63}$$

We see explicitly the changing of the Burgers vector on the dislocation and disclination lines. The effective Burgers vector differs from the constant value Ωz in the region from $r = 0$ to $r \simeq 6/\kappa$. We find $b_x(0) = 0$ and $b_x(\infty) = \Omega z$. In addition, the Burgers vector (4.63) depends on the position of z. At the position $z = 0$ it is zero. From (4.61) and (4.63) we obtain the relation between the effective Burgers and Frank vectors:

$$b_x(r) = z\Omega_y(r). \tag{4.64}$$

We find for the non-vanishing component of the disclination density (2.11) of a twist disclination

$$\Theta_{yz} = \frac{\Omega\kappa^2}{2\pi} K_0(\kappa r). \tag{4.65}$$

In the limit as $\kappa^{-1} \to 0$, the result (4.65) converts to the classical expression $\Theta_{yz} = \Omega\delta(r)$. The disclination density tensor (4.65) and the disclination torsion (4.62) of a twist disclination fulfil the equation (2.16) as follows:

$$\alpha_{xz} = z\Theta_{yz}. \tag{4.66}$$

Since the dislocation density (4.62) and the disclination density (4.65) are localized at the same position it seems that the dislocation density (disclination torsion) is coupled to the twist disclination. It is a characteristic quantity of a twist disclination which cannot be created by a pure edge dislocation without the presence of a twist disclination. In general, the disclination torsion is not independent of the disclination density of a straight twist disclination. Only in the xy-plane at $z = 0$ are the disclination torsion and the Burgers vector of the corresponding twist disclination zero.

If we use the decomposition (2.1) for the distortions (4.53)–(4.58), we may restore an effective displacement field and a properly incompatible distortion. The displacement is given by

$$u_x = \frac{\Omega z}{2\pi}\left\{\varphi(1 - \kappa r K_1(\kappa r)) + \frac{\pi}{2}\,\mathrm{sgn}(y)\kappa r K_1(\kappa r) + \frac{1}{2(1-\nu)}\frac{xy}{r^2}\left(1 - \frac{4}{\kappa^2 r^2} + 2K_2(\kappa r)\right)\right\}, \tag{4.67}$$

$$u_y = -\frac{\Omega z}{4\pi(1-\nu)}\left\{(1-2\nu)(\ln r + K_0(\kappa r)) + \frac{x^2}{r^2} - \frac{(x^2 - y^2)}{\kappa^2 r^4}(2 - \kappa^2 r^2 K_2(\kappa r))\right\}, \tag{4.68}$$

$$u_z = -\frac{\Omega}{2\pi}\left\{x\left[\varphi(1 - \kappa r K_1(\kappa r)) + \frac{\pi}{2}\,\mathrm{sgn}(y)\kappa r K_1(\kappa r)\right] + \frac{y}{2(1-\nu)}\left[(1-2\nu)(\ln r - 1 + K_0(\kappa r)) - \frac{1}{\kappa^2 r^2}(2 - \kappa^2 r^2 K_2(\kappa r))\right]\right\}. \tag{4.69}$$

These displacements (4.67)–(4.69) have no singularities at the disclination line. When $y \to 0$, the Bessel function terms in (4.67) lead to the symmetric smoothing of the displacement profile in contrast to the abrupt jump occurring in the profile of the classical solution (see figure 4(a)). Equations (4.68) and (4.69) demonstrate the elimination of 'classical' logarithmic singularities at the disclination line (see figure 4(b) where a constant term proportional to $\ln\kappa$ is neglected). When $y \to 0$, the Bessel function terms in (4.69)

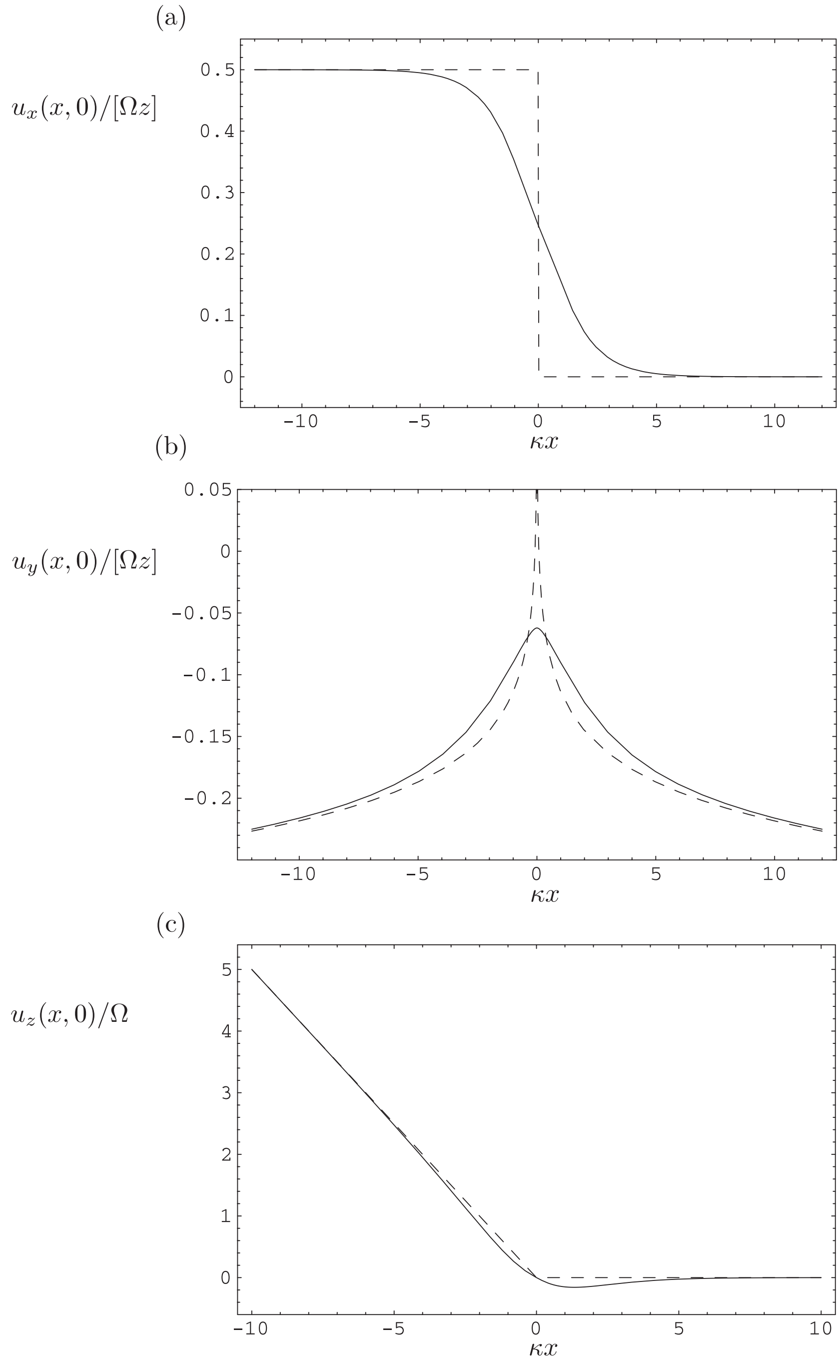


Figure 4. The displacement vector of a twist disclination: (a) $u_x(x, y \to +0)/[\Omega z]$, (b) $u_y(x, 0)/[\Omega z]$ with $\nu = 0.3$, (c) $u_z(x, y \to +0)/\Omega$. The dashed curves represent the classical solution.

smooth the displacement profile in the core region (see figure 4(c)). It is interesting to note that the non-classical parts of the displacements (4.67) and (4.68) caused by the straight twist disclination with the Frank vector $\boldsymbol{\Omega} \equiv (0, \Omega, 0)$ coincide with the non-classical parts of the displacements due to the straight edge dislocation with the Burgers vector $\boldsymbol{b} \equiv (b, 0, 0)$ if we replace Ωz by b (compare with equations (3.47) and (3.52) in [32]). In addition, the displacement (4.69) coincides with the displacement $-u_y$ of a wedge disclination (compare equation (43) for $C = 0$ in [34]). The classical parts of (4.67)–(4.69) agree with the displacement given by deWit [13]. The displacement values should be detectable for nanoparticle containing twist disclinations. Therefore, one could compare the displacements (4.67)–(4.69) with experimental and simulated results. In performing the differentiations of the displacements (4.67)–(4.69) we obtain the total distortion $\beta^T_{ij} \equiv \partial_j u_i$. Using (2.1) and comparing the total distortion with the elastic ones (4.53)–(4.60) the excess terms of the total distortion may be identified with the plastic part. So the incompatible distortion can be found as

$$\tilde{\beta}_{xx} = -\frac{\Omega z}{2\pi}\kappa^2 x K_0(\kappa r)\left(\varphi - \frac{\pi}{2}\,\mathrm{sgn}(y)\right), \tag{4.70}$$

$$\tilde{\beta}_{xy} = -\frac{\Omega z}{2\pi}\left\{\kappa^2 y K_0(\kappa r)\left(\varphi - \frac{\pi}{2}\,\mathrm{sgn}(y)\right) + \pi\delta(y)(1 - \mathrm{sgn}(x)[1 - \kappa r K_1(\kappa r)])\right\}, \tag{4.71}$$

$$\tilde{\beta}_{zx} = \frac{\Omega}{2\pi}\kappa^2 x^2 K_0(\kappa r)\left(\varphi - \frac{\pi}{2}\,\mathrm{sgn}(y)\right), \tag{4.72}$$

$$\tilde{\beta}_{zy} = -\frac{\Omega}{2\pi}\left\{\kappa r K_1(\kappa r) - \kappa^2 x y K_0(\kappa r)\left(\varphi - \frac{\pi}{2}\,\mathrm{sgn}(y)\right) - \pi\delta(y)x(1 - \mathrm{sgn}(x)[1 - \kappa r K_1(\kappa r)])\right\}. \tag{4.73}$$

Equations (4.70)–(4.73) satisfy the relation (2.7). The δ-terms in (4.71) and (4.73) have a similar form to deWit's plastic distortion [13] of a twist disclination $\beta^{\mathrm{P}}_{xy} = (\Omega z/2)\delta(y)(1 - \mathrm{sgn}(x))$ and $\beta^{\mathrm{P}}_{zy} = -(\Omega x/2)\delta(y)(1 - \mathrm{sgn}(x))$. But now the singularity surface is not strictly bounded by the disclination line. The incompatible distortions (4.70) and (4.71) coincide with the incompatible distortion of an edge dislocation if we replace Ωz by b (see [32]) and (4.72) and (4.73) agree with the incompatible distortions $-\tilde{\beta}_{yx}$ and $-\tilde{\beta}_{yy}$ of a wedge disclination (see [34]).

Using (2.15) we obtain for (4.70)–(4.73) the following decomposition:

$$\begin{aligned} \tilde{\beta}_{xx} &= z W_{yx}, \\ \tilde{\beta}_{xy} &= z W_{yy}, \\ \tilde{\beta}_{zx} &= -x W_{yx}, \\ \tilde{\beta}_{zy} &= \phi_{zy} - x W_{yy}, \end{aligned} \tag{4.74}$$

into the translational gauge field

$$\phi_{zy} = -\frac{\Omega}{2\pi}\kappa r K_1(\kappa r) \tag{4.75}$$

and the rotational gauge field

$$W_{yx} \equiv -\varphi^*_{yx}, \qquad W_{yy} \equiv -\varphi^*_{yy}. \tag{4.76}$$

Thus, the negative disclination loop density (4.51) is equivalent to the rotational gauge potential (4.76).

5. Conclusions

The field theory of elastoplasticity has been employed in the consideration of a straight twist disclination in an infinitely extended body. We were able to calculate the elastic and plastic fields. We found that the elastic stress, elastic strain, elastic bend–twist, dislocation density and disclination density are continuous and the displacement, plastic distortion, rotation and the disclination loop density of the twist disclination are discontinuous fields. Exact analytical solutions for all characteristic field quantities of a twist disclination have been reported which demonstrate the elimination of 'classical' singularities at the disclination line. The disclination core appears naturally as a result of the smoothing of the rotation vector profile. In addition, we pointed out and discussed the relation between the twist disclination with Frank vector $\boldsymbol{\Omega} \equiv (0, \Omega, 0)$ and an edge dislocation with Burgers vector $\boldsymbol{b} \equiv (b, 0, 0)$. We were able to calculate the effective Frank and Burgers vectors of the twist disclination. The force stress of a twist disclination calculated in the field theory of elastoplasticity agrees with the stress calculated within the theory of nonlocal elasticity and strain gradient elasticity. The reason is that in all three theories the fundamental equation for the force stress has the form of an inhomogeneous Helmholtz equation (see equation (2.19)). The solutions of a twist disclination considered in this paper could be help in studies of mechanical behaviour of nano-objects including nanotubes and nanomembranes and of disclinated nanoparticles. Last but not least, using the geometric framework of $ISO(3)$ gauge theory of defects we have found the translational and rotational gauge fields of a twist disclination. It turned out that the (negative) disclination loop density is equivalent to the rotational gauge field. In general, the (negative) gauge fields may be considered as the plastic parts in the field theory of elastoplasticity.

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