Riemann-Cartan Geometry of Nonlinear Disclination Mechanics*

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Abstract

In the continuous theory of defects in nonlinear elastic solids, it is known that a distribution of disclinations leads, in general, to a non-trivial residual stress field. To study this problem we consider the particular case of determining the residual stress field of a cylindrically-symmetric distribution of parallel wedge disclinations. We first use the tools of differential geometry to construct a Riemaniann material manifold in which the body is stress-free. This manifold is metric compatible, has zero torsion, but has non-vanishing curvature. The problem then reduces to embed this manifold in Euclidean 3-space following the procedure of a classical nonlinear elastic problem. We show that this embedding can be elegantly accomplished by using Cartan's method of moving frames and compute explicitly the residual stress field for various distributions in the case of a neo-Hookean material.

1 Introduction

Disclinations were introduced by Volterra [1907] more than a century ago. Disclinations are the rotational counterpart of dislocations (translational defects) but are not as well studied. For classical works on disclinations see [Anthony, 2002; de Wit, 1960, 1972, 1973; Eshelby, 1966; Kossecka and de Wit, 1977; Kröner and Anthony, 1975; Kroupa and Lejček, 2002; Kuo and Mura, 1972; Romanov and Vladimirov, 1983; Romanov, 1993] and references therein. See also [Romanov, 2003; Romanov and Kolesnikova, 2009] for recent reviews. Here, we are interested in the continuum mechanics of nonlinear solids with distributed disclinations and the residual stress field generated by distributed disclinations. Most of the existing treatments are linear with the exception of the monograph of Zubov [1997].

In §2 we briefly review some definitions and concepts from differential geometry and, in particular, Cartan's moving frames. In §3 we start with a single wedge disclination in an infinite body and motivated by Volterra's construction, we build a manifold with a singular distribution of Riemann curvature. We then look at the problem of a parallel cylindrically-symmetric distribution of wedge disclinations in §4. Using Cartan's structural equations we obtain an orthonormal coframe field and hence the material metric. Having the material metric we calculate the residual stress field. Conclusions are given in §5.

2 Cartan's Moving Frames and Geometric Elasticity

Throughout this paper, we rely on a comprehensive formulation of anelastic problems [Yavari and Goriely, 2011] using differential geometry. We tersely review the theory before proceeding with the application to disclinations.

Differential Geometry. We first review some facts about affine connections on manifolds and geometry of Riemann-Cartan manifolds. For more details see Nakahara [2003]. Let $\pi: E \to \mathcal{B}$ be a vector bundle over a manifold \mathcal{B} and let $\mathcal{E}(\mathcal{B})$ be the space of smooth sections of E. A connection in E is a map $\nabla: \mathcal{X}(\mathcal{B}) \times \mathcal{E}(\mathcal{B}) \to \mathcal{B}$

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 $\mathcal{E}(\mathcal{B})$ such that $\forall f, f_1, f_2 \in C^{\infty}(\mathcal{B}), \ \forall \ a_1, a_2 \in \mathbb{R}$:

$$i) \quad \nabla_{f_1 \mathbf{X}_1 + f_2 \mathbf{X}_2} \mathbf{Y} = f_1 \nabla_{\mathbf{X}_1} \mathbf{Y} + f_2 \nabla_{\mathbf{X}_2} \mathbf{Y}, \tag{2.1}$$

$$ii) \quad \nabla_{\mathbf{X}}(a_1\mathbf{Y}_1 + a_2\mathbf{Y}_2) = a_1\nabla_{\mathbf{X}}(\mathbf{Y}_1) + a_2\nabla_{\mathbf{X}}(\mathbf{Y}_2), \tag{2.2}$$

$$iii) \quad \nabla_{\mathbf{X}}(f\mathbf{Y}) = f\nabla_{\mathbf{X}}\mathbf{Y} + (\mathbf{X}f)\mathbf{Y}. \tag{2.3}$$

A linear connection on \mathcal{B} is a connection in $T\mathcal{B}$, i.e., $\nabla: \mathcal{X}(\mathcal{B}) \times \mathcal{X}(\mathcal{B}) \to \mathcal{X}(\mathcal{B})$. In a local chart $\{X^A\}$, $\nabla_{\partial_A}\partial_B = \Gamma^C{}_{AB}\partial_C$, where $\Gamma^C{}_{AB}$ are the Christoffel symbols of the connection and $\partial_A = \frac{\partial}{\partial x^A}$ are natural bases for the tangent space corresponding to a coordinate chart $\{x^A\}$. A linear connection is said to be compatible with a metric \mathbf{G} of the manifold if

$$\nabla_{\mathbf{X}} \langle \langle \mathbf{Y}, \mathbf{Z} \rangle \rangle_{\mathbf{G}} = \langle \langle \nabla_{\mathbf{X}} \mathbf{Y}, \mathbf{Z} \rangle \rangle_{\mathbf{G}} + \langle \langle \mathbf{Y}, \nabla_{\mathbf{X}} \mathbf{Z} \rangle \rangle_{\mathbf{G}}, \qquad (2.4)$$

where $\langle \langle .,. \rangle \rangle_{\mathbf{G}}$ is the inner product induced by the metric \mathbf{G} . It can be shown that ∇ is \mathbf{G} -compatible if and only if $\nabla \mathbf{G} = \mathbf{0}$, or in components

$$G_{AB|C} = \frac{\partial G_{AB}}{\partial X^C} - \Gamma^S{}_{CA}G_{SB} - \Gamma^S{}_{CB}G_{AS} = 0.$$
 (2.5)

We consider an *n*-dimensional manifold \mathcal{B} with the metric \mathbf{G} and a \mathbf{G} -compatible connection ∇ . Then $(\mathcal{B}, \mathbf{G}, \nabla)$ is called a Riemann-Cartan manifold [Cartan, 1924, 1955, 2001].

The torsion of a connection is a map $T: \mathcal{X}(\mathcal{B}) \times \mathcal{X}(\mathcal{B}) \to \mathcal{X}(\mathcal{B})$ defined by

$$T(\mathbf{X}, \mathbf{Y}) = \nabla_{\mathbf{X}} \mathbf{Y} - \nabla_{\mathbf{Y}} \mathbf{X} - [\mathbf{X}, \mathbf{Y}]. \tag{2.6}$$

In components in a local chart $\{X^A\}$, $T^A{}_{BC} = \Gamma^A{}_{BC} - \Gamma^A{}_{CB}$. The connection ∇ is symmetric if it is torsion-free, i.e. $\nabla_{\mathbf{X}}\mathbf{Y} - \nabla_{\mathbf{Y}}\mathbf{X} = [\mathbf{X}, \mathbf{Y}]$. It can be shown that on any Riemannian manifold $(\mathcal{B}, \mathbf{G})$ there is a unique linear connection ∇ that is compatible with \mathbf{G} and is torsion-free with the following Christoffel symbols

$$\Gamma^{C}{}_{AB} = \frac{1}{2}G^{CD}\left(\frac{\partial G_{BD}}{\partial X^{A}} + \frac{\partial G_{AD}}{\partial X^{B}} - \frac{\partial G_{AB}}{\partial X^{D}}\right). \tag{2.7}$$

This is called the Levi-Civita connection. In a manifold with a connection, the curvature is a map $\mathcal{R}: \mathcal{X}(\mathcal{B}) \times \mathcal{X}(\mathcal{B}) \to \mathcal{X}(\mathcal{B})$ defined by

$$\mathcal{R}(\mathbf{X}, \mathbf{Y})\mathbf{Z} = \nabla_{\mathbf{X}}\nabla_{\mathbf{Y}}\mathbf{Z} - \nabla_{\mathbf{Y}}\nabla_{\mathbf{X}}\mathbf{Z} - \nabla_{[\mathbf{X}, \mathbf{Y}]}\mathbf{Z},\tag{2.8}$$

or in components

$$\mathcal{R}^{A}{}_{BCD} = \frac{\partial \Gamma^{A}{}_{CD}}{\partial X^{B}} - \frac{\partial \Gamma^{A}{}_{BD}}{\partial X^{C}} + \Gamma^{A}{}_{BM}\Gamma^{M}{}_{CD} - \Gamma^{A}{}_{CM}\Gamma^{M}{}_{BD}. \tag{2.9}$$

Cartan's Moving Frames. We consider a frame field $\{\mathbf{e}_{\alpha}\}_{\alpha=1}^{N}$ that forms, at every point of a manifold \mathcal{B} , a basis for the tangent space. We assume that this frame is orthonormal, i.e. $\langle\!\langle \mathbf{e}_{\alpha}, \mathbf{e}_{\beta} \rangle\!\rangle_{\mathbf{G}} = \delta_{\alpha\beta}$. This is, in general, a non-coordinate basis for the tangent space. Given a coordinate basis $\{\partial_{A}\}$ an arbitrary frame field $\{\mathbf{e}_{\alpha}\}$ is obtained by an $SO(N, \mathbb{R})$ -rotation of $\{\partial_{A}\}$ as $\mathbf{e}_{\alpha} = \mathsf{F}_{\alpha}{}^{A}\partial_{A}$. We know that for the coordinate frame $[\partial_{A}, \partial_{B}] = 0$ but for the non-coordinate frame field we have

$$[\mathbf{e}_{\alpha}, \mathbf{e}_{\alpha}] = -c^{\gamma}{}_{\alpha\beta}\mathbf{e}_{\gamma},\tag{2.10}$$

where $c^{\gamma}{}_{\alpha\beta}$ are components of the object of anhonolomy.

Connection 1-forms are defined as

$$\nabla \mathbf{e}_{\alpha} = \mathbf{e}_{\gamma} \otimes \omega^{\gamma}{}_{\alpha}. \tag{2.11}$$

The corresponding connection coefficients are defined as $\nabla_{\mathbf{e}_{\beta}}\mathbf{e}_{\alpha} = \langle \omega^{\gamma}{}_{\alpha}, \mathbf{e}_{\beta} \rangle \mathbf{e}_{\gamma} = \omega^{\gamma}{}_{\beta\alpha}\mathbf{e}_{\gamma}$. In other words $\omega^{\gamma}{}_{\alpha} = \omega^{\gamma}{}_{\beta\alpha}\vartheta^{\beta}$. Similarly, we have

$$\nabla \vartheta^{\alpha} = -\omega^{\alpha}{}_{\gamma}\vartheta^{\gamma},\tag{2.12}$$

and, $\nabla_{\mathbf{e}_{\beta}} \vartheta^{\alpha} = -\omega^{\alpha}{}_{\beta\gamma} \vartheta^{\gamma}$. In the non-coordinate basis, torsion has the following components

$$T^{\alpha}{}_{\beta\gamma} = \omega^{\alpha}{}_{\beta\gamma} - \omega^{\alpha}{}_{\gamma\beta} + c^{\alpha}{}_{\beta\gamma}. \tag{2.13}$$

Similarly, the curvature tensor has the following components with respect to the frame field

$$\mathcal{R}^{\alpha}{}_{\beta\lambda\mu} = \partial_{\beta}\omega^{\alpha}{}_{\lambda\mu} - \partial_{\lambda}\omega^{\alpha}{}_{\beta\mu} + \omega^{\alpha}{}_{\beta\xi}\omega^{\xi}{}_{\lambda\mu} - \omega^{\alpha}{}_{\lambda\xi}\omega^{\xi}{}_{\beta\mu} + \omega^{\alpha}{}_{\xi\mu}c^{\xi}{}_{\beta\lambda}. \tag{2.14}$$

The metric tensor has the simple representation $\mathbf{G} = \delta_{\alpha\beta} \vartheta^{\alpha} \otimes \vartheta^{\beta}$. Assuming that the connection ∇ is \mathbf{G} -compatible, we obtain the following metric compatibility constraints on the connection 1-forms:

$$\delta_{\alpha\gamma}\omega^{\gamma}{}_{\beta} + \delta_{\beta\gamma}\omega^{\gamma}{}_{\alpha} = 0. \tag{2.15}$$

Torsion and curvature 2-forms are defined as

$$\mathcal{T}^{\alpha} = d\vartheta^{\alpha} + \omega^{\alpha}{}_{\beta} \wedge \vartheta^{\beta}, \tag{2.16}$$

$$\mathcal{R}^{\alpha}{}_{\beta} = d\omega^{\alpha}{}_{\beta} + \omega^{\alpha}{}_{\gamma} \wedge \omega^{\gamma}{}_{\beta}, \tag{2.17}$$

where d is the exterior derivative. These are called Cartan's structural equations. Bianchi identities read:

$$D\mathcal{T}^{\alpha} := d\mathcal{T}^{\alpha} + \omega^{\alpha}{}_{\beta} \wedge \mathcal{T}^{\beta} = \mathcal{R}^{\alpha}{}_{\beta} \wedge \vartheta^{\beta}, \tag{2.18}$$

$$D\mathcal{R}^{\alpha}{}_{\beta} := d\mathcal{R}^{\alpha}{}_{\beta} + \omega^{\alpha}{}_{\gamma} \wedge \mathcal{R}^{\gamma}{}_{\beta} - \omega^{\gamma}{}_{\beta} \wedge \mathcal{R}^{\alpha}{}_{\gamma} = 0, \tag{2.19}$$

where D is the covariant exterior derivative.

Geometric Elasticity. Next we review a few of the basic notions of geometric continuum mechanics. A body \mathcal{B} is identified with a Riemannian manifold \mathcal{B} and a configuration of \mathcal{B} is a mapping $\varphi: \mathcal{B} \to \mathcal{S}$, where \mathcal{S} is another Riemannian manifold. The set of all configurations of \mathcal{B} is denoted by \mathcal{C} . A motion is a curve $c: \mathbb{R} \to \mathcal{C}; t \mapsto \varphi_t$ in \mathcal{C} . It is assumed that the body is stress free in the material manifold. For a fixed t, $\varphi_t(\mathbf{X}) = \varphi(\mathbf{X}, t)$ and for a fixed $\mathbf{X}, \varphi_{\mathbf{X}}(t) = \varphi(\mathbf{X}, t)$, where \mathbf{X} is position of material points in the undeformed configuration \mathcal{B} . The material velocity is the map $\mathbf{V}_t: \mathcal{B} \to T_{\varphi_t(\mathbf{X})} \mathcal{S}$ given by

$$\mathbf{V}_{t}(\mathbf{X}) = \mathbf{V}(\mathbf{X}, t) = \frac{\partial \varphi(\mathbf{X}, t)}{\partial t} = \frac{d}{dt} \varphi_{\mathbf{X}}(t). \tag{2.20}$$

Similarly, the material acceleration is defined by

$$\mathbf{A}_{t}(\mathbf{X}) = \mathbf{A}(\mathbf{X}, t) = \frac{\partial \mathbf{V}(\mathbf{X}, t)}{\partial t} = \frac{d}{dt} \mathbf{V}_{\mathbf{X}}(t). \tag{2.21}$$

In components, $A^a = \frac{\partial V^a}{\partial t} + \gamma^a{}_{bc}V^bV^c$, where γ^a_{bc} is the Christoffel symbol of the local coordinate chart $\{x^a\}$. Note that \mathbf{A} does not depend on the connection coefficients of the material manifold. Here it is assumed that φ_t is invertible and regular. The spatial velocity of a regular motion φ_t is defined as $\mathbf{v}_t : \varphi_t(\mathcal{B}) \to T_{\varphi_t(\mathbf{X})}\mathcal{S}$, $\mathbf{v}_t = \mathbf{V}_t \circ \varphi_t^{-1}$, and the spatial acceleration \mathbf{a}_t is defined as $\mathbf{a} = \dot{\mathbf{v}} = \frac{\partial \mathbf{v}}{\partial t} + \nabla_{\mathbf{v}}\mathbf{v}$. In components $a^a = \frac{\partial v^a}{\partial t} + \frac{\partial v^a}{\partial x^b}v^b + \gamma^a{}_{bc}v^bv^c$. The deformation gradient is the tangent map of φ and is denoted by $\mathbf{F} = T\varphi$. Thus, at each point $\mathbf{X} \in \mathcal{B}$, it is a linear map

$$\mathbf{F}(\mathbf{X}): T_{\mathbf{X}}\mathcal{B} \to T_{\varphi(\mathbf{X})}\mathcal{S}.$$
 (2.22)

If $\{x^a\}$ and $\{X^A\}$ are local coordinate charts on \mathcal{S} and \mathcal{B} , respectively, the components of \mathbf{F} are

$$F^{a}{}_{A}(\mathbf{X}) = \frac{\partial \varphi^{a}}{\partial X^{A}}(\mathbf{X}). \tag{2.23}$$

 $^{^{1}}$ A material manifold is a differentiable manifold \mathcal{B} equipped with the appropriate geometry such that the body is stress free. The appropriate geometry is problem dependent.

The transpose of \mathbf{F} is defined by $\mathbf{F}^{\mathsf{T}}: T_{\mathbf{x}}\mathcal{S} \to T_{\mathbf{X}}\mathcal{B}$, $\langle \langle \mathbf{F}\mathbf{V}, \mathbf{v} \rangle \rangle_{\mathbf{g}} = \langle \langle \mathbf{V}, \mathbf{F}^{\mathsf{T}}\mathbf{v} \rangle \rangle_{\mathbf{G}}$, for all $\mathbf{V} \in T_{\mathbf{X}}\mathcal{B}$, $\mathbf{v} \in T_{\mathbf{x}}\mathcal{S}$. In components $(F^{\mathsf{T}}(\mathbf{X}))^{A}{}_{a} = g_{ab}(\mathbf{x})F^{b}{}_{B}(\mathbf{X})G^{AB}(\mathbf{X})$, where \mathbf{g} and \mathbf{G} are metric tensors on \mathcal{S} and \mathcal{B} , respectively. **F** has the following local representation

$$\mathbf{F} = F^a{}_A \frac{\partial}{\partial x^a} \otimes dX^A. \tag{2.24}$$

The right Cauchy-Green deformation tensor is defined by

$$\mathbf{C}(X): T_{\mathbf{X}}\mathcal{B} \to T_{\mathbf{X}}\mathcal{B}, \quad \mathbf{C}(\mathbf{X}) = \mathbf{F}(\mathbf{X})^{\mathsf{T}}\mathbf{F}(\mathbf{X}).$$
 (2.25)

In components, $C_B^A = (F^{\mathsf{T}})^A{}_a F^a{}_B$. It is straightforward to show that $\mathbf{C}^{\flat} = \varphi^*(\mathbf{g}) = \mathbf{F}^* \mathbf{g} \mathbf{F}$, i.e. $C_{AB} = (g_{ab} \circ \varphi) F^a{}_A F^b{}_B$. The following are the governing equations of nonlinear elasticity in material coordinates [Yavari, et al, 2006]

$$\frac{\partial \rho_0}{\partial t} = 0,$$

$$\text{Div } \mathbf{P} + \rho_0 \mathbf{B} = \rho_0 \mathbf{A},$$
(2.26)

$$Div \mathbf{P} + \rho_0 \mathbf{B} = \rho_0 \mathbf{A}, \tag{2.27}$$

$$\boldsymbol{\tau}^{\mathsf{T}} = \boldsymbol{\tau},\tag{2.28}$$

where **P** is the first Piola-Kirchhoff stress and $\tau = J\sigma$ is the Kirchhoff stress. σ is the Cauchy stress, J = $\sqrt{\det \mathbf{g}/\det \mathbf{G}} \det \mathbf{F}$ is the Jacobian, and $\sigma^{ab} = \frac{1}{I} P^{aA} F^b{}_A$.

Continuum mechanics of solids with distributed disclinations. A body with distributed disclinations has residual stresses, in general. This means that classical nonlinear elasticity based on a stress-free reference configuration cannot be directly used. One idea would be to locally decompose the deformation gradient into elastic and in-elastic parts. This has been the main idea behind almost all the existing treatments of solids with distributed defects. Here, instead we try to geometrically characterize a stress-free reference configuration. In the case of solids with distributed disclinations this stress-free state can be realized as a Riemannian manifold with a non-trivial geometry (see Fig. 2.1). This idea in the case of solids with distributed dislocations goes back to Kondo [Kondo, 1955] and Bilby [Bilby, et al., 1955]. See also Yavari and Goriely [2011] for more details. A similar idea was developed in [Ozakin and Yavari, 2009] for nonlinear thermoelasticity and in [Yavari, 2010] for solids with bulk growth. Here, we use a geometric framework for solids with distributed disclinations. We assume a fixed given distribution of wedge disclinations and calculate the residual stress field induced by disclinations.

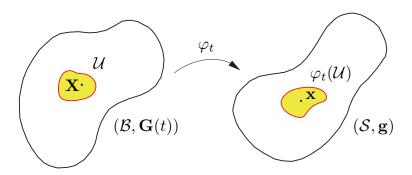


Figure 2.1: Kinematic description of a continuum with distributed disclinations. The material manifold has a dynamic metric $\mathbf{G}(t)$.

A Single Wedge Disclination 3

We start with a single wedge disclination in an infinite elastic solid. We use Volterra's cut-and-weld approach to construct the material manifold. We do this more systematically in the next section using Cartan's method of moving frames. This was done elsewhere for dislocations [Yavari and Goriely, 2011].

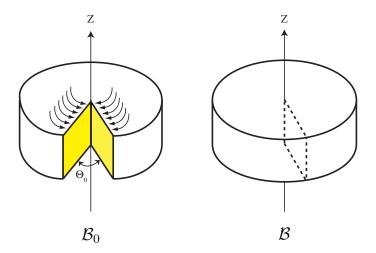


Figure 3.1: Material manifold of a single positive wedge disclination. \mathcal{B} is constructed from \mathcal{B}_0 using Volterra's cut-and-weld operation.

Material manifold. Let us denote the Euclidean 3-space by \mathcal{B}_0 with the flat metric

$$dS^2 = dR_0^2 + R_0^2 d\Phi_0^2 + dZ_0^2, (3.1)$$

in the cylindrical coordinates (R_0, Φ_0, Z_0) . Now cut \mathcal{B}_0 along the half 2-planes $\Phi_0 = 0$ and $\Phi_0 = \Theta_0$ $(0 < \Theta_0 < 2\pi)$. We remove the line R = 0 and the region $0 < \Phi_0 < \Theta_0$ and then identify the two half 2-planes (see Fig. 3.1). We denote the identified manifold by \mathcal{B} . Following Tod [1994] we define the following smooth coordinates on \mathcal{B} :

$$R = R_0, \quad \Phi = \beta(\Phi_0 - \Theta_0), \quad Z = Z_0,$$
 (3.2)

where

$$\beta = \frac{2\pi}{2\pi - \Theta_0} > 1. \tag{3.3}$$

Note that if instead of removing the region $0 < \Phi_0 < \Theta_0$ (positive disclination) we insert it in (negative disclination) we would have a wedge disclination of the opposite sign and in this case

$$\beta = \frac{2\pi}{2\pi + \Theta_0} < 1. \tag{3.4}$$

In constructing \mathcal{B} from \mathcal{B}_0 , the Z-axis is removed. In the new coordinate system the flat metric (3.1) has the following form

$$dS^2 = dR^2 + \frac{R^2}{\beta^2} d\Phi^2 + dZ^2. {(3.5)}$$

Following Yavari and Goriely [2011], we define the following orthonormal coframe field

$$\vartheta^1 = dR, \quad \vartheta^2 = \frac{R}{\beta} d\Phi, \quad \vartheta^3 = dZ.$$
(3.6)

Note that $d\vartheta^1 = d\vartheta^3 = 0$ but $d\vartheta^2 = \frac{1}{\beta}dR \wedge d\Phi = \frac{1}{R}\vartheta^1 \wedge \vartheta^2$. Note also that \mathcal{B} has the following given singular curvature 2-form:

$$\mathcal{R}^{R}{}_{\Phi} = -\Theta_{0}\delta(R)dR \wedge d\Phi = -\frac{\beta\Theta_{0}}{R}\vartheta^{1} \wedge \vartheta^{2}, \tag{3.7}$$

where $\delta^2(R)$ is the 2-dimensional Dirac delta distribution. In the next section we show how to use Cartan's moving frames to systematically construct the material manifold without any need for Volterra's cut-and-weld

process. The material metric for the disclinated body has the following representation

$$\mathbf{G} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{R^2}{\beta^2} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{3.8}$$

Residual stresses. In the absence of external forces we embed the body in the ambient space (S, \mathbf{g}) , which is the flat Euclidean 3-space. We look for solutions of the form $(r, \phi, z) = (r(R), \Phi, Z)$. Note that putting the disclinated body in the appropriate material manifold the anelasticity problem is transformed to an elasticity problem from a material manifold with a non-trivial geometry to the Euclidean ambient space. The deformation gradient is $\mathbf{F} = \mathrm{diag}(r'(R), 1, 1)$ and hence the incompressibility condition reads

$$J = \sqrt{\frac{\det \mathbf{g}}{\det \mathbf{G}}} \det \mathbf{F} = \frac{r'(R)r(R)}{R/\beta} = 1.$$
 (3.9)

Assuming that r(0) = 0 to fix the translation invariance, this tells us that $r = \frac{1}{\sqrt{\beta}}R$ so that

$$\mathbf{F} = \begin{pmatrix} \frac{1}{\sqrt{\beta}} & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1 \end{pmatrix}. \tag{3.10}$$

For a neo-Hookean material we have [Marsden and Hughes, 1983]

$$P^{aA} = \mu F^{a}{}_{B}G^{AB} - p \left(F^{-1}\right)_{b}{}^{A}g^{ab}, \tag{3.11}$$

where p = p(R) is the unknown pressure field. The non-zero stress components read

$$P^{rR} = \frac{\mu}{\sqrt{\beta}} - \sqrt{\beta} \ p(R), \quad P^{\phi\Phi} = \frac{\mu \beta^2}{R^2} - \frac{\beta}{R^2} p(R), \quad P^{zZ} = \mu - p(R). \tag{3.12}$$

The corresponding Cauchy stresses are

$$\sigma^{rr} = \frac{\mu}{\beta} - p(R), \quad \sigma^{\phi\phi} = \frac{\mu\beta^2}{R^2} - \frac{\beta}{R^2}p(R), \quad \sigma^{zZ} = \mu - p(R).$$
 (3.13)

The only no-trivial equilibrium equation is $P^{rA}{}_{|A}=0$, which reads (note that $\Gamma^{R}{}_{\Phi\Phi}=-R/\beta^2,\ \Gamma^{\Phi}{}_{R\Phi}=1/R$)

$$\frac{\partial P^{rR}}{\partial R} + \frac{1}{R}P^{rR} - \frac{R}{\sqrt{\beta}}P^{\phi\Phi} = 0. \tag{3.14}$$

Thus

$$\frac{dp(R)}{dR} = \mu \left(\frac{1}{\beta} - \beta\right) \frac{1}{R}.$$
(3.15)

If we consider a finite cylinder with outer radius R_o and zero traction at $R = R_o$, we have

$$p(R) = \frac{\mu}{\beta} - \mu \left(\beta - \frac{1}{\beta}\right) \ln \frac{R}{R_o}.$$
 (3.16)

The nonzero first Piola-Kirchhoff stress components read

$$P^{rR} = \mu \sqrt{\beta} \left(\beta - \frac{1}{\beta}\right) \ln \frac{R}{R_o}, \ P^{\phi\Phi} = \frac{\mu(\beta^2 - 1)}{R^2} \left(1 + \ln \frac{R}{R_o}\right), \ P^{zZ} = \mu \left(1 - \frac{1}{\beta}\right) + \mu \left(\beta - \frac{1}{\beta}\right) \ln \frac{R}{R_o}. \ (3.17)$$

Similarly, the Cauchy stresses (expressed as functions of R) read

$$\sigma^{rr} = \mu \left(\beta - \frac{1}{\beta} \right) \ln \frac{R}{R_o}, \quad \sigma^{\phi\phi} = \frac{\mu(\beta^2 - 1)}{R^2} \left(1 + \ln \frac{R}{R_o} \right), \quad \sigma^{zz} = \mu \left(1 - \frac{1}{\beta} \right) + \mu \left(\beta - \frac{1}{\beta} \right) \ln \frac{R}{R_o}. \quad (3.18)$$

Remark 3.1. Note that in curvilinear coordinates, the components of a tensor may not have the same physical dimensions. The stress components shown above are not the so-called *physical components* of Cauchy stress. The following relation holds between the Cauchy stress components (unbarred) and its physical components (barred) [Truesdell, 1953]

$$\bar{\sigma}^{ab} = \sigma^{ab} \sqrt{g_{aa}g_{bb}}$$
 no summation on a or b . (3.19)

Note that the spatial metric in cylindrical coordinates has the form $diag(1, r^2, 1)$. This means that for the nonzero Cauchy stress components we have

$$\bar{\sigma}^{rr} = \sigma^{rr}, \quad \bar{\sigma}^{\phi\phi} = r^2 \sigma^{\phi\phi} = \frac{R^2}{\beta} \sigma^{\phi\phi} = \mu \left(\beta - \frac{1}{\beta} \right) \left(\ln \frac{R}{R_0} + 1 \right), \quad \bar{\sigma}^{zz} = \sigma^{zz}. \tag{3.20}$$

Remark 3.2. When $\Theta_0 \ll 1$, we have

$$\bar{\sigma}^{rr} = \frac{\mu\Theta_0}{\pi} \ln \frac{R}{R_o}, \quad \bar{\sigma}^{\phi\phi} = \frac{\mu\Theta_0}{\pi} \left(\ln \frac{R}{R_o} + 1 \right), \quad \bar{\sigma}^{zz} = \frac{\mu\Theta_0}{\pi} \left(\ln \frac{R}{R_o} + \frac{1}{2} \right). \tag{3.21}$$

These are identical to the classical solutions using linearized elasticity [Eshelby, 1966; de Wit, 1972] when $\nu = \frac{1}{2}$.

4 A Parallel Cylindrically-Symmetric Distribution of Wedge Disclinations

Given a torsion 2-form one can integrate it over an infinitesimal 2-manifold. Given a dislocation distribution with a known dislocation density tensor we know the torsion tensor. Therefore, we can compute the torsion 2-form. Knowing that the material connection is flat and metric compatible we can find the connection coefficients [Yavari and Goriely, 2011]. In the case of disclinations the material connection is torsion-free but has a non-vanishing curvature. Again, knowing that the material connection is metric compatible one can calculate the connection 1-forms given a distributed disclination. We show this in the following example.

Motivated by the first example, let us consider a cylindrically-symmetric distribution of wedge disclinations parallel to the Z-axis in the cylindrical coordinate system (R, Φ, Z) . We use the following ansatz for the coframe field

$$\vartheta^1 = dR, \quad \vartheta^2 = f(R)d\Phi, \quad \vartheta^3 = dZ,$$
 (4.1)

for some unknown function f to be determined. Assuming metric compatibility the unknown connection 1-forms are: $\omega^1_2, \omega^2_3, \omega^3_1$, i.e. the matrix of connection 1-forms has the following form

$$\boldsymbol{\omega} = [\omega^{\alpha}{}_{\beta}] = \begin{pmatrix} 0 & \omega^{1}{}_{2} & -\omega^{3}{}_{1} \\ -\omega^{1}{}_{2} & 0 & \omega^{2}{}_{3} \\ \omega^{3}{}_{1} & -\omega^{2}{}_{3} & 0 \end{pmatrix}. \tag{4.2}$$

For our disclinated body the material manifold is torsion-free and hence

$$\mathcal{T}^1 = \mathcal{T}^2 = \mathcal{T}^3 = 0. \tag{4.3}$$

Note that

$$d\vartheta^{1} = 0, \quad d\vartheta^{2} = f'(R)dR \wedge d\Phi = \frac{f'(R)}{f(R)}\vartheta^{1} \wedge \vartheta^{2}, \quad d\vartheta^{3} = 0.$$
 (4.4)

²A similar problem was considered in [Derezin and Zubov, 2011] but in 2D.

By using Cartan's first structural equations: $\mathcal{T}^{\alpha} = d\vartheta^{\alpha} + \omega^{\alpha}{}_{\beta} \wedge \vartheta^{\beta}$, for $\alpha = 1, 2, 3$ we obtain

$$\omega^{1}_{12} = \omega^{3}_{11} = 0, \quad \omega^{3}_{21} + \omega^{1}_{32} = 0,$$
 (4.5)

$$\omega^{1}_{22} = -\frac{f'(R)}{f(R)}, \quad \omega^{2}_{231} = 0, \quad \omega^{1}_{32} + \omega^{2}_{13} = 0,$$
 (4.6)

$$\omega^3_{31} = \omega^2_{33} = 0, \quad \omega^3_{21} + \omega^2_{13} = 0.$$
 (4.7)

Therefore, the only nonzero connection coefficient is ω^{1}_{22} . Hence, the connection 1-forms read

$$\omega^{1}_{2} = -\frac{f'(R)}{f(R)}\vartheta^{2}, \quad \omega^{2}_{3} = \omega^{3}_{1} = 0.$$
 (4.8)

In turn, this implies

$$d\omega^{1}_{2} = -\frac{f''(R)}{f(R)}\vartheta^{1} \wedge \vartheta^{2}, \quad d\omega^{2}_{3} = d\omega^{3}_{1} = 0.$$
(4.9)

We know that for the cylindrically symmetric disclination distribution the curvature 2-forms have the following forms:

$$\mathcal{R}^{1}{}_{2} = \frac{w(R)}{2\pi} dR \wedge R d\Phi = \frac{Rw(R)}{2\pi f(R)} \vartheta^{1} \wedge \vartheta^{2}, \quad \mathcal{R}^{2}{}_{3} = \mathcal{R}^{3}{}_{1} = 0, \tag{4.10}$$

where w(R) is the radial density of the wedge disclinations. The second Cartan's structural equations: $\mathcal{R}^{\alpha}{}_{\beta} = d\omega^{\alpha}{}_{\beta} + \omega^{\alpha}{}_{\gamma} \wedge \omega^{\gamma}{}_{\beta}$ give

$$\mathcal{R}^{2}_{3} = d\omega^{2}_{3} + \omega^{1}_{2} \wedge \omega^{3}_{1} = 0, \tag{4.11}$$

$$\mathcal{R}^{3}_{1} = d\omega^{3}_{1} + \omega^{2}_{3} \wedge \omega^{1}_{2} = 0, \tag{4.12}$$

$$\mathcal{R}^{1}{}_{2} = d\omega^{1}{}_{2} + \omega^{3}{}_{1} \wedge \omega^{2}{}_{3} = -\frac{f''(R)}{f(R)} \vartheta^{1} \wedge \vartheta^{2}. \tag{4.13}$$

Comparing $(4.10)_1$ and (4.13) we see that

$$f''(R) = -\frac{R}{2\pi}w(R). \tag{4.14}$$

Calculation of residual stresses. The material metric has the following form:

$$\mathbf{G} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & f^2(R) & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{4.15}$$

Note that det $\mathbf{G} = 1$. From the material manifold, we obtain the residual stress field by embedding it into the ambient space, which is assumed to be the Euclidean 3-space. We look for solutions of the form $(r, \phi, z) = (r(R), \Phi, Z)$, and hence det $\mathbf{F} = r'(R)$. Assuming an incompressible neo-Hookean material, incompressibility dictates

$$J = \sqrt{\frac{\det \mathbf{g}}{\det \mathbf{G}}} \det \mathbf{F} = \frac{r}{f(R)} r'(R) = 1.$$
 (4.16)

Assuming that r(0) = 0, we have

$$r(R) = \left(2\int_0^R f(\xi)d\xi\right)^{\frac{1}{2}},\tag{4.17}$$

with the condition $\int_0^R f(\xi)d\xi > 0$.

For a neo-Hookean material we have $P^{aA} = \mu F^a{}_B G^{AB} - p \left(F^{-1}\right)_b{}^A g^{ab}$, where p = p(R) is the pressure

field. The first Piola-Kirchhoff stress tensor reads

$$\mathbf{P} = \begin{pmatrix} \mu r'(R) - \frac{p(R)}{r'(R)} & 0 & 0 \\ 0 & \frac{\mu}{f^{2}(R)} - \frac{p(R)}{r(R)^{2}} & 0 \\ 0 & 0 & \mu - p \end{pmatrix}$$

$$= \begin{pmatrix} \mu \frac{f(R)}{r(R)} - p(R) \frac{r(R)}{f(R)} & 0 & 0 \\ 0 & \frac{\mu}{f^{2}(R)} - \frac{p(R)}{r(R)^{2}} & 0 \\ 0 & 0 & \mu - p \end{pmatrix}. \tag{4.18}$$

Similarly, the Cauchy stress reads

$$\boldsymbol{\sigma} = \begin{pmatrix} \mu \frac{f^2(R)}{r^2(R)} - p(R) & 0 & 0\\ 0 & \frac{\mu}{f^2(R)} - \frac{p(R)}{r^2(R)} & 0\\ 0 & 0 & \mu - p \end{pmatrix}.$$
 (4.19)

The only non-trivial equilibrium equation is $\sigma^{ra}_{|a} = \sigma^{rr}_{,r} + \frac{1}{r}\sigma^{rr} - r\sigma^{\phi\phi} = 0$. This gives us the following differential equation for p(R):

$$p'(R) = \mu \left(2r'r'' + \frac{r'^3}{r} - \frac{rr'}{f^2} \right). \tag{4.20}$$

Knowing that r' = f/r, this differential equation is simplified to read

$$p'(R) = \mu \left[\frac{f(R)f'(R)}{\int_0^R f(\xi)d\xi} - \frac{f^3(R)}{4\left(\int_0^R f(\xi)d\xi\right)^2} - \frac{1}{f(R)} \right]. \tag{4.21}$$

We know that traction vanishes on the outer boundary $(R = R_o)$, and hence

$$p_o = \mu \frac{f^2(R_o)}{r^2(R_o)}. (4.22)$$

Therefore

$$p(R) = \mu \frac{f^2(R_o)}{r^2(R_o)} - \mu \int_R^{R_o} \left[\frac{f(\eta)f'(\eta)}{\int_0^{\eta} f(\xi)d\xi} - \frac{f^3(\eta)}{4\left(\int_0^{\eta} f(\xi)d\xi\right)^2} - \frac{1}{f(\eta)} \right] d\eta.$$
 (4.23)

Example 4.1. Let us look at a single wedge disclination for which $\omega(R) = 2\pi\Theta_0\delta^2(R)$. Thus, $f''(R) = -\frac{\Theta_0}{2\pi}\delta(R)$. Hence

$$f(R) = -\frac{\Theta_0}{2\pi}RH(R) + C_1R + C_2. \tag{4.24}$$

We know that when $\Theta_0 = 0$, f(R) = R and thus $C_1 = 1$, $C_2 = 0$. Therefore, because R > 0, we have

$$f(R) = R\left(1 - \frac{\Theta_0}{2\pi}\right)R = \frac{R}{\beta}.$$
 (4.25)

This is exactly what we obtained earlier using Volterra's cut-and-weld construction. See Eq. (3.6). Fig. 4.1 shows σ^{rr} distribution for both positive and negative single wedge disclinations.

Example 4.2. Uniform disclination distribution $\omega(R) = \omega_0$. In this case

$$f(R) = R - \frac{\omega_0}{12\pi} R^3. \tag{4.26}$$

Thus

$$r(R) = R\sqrt{1 - \frac{\omega_0}{24\pi}R^2},\tag{4.27}$$

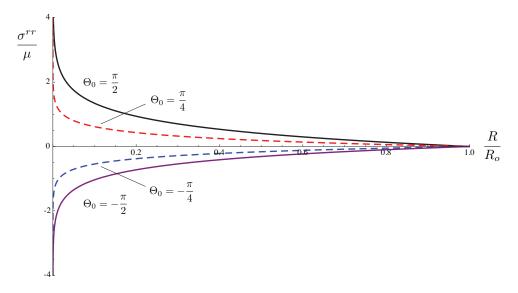


Figure 4.1: σ^{rr} distributions for positive and negative single wedge disclinations.

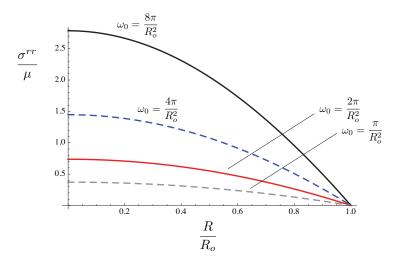


Figure 4.2: σ^{rr} distributions for different values of ω_0 (uniform disclination distribution).

provided that $\omega_0 < 24\pi/R_0^2$. Fig. 4.2 shows σ^{rr} distribution for different values of ω_0 .

Example 4.3. In this example $\omega(R) = \frac{\omega_0 R_0}{\pi R} \sin \frac{\pi R}{R_0}$ ($\omega_0 > 0$). Therefore

$$f(R) = R + \frac{\omega_0 R_0^3}{2\pi^4} \sin \frac{\pi R}{R_0}.$$
 (4.28)

Thus

$$r(R) = R \left[1 + \frac{2\omega_0}{\pi^5} \frac{R_0^4}{R^2} \sin^2 \left(\frac{\pi R}{2R_0} \right) \right]^{\frac{1}{2}}.$$
 (4.29)

Fig. 4.3 shows σ^{rr} distribution for different values of ω_0 .

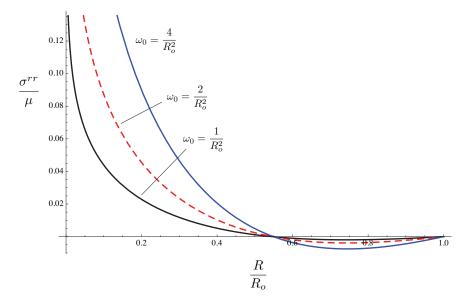


Figure 4.3: σ^{rr} distributions for the disclination distribution $\omega(R) = \frac{\omega_0 R_0}{\pi R} \sin \frac{\pi R}{R_0}$ for different values of ω_0 .

5 Concluding Remarks

The material manifold of a distributed disclination – where the body is stress free – is a Riemannian manifold whose curvature tensor is identified with the disclination density tensor. We started with a single wedge disclination in an infinite body and using Volterra's cut-and-weld process we constructed its material manifold. From the material manifold, calculating the stress field of the disclination amounts to a classical nonlinear elasticity problem; one simply needs to find an embedding into the Euclidean 3-space. We calculated the stress field of the single wedge disclination in an incompressible neo-Hookean solid. For small wedge angles our solution is reduced to the classical linear elasticity solution (when $\nu = \frac{1}{2}$). We then considered a distribution of cylindrically symmetric parallel wedge disclinations. Using Cartan's methods of moving frames we constructed its material manifold. For an incompressible neo-Hookean material we calculated the corresponding residual stress field.

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References

Anthony, K. H. [2002], Crystal disclinations versus continuum theory, Solid State Phenomena 87:15-46.

Bilby, B. A., R., Bullough, and E., Smith [1955], Continuous distributions of dislocations: a new application of the methods of non-Riemannian geometry, *Proceedings of the Royal Society of London* **A231**(1185): 263-273.

Cartan, E. [1924], Sur les variétés a connexion affine et la théorie de la relativité généralisée (première partie suite). Annales Scientifiques de l'Ecole Normale Supérieure 41:1-25.

Cartan, E. [1995], On Manifolds with an Affine Connection and the Theory of General Relativity. Bibliopolis, Napoli.

Cartan, E. [2001], Riemannian Geometry in an Orthogonal Frame. World Scientific, New Jersey.

- Derezin, S. V. and Zubov, L. M. [2011], Disclinations in Nonlinear Elasticity. ZAMM 91(6):433-442.
- de Wit, R. [1960], The continuum theory of stationary disclinations, Solid State Physics-Advances in Research and Applications 10: 249-292.
- de Wit, R. [1972], Partial disclinations, Journal of Physics C: Solid State Physics 5(5): 529-534.
- de Wit, R. [1972], Theory of disclinations: IV. Straight disclinations, Journal of Research of the National Bureau of Standards Section a-Physics and Chemistry A 77(5): 607-658.
- Eshelby, J. D. [1966], A simple derivation of elastic field of an edge dislocation, *British Journal of Applied Physics* **17**(9): 1131-1135.
- Hehl, F. W. and Y. N. Obukhov [1983], Foundations of Classical Electrodynamics Charge, Flux, and Metric, Birkhäuser, Boston.
- Kondo, K. [1955], Non-Riemannien geometry of imperfect crystals from a macroscopic viewpoint, Memoirs of the Unifying Study of the Basic Problems in Engineering Science by Means of Geometry, (K. Kondo, ed.), vol. 1, Division D-I, Gakujutsu Bunken Fukyo-Kai, 1955, pp. 6-17
- Kossecka, E. and R. Dewit [1977], Disclination kinematics, Archives of Mechanics 29(5): 633-651.
- Kröner, E. and Anthony, K. H. [1975], Dislocations and disclinations in material structures Basic topological concepts. *Annual Review of Materials Science* **5**:43-72.
- Kroupa, F. and Lejček, L. [2002], Development of the disclination concept. Solid State Phenomena 87:1-14.
- Kuo, H. H. and Mura, T. [1972], Elastic field and strain energy of a circular wedge disclination. *Journal of Applied Physics* 43(4):1454-1457.
- Marsden, J.E. and T.J.R. Hughes [1983], Mathematical Foundations of Elasticity, Dover, New York.
- Nakahara, M. [2003], Geometry, Topology and Physics, Taylor & Francis, New York.
- Ozakin, A. and A. Yavari [2009], A geometric theory of thermal stresses, *Journal of Mathematical Physics* **51**, 032902, 2010.
- Romanov, A. E. and Vladimirov, V. I. [1983], Disclinations in solids. *Physica Status Solidi A-Applied Research* **78**(1):11-34.
- Romanov, A. E. [1993], Screened disclinations in solids. *Materials Science and Engineering A-Structural Materials Properties Microstructure and Processing* **164**(1-2):58-68.
- Romanov, A. E. [2003], Mechanics and physics of disclinations in solids. *European Journal of Mechanics A-Solids* **22**(5):727-741.
- Romanov, A. E. and Kolesnikova, A. L. [2009], Application of disclination concept to solid structures. *Progress in Materials Science* **54**(6):740-769.
- Tod, K. P. [1994], Conical singularities and torsion. Classical and Quantum Gravity 11:1331-1339.
- Truesdell, C. [1953], The physical components of vectors and tensors, ZAMM 33: 345-356.
- Volterra, V. [1907], Sur l'équilibre des corps élastiques multiplement connexes. Annales Scientifiques de l'Ecole Normale Supérieure, Paris 24(3):401-518.
- Yavari, A., J. E. Marsden and M. Ortiz [2006], On the spatial and material covariant balance laws in elasticity, *Journal of Mathematical Physics* 47: 042903; 85 112.
- Yavari, A. [2010] A geometric theory of growth mechanics. Journal of Nonlinear Science 20(6):781-830.
- Yavari, A. and A. Goriely [2011] Riemann-Cartan geometry of nonlinear dislocation mechanics, under review.
- Zubov, L.M. [1997], Nonlinear Theory of Dislocations and Disclinations in Elastic Bodies, Springer, Berlin.