4.1 Introduction

As we estimate the fracture parameter for a cracked body in quantitative fracture mechanics therefore, modeling of fracture and failure is an important and challenging task. In last chapter we have discussed the basics of large deformation formulation based on conventional as well as convected coordinates approach. Now in this chapter we will discuss the constitutive modeling used in the present research work for plastically compressible rate dependent solids. While modeling the behavior of VACNTs, the complex and hierarchical nature of it makes the choice of scale non-trivial. They appear as arrays of vertically aligned tubes at magnifications of 1000x, markedly anisotropic. While it is magnified 100 times more it reveals a highly interconnected foam like structure and the network of CNTs starts to appear almost isotropic. After magnifying another 100 times, one finds a view of the individual CNTs themselves. The present work makes use of a model which smooths over the discrete nature of the individual CNTs and also approximates the overall material behavior through an isotropic continuum constitutive relation (Deshpande and Fleck, 2000). Here the focus is on the scale at which the material appears to be a nominally aligned array of tubes (Cao et al., 2005; Pathak et al., 2009; Zbib et al., 2008). Thus, the rich deformation and stress-strain behavior of VACNTs which was observed by Hutchens et. al. (2012) serves as inspiration as well as validation for the choice of constitutive relation.

In order to analyze the deformation of any body under prescribed surface tractions, body forces and boundary conditions using the incremental virtual work equations, the Kirchhoff stress tensor within the body must be related to Lagrangian strain tensor. Without such a constitutive relationship an analysis cannot proceed since there would be then an infinite number of possible solutions for the deformation of the body.

4.2 Constitutive Relations

The material model employed in the present work is same as that given in Hutchens et. al. (2011), Needleman et. al. (2012), Mohan et. al. (2013), Khan et. al. (2017) with the use of normality and non-normality flow rule. However, for completeness, here a recapitulation of the material model is provided. Any constitutive model can be properly framed in terms of field quantities corresponding to the deformed state of the material, such as the Cauchy stress tensor σ and the rate of deformation tensor D. The rate of deformation tensor, D is symmetric part of $\dot{\mathbf{F}} \cdot \mathbf{F}^{-1}$, where \mathbf{F} is the deformation gradient and the Kirchhoff stress $\tau = J\sigma$, where $J = \det(\mathbf{F})$. A superposed dot denotes the partial derivative with respect to time.

The rate of deformation tensor is taken to be the sum of elastic $(D^{ij})^e$ and plastic $(D^{ij})^p$ parts.

$$D^{ij} = \left(D^{ij}\right)^e + \left(D^{ij}\right)^p \tag{4.1}$$

Elastic strains are assumed to be small and the elastic part of the response is taken to be governed by the hypo-elastic law

$$\left(D^{ij}\right)^e = \frac{1+\nu}{E}\hat{\tau}^{ij} - \frac{\nu}{E}\operatorname{tr}\left(\hat{\tau}^{ij}\right)\bar{g}^{ij} \tag{4.2}$$

Where $\hat{\tau}^{ij}$ is the Jaumann rate of Kirchhoff stress, *E* is Young's modulus, *v* is Poisson's ratio, tr (.) denotes the trace and \bar{g}^{ij} is the metric tensor in current configuration.

The plastic part of the rate of deformation tensor is taken to be specified through the viscoplastic constitutive equation

$$\left(D^{ij}\right)^p = \frac{3}{2} \frac{\dot{\epsilon}_{\rm p}}{\sigma_{\rm e}} p^{ij} \tag{4.3}$$

Where, $\dot{\epsilon}_p$ is plastic strain rate, σ_e is effective equivalent stress corresponding to the instantaneous $\dot{\epsilon}_p$ and p^{ij} is deviatoric part of Kirchhoff stress tensor. This deviatoric part of Kirchhoff stress p^{ij} is given by

$$p^{ij} = \tau^{ij} - \beta_{\rm p} {\rm tr} \left(\tau^{ij}\right) \bar{g}^{\rm ij} \tag{4.4}$$

In the numerical example a viscoplastic strain rate relation of the following form is employed

$$\dot{\epsilon}_{\rm p} = \dot{\epsilon}_0 \left(\frac{\sigma_{\rm e}}{\rm g}\right)^{1/m} \tag{4.5}$$

Here $\dot{\epsilon}_0$ is a reference strain rate, *m* is the rate hardening exponent and the function $g(\epsilon_P)$ are of various types but here in Eq. (4.5) we are using as shown in Eq. (4.6) is taken to be a trilinear hardening relation of the form

$$g(\epsilon_{p}) = \sigma_{0} \begin{cases} 1 + h_{1}\epsilon_{p}, & \epsilon_{p} < \epsilon_{1} \\ 1 + h_{1}\epsilon_{1} + h_{2}(\epsilon_{p} - \epsilon_{1}), & \epsilon_{1} < \epsilon_{p} < \epsilon_{2} \\ 1 + h_{1}\epsilon_{1} + h_{2}(\epsilon_{2} - \epsilon_{1}) + h_{3}(\epsilon_{p} - \epsilon_{2}), & \epsilon_{p} > \epsilon_{2} \end{cases}$$

$$(4.6)$$

Where, σ_0 is a reference stress. The effective stress, σ_e is defined by

$$\sigma_{\rm e}^2 = \frac{3}{2} \tau^{ij} q^{ij} = \frac{3}{2} \left[\tau^{ij} \tau^{ij} - \alpha_{\rm p} \left({\rm tr} \left(\tau^{ij} \right) \right)^2 \right] \tag{4.7}$$

With

$$q^{ij} = \tau^{ij} - \alpha_{\rm p} {\rm tr}(\tau^{ij}) \bar{g}^{\rm ij} \tag{4.8}$$

Here q^{ij} is introduced to induce plastic non-normality. For $\alpha_p = \beta_p$ the plastic constitutive relation satisfies plastic normality and when $\alpha_p \neq \beta_p$ the constitutive relation is said to show evidence of plastic non-normality. For $\alpha_p = \beta_p = 1/3$ it further reduces to the well known von-Mises isotropic hardening solid. As per the laws of thermodynamics, it is made sure that the dissipation is positive. For this purpose, the dissipation rate calculation was checked as follows:

$$\tau^{ij} \left(D^{ij} \right)^p = \sigma_{\rm e} \dot{\epsilon}_{\rm p} \left[1 + \frac{3}{2} \left(\alpha_{\rm p} - \beta_{\rm p} \right) \left(\frac{\operatorname{tr}(\tau^{ij})}{\sigma_{\rm e}} \right)^2 \right]$$
(4.9)

So the above equation dictates that the plastic dissipation is always non-negative for $\alpha_p \ge \beta_p$ and when $\alpha_p = \beta_p = 1/3$ the constitutive relation reduces to that of an isotropic hardening viscoplastic Mises solid.

Constitutive relations exhibiting plastic non-normality are widely used to model frictional, dilatant solids. For instance, in soil mechanics, this non-normality condition has been commonly utilized in modeling and shown to account for the frictional dissipations. In recent times, the role of non normality in localized deformation is illustrated by a number of researchers (Drucker and Prager, 1952; Rice, 1977; Needleman, 1979; Leroy and Ortiz, M., 1989). The term in eq. (4.7) is non-negative for $\alpha_p \leq 1/3$ with $\alpha_p = 1/3$ corresponding to a plastically incompressible Mises Solid.



Figure 4.1: The typical definition of the hardening-softening-hardening flow stress function with the transition strains denoted by ϵ_1 and ϵ_2 and the slope of the three piece wise linear functions given by h_1 , h_2 and h_3 , respectively

The function of flow stress would be better envisaged as the material's relative yield strength as a function of plastic strain, Fig. 4.1. It permits for tailoring the material hardening/softening characterization over the range of plastic strain as a hardening back stress. The value of ϵ_1 specifies the plastic strain at which the transition from hardening to softening takes place while the ϵ_2 value indicates the strain at which the transition back to hardening occurs. In this thesis work, a wider range of possibilities is explored including, for example, cases where h_2 is positive and other cases where $h_2 = h_3$, in which case the value of ϵ_2 is irrelevant.

The work conjugate effective stress, σ_e , defined in equation (4.7), has both hydroststic as well as shear contributions. To show these explicitly, σ_e^2 in equation (4.7) can be rewritten as

$$\sigma_{\rm e}^2 = \sigma_{\rm M}^2 + 9\left(\frac{1-3\alpha_{\rm p}}{2}\right)\sigma_{\rm h}^2 = \sigma_{\rm M}^2 + \sigma_{\rm DF}^2\sigma_{\rm h}^2 \tag{4.10}$$

where

$$\sigma_{\rm M}^2 = \frac{3}{2} (\tau^{ij})' (\tau^{ij})', \qquad \sigma_{\rm h} = \frac{1}{3} {\rm tr} (\tau^{ij}) \qquad (4.11)$$

with

$$\left(\tau^{ij}\right)' = \tau^{ij} - \sigma_h \bar{g}^{ij} \tag{4.12}$$

The connection with the Deshpande-Fleck constitutive relation parameter α_{DF} (Deshpande and Fleck, 2000) is through the relation (Needleman et al., 2015)

$$\alpha_{\rm DF} = \sqrt{9\left(\frac{1-3\alpha_{\rm p}}{2}\right)} \tag{4.13}$$

Now it is also worth noting that the plastic dissipation in equation (4.9) can also be written as

$$\tau^{ij} \left(D^{ij} \right)^p = \frac{\dot{\epsilon}_{\rm p}}{\sigma_{\rm e}} \left[\sigma_{\rm M}^2 + 9 \left(\frac{1 - 3\alpha_{\rm p}}{2} \right) \sigma_{\rm h}^2 \right] \tag{4.14}$$

4.3 Concluding Remarks

In this chapter the constitutive equations of isotropic, plastically compressible rate dependent elastic-viscoplastic solids with hardening-hardening and hardening-softening-hardening form of flow strength as a function of plastic strain have been presented in classical form. Constitutive equations have been made available for both normality and normality flow rules. The constitutive equations developed in this chapter are implemented into finite element based program to examine various performance characteristics in chapter 5.