1.1 Background

The structural failure may occur due to pre-existing flaws/ defects or through nucleation of crack and its subsequent growth to the defect free regions with catastrophic consequences to human life, normally involving large scale financial loss. The strength of structures is reduced by the presence of defects or cracks under normal operating conditions. It is therefore necessary to characterize the remaining strength of material in the presence of cracks or crack like defects. Over the years, the improvement of methodology and criteria for correct failure prediction has been the key focus of research to the material engineers and scientists. With a view to characterize the material resistance to crack growth it is essential to describe the mechanical state of a deforming cracked body. The field of fracture mechanics is generally concerned with such description of the mechanical state and it is based on the energetic concepts correlated to crack extension. Therefore, fracture mechanics is a relatively new branch in solid mechanics where the behavior of solid system containing one or more cracks is dealt. Traditionally, the description of the mechanical state of a particular system needs the solution of complex partial differential governing equations of an idealized geometrical configuration of the deforming body with cracks.

Considerable attention, in recent years, has been devoted to computer-based simulation and modeling of various fracture phenomena since computer based analyses are often able to generate results within a short time compared to that required in real life experiments. In continuum mechanics based fracture analyses, the Finite Element Method (FEM) and the Boundary Element Method (BEM) are the two most popular numerical techniques. However, the FEM is very suitable for practical engineering problems with complex geometries compared to BEM (Becker, 1992).

In practical situation the three-dimensional (3-D) structures are generally encountered and for any practical purpose their analyses are of utmost importance. Two-dimensional (2-D) cases are generally idealization of 3-D problems to simplify the mathematical complexities or to reduce computational efforts. When 2-D modeling of the cracked geometry is not possible or does not provide adequate computational accuracy, the 3-D analyses have to be carried out.

Ductile behavior results in metal failure due to significant or large amount of plastic deformation, whereas brittle behavior results in metal failure with little or no associated plastic deformation. In the former case, fracture occurs due to gradual crack extension, while in the latter case, fractures occur due to rapid unstable crack growth, and as such there is little warning prior to failure. However, there are situations where brittle failure may occur in metals and alloys considered to be normally ductile, such as that may be seen in notched components or in sudden impact of large objects. In brittle fracture the linear elastic material behavior is a basis for fracture control while in the other category, fracture is preceded by considerable plastic deformation. The linear elastic condition cannot be used due to inelastic behavior and yielding fracture mechanics is necessary in such a case.

Therefore, the analysis of fracture can be based on simple linear or more complex nonlinear elastic plastic material models. At present it is well-known that the nonlinear fracture mechanics methods offer more realistic measures of fracture behavior for high toughness and

low strength materials compared to the elastic methods. However, even for linear elastic material model a plastic zone is formed at the crack tip.

In cases where the plastic zone surrounding the crack tip is of small magnitude, Linear Elastic Fracture Mechanics (LEFM) may be applied for a simple determination of failure loads and related fracture quantities. For the elastic case, the Stress Intensity Factor (SIF) K is the most widely used fracture parameter. However, in many practical problems due to large stress gradients, the existence of severe plastic deformation around the crack tip regions disqualifies the application of LEFM theory. For limited amount of plasticity, the extended elastic models incorporating correction factors to characterize the plasticity effects are often advantageous (Broek, 1982).

Now, in order to develop the field of elastic plastic fracture mechanics (EPFM), the necessity to incorporate the influence of significant plastic deformation that may accompany crack initiation and the subsequent stable growth has been the main impetus. In EPFM, the crack driving force or the crack extension force is frequently explained in terms of crack tip opening displacement (CTOD) and the *J* contour integral. Both the CTOD and *J* contour integral describe crack tip conditions in elastic plastic materials and each of these parameters can be used as a fracture criterion. Critical values of CTOD or *J* give almost size independent measures of fracture toughness, even for relatively large amounts of crack tip plasticity (Anderson, 2005).

At high loading rates, LEFM and EPFM, which assume quasi-static, rate-independent deformation, are inadequate and require the use of dynamic fracture mechanics methods. For dynamic fracture mechanics, the additional factors considered are inertia forces on the

cracked body, rate dependent material behavior and reflected stress waves. When the load changes abruptly or the crack grows rapidly, inertia effects become very important; a portion of the work applied to the specimen is converted into kinetic energy. The crack speed is dictated by the magnitude of the kinetic energy. Near ambient temperature, most metals are not sensitive to reasonable variations in strain rate; however the flow stress can increase substantially when there is increase in strain rate by several orders of magnitude. When there is abrupt change in load or the crack grows very fast, stress waves propagate through the material and reflect from the specimen boundaries and the crack plane. Reflecting stress waves influence the local crack tip fields, and therefore, affect the fracture behavior. In certain problems, we may ignore one or more of the above effects. There are mainly two types of dynamic fracture problems, namely, the fracture initiation due to rapid loading and rapid propagation of a crack. When the crack driving force reaches beyond the material resistance, the structure becomes unstable and rapid crack propagation occurs (Anderson, 2005).

There has also been a tremendous interest in the fracture behavior of polymer based composite materials, especially the fiber reinforced composites. One reason for this is the increasing use of composites in structural components in aircraft, automotive and other industries. The characteristic behavior of composite materials and their response to a tensile or compressive loading, however, are considerably different from those of metals. In metals, damage development under static loading exhibits only one primary failure mode, whereas composite materials exhibit a combination of different failure modes (Kanninen and Popelar, 1985).

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In recent times, materials like toughened structural polymers, metallic foam, plastics, transformation toughened ceramics and vertically aligned carbon nanotubes (VACNTs) have attracted tremendous research attention due to some of their outstanding mechanical properties, for example, toughened structural polymers are widely used in structures due to their light weight and relatively high strength and toughness, foams are interesting for their energy absorption mechanism and the highly desired thermal, electrical, acoustic and radiation-resistant properties etc. Experimental results on the mechanical behavior of these above mentioned materials support a constitutive description that accounts for pressuresensitive yielding. In classical plasticity theory on the other hand, it is assumed that hydrostatic pressure has no effect on material plastic deformation and therefore, the effect of plastic dilatancy is neglected. For the plastically dilatant materials mentioned above, volumetric strains are usually closely related to the pressure sensitivity. Analyses of asymptotic crack tip fields for pressure sensitive materials have been done by a number of researchers to show the effect of plastic dilatancy factor on near tip plastic strain, hydrostatic and effective stresses. It is considered that pressure sensitive yielding and plastic volumetric strains of these materials stem from a variety of factors like basic flow mechanism, cavitation, crazing in glassy polymers and several other interacting micro-mechanisms (Altenbach and Ochsner, 2014; Rudnicki and Rice, 1975; Spitzig and Richmond, 1979; Hwang and Luo, 1988; Li and Pan, 1990; Yuan and Lin, 1993; Yuan, 1994; Chang et al., 1997). Additionally, it is believed that plastic non-normality appears as a result of dilatancy effect. Consequently, the reliable modeling of such materials induces necessary implementation of the non-normality flow rule concept. Even though the normality rule concept is widely used in metal plasticity, experimental data suggest that this normality rule

is not applicable for geomaterials. Also for making the predictions of the model more accurate in crystal plasticity, a deviation from the normality rule is needed. The problem is that the normality rule has initially been assumed as a postulate for all materials and if the normality flow rule holds true, important theorems can be proven (Nova, 2004; Sumelka and Nowak, 2016).

Whenever an elastic plastic body with a sharp crack is subjected to a load of the mode I type (monotonically increasing), crack tip blunting by intense straining will take place until some mechanism of crack extension takes over. There are several situations where fracture mechanisms generally involve significant plastic flow. Representative applications include models of metal forming, crash simulations, various military applications etc. Even for some high-strength materials such as steels, aluminum alloys and superalloys, the fracture surfaces confirm local strain of the order of unity. On the other hand for macroscopic scale in such materials, the fracture process under monotonically increasing loading consists of crack-tip blunting followed often by a regime of stable crack advance before catastrophic failure occurs. Successful ductile crack growth criteria are based on some measure of the deformation field at or within a small characteristic distance from a crack tip. Within a certain near-tip radius the deformation is so intense that it violates the small-displacementgradient condition and hence the usual "small strain" idealization. Therefore, large deformation numerical solutions are generated to elucidate the peculiarities of the near tip large deformation, strain and stress fields in elastoplastic solids.

In many applications the load may be repetitive or cyclic such that the total accumulated damage results in failure, commonly known as fatigue failure. As far as fatigue fractures of engineering structure are concerned, the following two types of fractures are important

- High cycle, low stress fatigue
- Low cycle, high stress fatigue

In high cycle fatigue, the endurance limit of a material after several million cycles or more is usually the consideration. This kind of fatigue is a problem in those portions of structure subjected to fast, repeated loads, such as areas close to propellers, rotating machinery, and areas under constant vibrations where several million stress cycles may be achieved in a relatively short period of time. In low cycle fatigue, on the other hand, fracture after repeated loading of less than 10^5 cycles is usually considered. There are many structural components in which low cycle fatigue, rather than high cycle fatigue, is usually the problem. For example, cracks frequently found in the hull structure of a ship are caused by low cycle fatigue. A fatigue fracture goes through the stages like the initiation of crack, the slow growth of cracks and onset of the unstable fracture. Though the applicability of *J* concept is not uncommon in this area but the use of Paris law is most popular (Anderson, 2005).

For realistic evaluation of fracture response and reliability of cracked structures, Probabilistic Fracture Mechanics (PFM) is getting more and more popular now-a-days. By means of PFM, one can incorporate statistical uncertainties in engineering design and evaluation. The fracture mechanics theory based on continuum approach provides a relationship between the maximum permissible load acting on a structural component to the size and location of a crack in that component. On the other hand, the theory of probability determines how the uncertainties in crack size, loads, and material properties, if modeled accurately, have an effect on the integrity of cracked structure. PFM, which combines these two theories, accounts for both mechanistic and statistical aspects of fracture problems, and therefore, provides a more rational way of describing the actual behavior and reliability of structures as compared to the traditional deterministic models (Rahman, 2001; Rahman and Kim, 2001).

The advancement of science and technology has evolved into the new area of nanotechnology. Atomic components e.g. atomic wire and carbon nano-tube etc possess remarkable mechanical, thermal and electrical properties. These properties combined with their low density and high aspect ratio; make them a very attractive candidate as reinforcing materials for the development of an entirely new class of composites. However, there is still a lack of fundamental knowledge about the strength and failure behavior of such atomic components. The most distinct characteristics of nano-technology is that the properties of nano-materials are size dependent. Due to the extremely small size, the evaluation of their mechanical properties, such as elastic modulus, tensile/ compressive strength, buckling resistance and fracture properties present significant challenges to researchers. While the experimental works brought about striking progress in the research of this area, many researchers have also resorted to the computational nano-mechanics. Due to nano-scale most of the continuum based classical fracture mechanics are not really suitable to describe the failure evolution. Molecular-mechanics based finite element approach is often now used to predict the failure behavior of such atomic components and therefore, combination of atomistic/ molecular dynamics and continuum methods leading to quasi-continuum type modeling are in use in recent times (Li and Chou, 2003; Sun and Zhao, 2005; Meo and Rossi, 2006).

1.2 Motivation for the Research

Foams and entangled arrays of carbon nanotubes or VACNTs have revealed remarkable mechanical properties in a variety of applications, such as, viscoelastic energy absorption (Cao et al., 2005; Gogotsi, 2010; Misra et al., 2009; Pathak et al., 2009; Zhang et al., 2010), recoverability under cyclic loading, impact resistance (Misra et al., 2009), compliant thermal interfaces (Cola et al., 2009; McCarter et al., 2006; Zbib et al., 2008), and biomimetic dry adhesives (Boesel et al., 2010). In order to provide the basis for design in such applications, a fundamental understanding of their mechanical behavior is required. Over the years a number of researchers have studied the mechanical properties of VACNTs through various experimental techniques like nanoindentation, uniaxial compression, impact testing etc. It has been observed in the literature that VACNTs exhibit considerable variations in the mechanical properties, deformation morphology, the amount of post deformation recovery, and the elastic modulus. For instance, in case of compression and flat punch indentation, some VACNTs display essentially a fully elastic or viscoelastic mechanical response whereas others deform permanently. Some VACNTs also display high recoverability after significant strain. VACNTs have been observed to deform in a progressive buckling-like deformation mode during uniaxial compression. A phenomenological elastic-viscoplastic constitutive relation, which incorporated plastic compressibility, plastic non-normality, and a hardening-softening-hardening type of hardness function (Hutchens et al., 2011; Needleman et al., 2012) qualitatively, reproduced the experimentally observed deformation mode and overall stress-strain behavior (Hutchens et al., 2010; Pathak et al., 2013). Till now, the existing experimental and computational studies on the deformation of the entangled arrays of carbon nanotubes have mostly been limited to compressive loading – either compression or indentation. However, as VACNTs have potential uses in a variety of applications as stated above, therefore it is useful to develop a predictive framework for the mechanical behavior of VACNTs under a wide range of loadings.

From the perspective of phenomenological fracture mechanics, the crack initiation and its subsequent growth depend on the surrounding stress and deformation fields near the tip. Thus, analyses of the near crack tip stress and deformation fields are important in order to relate continuum stress analyses to micromechanical failure mechanism. Despite the availability of various fracture related studies of plastically incompressible and compressible materials for small deformation formulation, pressure sensitive yielding effects on crack tip finite deformation fields of plastically compressible material has not been addressed in open literature so far.

Contrary to the analysis of hardening materials, the constitutive equations of many materials include material softening in various engineering applications. The physical mechanism responsible for activating localization often is a consequence of some softening process, including, for example, thermal softening, textural softening, phase change, dynamic recrystallization, microcracking, or microvoid nucleation and growth (Needleman, 2015). In various circumstances, once softening initiates, there is decrease in the material's stress carrying capacity monotonically so that softening can also lead to material failure. To the best of the author's knowledge there is no such study exists so far which explores the combined effects of pressure sensitive yielding and material softening in the hardness function on the near crack tip finite deformation and stress fields.

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1.3 Objectives and Scope of Study

The primary goal of this study is finite element finite deformation quasi-static mode I plane strain small scale yielding analyses of crack tip blunting and near crack tip fields for plastically compressible solids exhibiting a variety of uniaxial stress – strain responses. In particular solids with hardening-softening-hardening responses as can occur for foams and VACNTs have been considered. The novelty of this model comprises unique characteristics as mentioned earlier like the hardening-softening-hardening material response, strain rate-dependence, and plastically compressible solids with plastic non-normality.

As for localization studies it needs a finite strain plasticity description, initially, the governing/field equations are outlined based on a Lagrangian framework with convected coordinates. Quasi-static deformation conditions are assumed and the equilibrium equations are expressed through the virtual work principle. Full derivation of the finite element equations have been provided as an approximate solution of the variation principle in terms of a displacement field with a finite number of degrees of freedom.

Next, finite element program using FORTRAN has been developed by the author for getting the stress and displacement quantities. The initial part of the investigation refers to crack tip blunting and field quantities analyses under monotonic load while in the next part studies have been conducted for fatigue loading to find the key results of crack tip blunting and fields.

• The present simulation aims to understand the process of mode I crack growth, kinematics of the near tip finite deformations, crack tip fields in plastically compressible rate dependent elastic-viscoplastic constitutive relation with hardening-

softening-hardening type of hardness function from continuum descriptions under monotonic load.

- Study also aims to compare the crack tip fields and deformation pattern of plastically compressible hardening solids with those of hardening-softening-hardening solids.
- Since plastic zone shapes and sizes are important in fracture studies, a number of such studies have been performed under various conditions.
- Effects of cyclic loading on the near tip deformation and fields for plastically compressible rate dependent hardening-softening-hardening solids are investigated.
- Plastically incompressible solids are also considered in many cases for comparison purpose of the results under both monotonic and cyclic loading.
- Even though most of the computations are restricted to plastic normality condition, however for comparison purpose the effect of plastic non-normality is explored in a few calculations.

1.4 Organization of the Thesis

The thesis deals with the finite deformation analysis of crack tip fields in plastically compressible hardening and hardening-softening-hardening solids under monotonic and fatigue loading. The introduction provides an overview of the topics contained therein while the summary highlights the important points discussed in the chapter. Moreover, it also provides a smooth transition to the next chapter. The contents of each chapter are briefly outlined in the following.

Chapter 2 is a brief historical review of the early development of fracture mechanics and contains a survey of relevant literature that is both of general interest and of particular importance pertinent to the present problem. This also partially introduces some of the crack growth modeling strategies developed over the years. Further, this chapter as well includes a comprehensive literature on different analytical/ numerical techniques used in fracture mechanics problems.

Chapter 3 provides a brief overview of the basics of continuum mechanics, which includes kinematics and balance laws. After explaining the various terms and equations related to continuum mechanics, finite strain descriptions of the governing/field equations have been provided based on a Lagrangian formulation and using convected coordinates. Since the convected coordinate net can undergo a general transformation it will not necessarily remain orthogonal and therefore general metric tensor needs to be used. Various rules of tensor transformation and differentiation have been extensively used in the formulation and it has become necessary to provide a description of this mathematical background in a comprehensive manner. Quasi-static deformations have been assumed throughout the loading history and the equilibrium equations are expressed through the virtual work principle.

Chapter 4 deals with the constitutive equations used in the research work. The present work considers elastic-viscoplastic constitutive relation which incorporates plastic compressibility, plastic non-normality and hardening-softening-hardening as well as hardening-hardening type hardness functions. The constitutive model is conveniently formulated in terms of quantities referring to the deformed state of the material and the rate of deformation tensor. This chapter covers the mathematical description of the formulation in a step-by-step procedure to increase the readers' acceptability.

Chapter 5 describes the numerical methods used in this work. As the equilibrium equations are expressed through the virtual work principle, the conditions for satisfying incremental equilibrium during a time step are obtained by expanding the principle of virtual work about the current state. Also, since numerical stability is always a key concern, the deformation history is calculated here in a linear incremental manner and in order to increase the stable time step, the rate tangent modulus method is used. As the rate tangent formulation of the constitutive equations is in the classical form of elastic-viscoplastic equations, the implementation in the numerical scheme needs to write these into finite element equations. The geometry on which these methods have been numerically tested is also described. Subsequently, some finite element issues like mesh convergence, type of element for mesh generation, material model, equation solver, nonlinear solution control options etc in the context of finite element program, relevant to the present problems, are also briefly outlined.

In chapter 6 some numerical results have been presented. The initial part of the investigation refers to crack tip blunting and analyses of field quantities under monotonic load while in the next part studies were conducted for fatigue loading. Although most of the results presented are for plastic normality condition, however for comparison purpose some results have also been demonstrated for constitutive relations showing plastic non-normality.

Chapter 7 concludes this thesis with key summaries based on the contents of current work and recommendations for future research possible in areas related to this work.