Chapter 1

Introduction

Solid fracture under high strain-rate deformation is of interest for high-velocity impact and penetration problems. High velocity projectiles impacting on a target produce shock waves in both the target and the projectile. Under certain conditions, this creates tensile pressures that can lead to nucleation, growth and coalescence of voids which, in turn, cause material fracture [5].

In plate impact experiments, a flyer plate is accelerated by some means, such as gas, explosives, lasers, etc., depending on the strain rate requirement, on to a target plate. The impact of a flyer plate produces compressive stress waves at the point of impact which travel toward the free surfaces of the flyer and target plates. When they reach the respective free surfaces of the flyer and the target, they reflect as release waves and interact at some location within the target plate, depending upon the thicknesses of the plates. The interaction of these waves leads to a state of tension in the material. If the tension created exceeds the tensile strength of the material, nucleation, growth and coalescence of voids take place, leading to fracture of the material. This process is called spallation and the fracture of the material is called spall fracture. The nucleation, growth and coalescence of voids in 1145 aluminum resulting from such impact is illustrated in Figure 1.1.

In order to model the fracture of materials under extreme conditions of pressure and temperature, it is necessary to develop an understanding of the basic mechanism of fracture and behaviour of materials under these conditions. Spall fracture takes place when release waves from the free surfaces of the flyer and target interact to produce tension in the target material. The interaction of these waves leads to a triaxial state of stress following uniaxial strain [7, 8]. It is during the triaxial state...
of stress that voids nucleate, grow and coalesce if the tension developed during this phase exceeds the tensile strength of the material.

Many researchers have studied the process of material failure through experiments [9–12], atomistic simulations using molecular dynamics [7, 8, 13–15], multiscale simulations [16] and hydrodynamic simulations [17].

Spallation studies have been carried out at different levels of strain rates. Plate impact experiments result in strain rates of $10^5$–$10^6$/s [12]. Strain rates exceeding $10^7$/s can be achieved by shock loading produced by nanosecond laser pulses [10]. Ultra-high strain rates (exceeding $10^8$/s) can be obtained by femto-second laser pulses [11]. An extremely high strain rate of $10^{10}$/s using high power laser pulses has been reported in the literature [18].

Computer simulations of high strain-rate failure of materials have been performed at various length scales. At the atomistic scale, Molecular Dynamics (MD) simulations have been carried out to study various features of fracture at high strain rates. Belak’s study [13] of nucleation and growth of voids in polycrystalline copper showed that voids at grain junctions yield at a lower strain than those at grain centres. Rudd et al [7], examining polycrystalline copper under triaxial expansion, found that voids nucleate at weaker junctions and this void nucleation does not take place at all available junctions. Traiviratana et al [14] simulated pre-existing voids in mono-crystalline and bi-crystalline copper at strain rates of $10^5$/s and $5\times10^9$/s and estimated the void-size dependence of the stress threshold for dislocation emission.
in mono-crystalline and bi-crystalline copper. Seppala et al [8] studied the effect of stress triaxiality on the growth of pre-existing voids in single crystal copper. Many workers have also studied the coalescence of voids. Seppala and others [15], in their coalescence study, estimated the inter-void ligament distance to be one void radius to coalesce the voids. Davila and others [19], in their study of void coalescence, found that shear loops nucleation based model is in good agreement with the observed molecular dynamics (MD) mechanism. These shear loops are also responsible for hardening the material near the void. Potirniche et al [20] simulated void growth and coalescence in single crystal nickel at high strain rate (10^8 - 10^{10}/s) and showed that the material length scale affects the stress-strain response of the material. It was also found that void growth dominates over void coalescence for the conditions examined in that study. Wang and co-workers [21] have studied instabilities in a perfect lattice at finite deformation using MD simulations. They showed that instabilities in the lattice lead to the nucleation of a small disordered region which grows as a void.

Molecular Dynamics simulations are generally confined to very small length scales (few hundreds nm) due to limitations of computing power. To bridge the atomistic (MD) and continuum length scales, multi-scale simulations have been done by several workers. In the multi-scale approach of Zhuang et al [22], the finite element method (FEM) is combined with discrete dislocation dynamics (DD). The plastic strain is calculated by the DD code and the material parameters are obtained by MD. The DD code works as a substitute for the constitutive form in the FEM code. Shehadeh et al [16] performed multi-scale simulation to study shock propagation and interaction of dislocations in single crystal copper at high strain rates (>10^6/s). He used the multi-scale dislocation dynamics plasticity (MDDP) model which couples discrete DD with FEM analysis. Rudd et al [23,24] have proposed the multi-scale simulation of voids by coupling MD to FEM. This technique is known as coarse grained molecular dynamics (CGMD).

1.1 Objective of this thesis

Hydrodynamic simulations of high velocity impact problems divide the domain of interest into computational cells. Such simulations require, as input, the following information for each of the materials involved in the problem:
1. An equation of state, which allows calculation of the pressure and specific internal energy in terms of the temperature and density of the material.

2. A model to predict the strength of the material during high strain-rate deformation, i.e., the variation of yield strength and shear modulus of the material with temperature, pressure, plastic strain, etc. [25,26] and [27–31].

3. A dynamic fracture model, e.g., void nucleation and growth (NAG) model, where fracture properties depend upon the temperature and pressure values in the cell [17].

For a given cell in the hydrodynamic simulations, the temperature and pressure are taken to be constant during each hydrodynamic timestep. Hence it is sufficient to use a fracture model that describes the nucleation/growth of voids at a specified temperature and pressure.

This thesis studies the high strain rate deformation of single crystal copper, using both simulations and experiments, and involves generation of the following materials data:

- Void NAG model [5] which is one of the fracture models. The parameters for this model are determined by molecular dynamics simulations and checked using multi-scale simulations.

- Johnson-Cook model [27] which is one of the material strength models. The parameters are obtained by high strain rate compression experiments on single crystal copper using a Split Hopkinson Pressure bar (SHPB).

These models involve several parameters. For example, the NAG model involves parameters such as the void nucleation threshold, void growth threshold, pressure sensitivity of void nucleation, material viscosity and void nucleation rate at threshold. In the literature, the parameters for these models are available only for a few materials; even for these materials, the parameters are only available at a single temperature. Therefore, for predictive simulations, it is necessary to generate these parameters for different materials of interest to the Department of Atomic Energy (DAE), either by experiments or by atomistic simulations.

This thesis covers the following areas which have not been addressed by earlier workers:
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- Validation of a macroscopic NAG model, which was originally developed for polycrystalline materials at macro scales, for single crystals at atomistic scales. Determination of best-fit NAG model parameters for single crystal copper deformed at high strain rates.

- Validation of void nucleation threshold obtained above for single crystal copper, using shock wave simulations at atomistic scales.

- Determination of the variation with temperature of NAG parameters for single crystal copper. It also includes a detailed analysis for unusual features observed at temperatures close to the melting point.

- Effect of pre-existing defects in the crystal on the spallation threshold of single crystal copper. In addition to this, studies have been performed to analyse:
  
  - Nucleation and growth mechanism under threshold conditions, when the impact velocity is close to the threshold for causing spallation.
  
  - Effect of crystal orientation and grain boundary on the fracture mechanism.
  
  - Stochastic effects on the spallation process for impact velocities close to the spallation threshold of the material.

- Multi-scale simulations of damage in single crystal copper: NAG parameters are generated using MD for single crystal copper with pre-existing defects. These parameters are then used in a hydrodynamic code to generate spall data, and the results compared with published experimental data.

1.2 Structure of the thesis

This thesis is organized as follows:

Chapter 2 describes the computational techniques used in this study. This covers a) Techniques used in molecular dynamics simulations, b) Details of the post-processor used for analysing the void distribution, c) An introduction to statistical methods used for analysing the crystal structure, such as centro-symmetry parameter, common neighbor analysis, structure factor, radial distribution function, d) An
outline of the singular value decomposition analysis used for determining characteristic modes of the crystal.

Chapter 3 covers MD simulations of uniform triaxial expansion of a perfect crystal, the resulting void nucleation and growth, and the use of MD data to determine best-fit values of NAG parameters. These NAG parameters, obtained using triaxial expansion, are then checked against shock-wave simulations. The location of the first nucleation site is also analyse in terms of characteristic modes of the crystal.

Chapter 4 discusses the temperature dependence of the NAG parameters for single crystal copper. Anomalous behaviour observed near the melting point is analyse in some detail.

Chapter 5 describes the effect of high strain rate history of the material on the spall threshold. Stochastic effects observed at impact velocities close to spall threshold are also presented.

Chapter 6 presents multi-scale simulations for the computation of spall data for single crystal copper. It describes the creation of various kinds of defects in the material and their effect on the NAG parameters.

Chapter 7 discusses the experiments on single crystal copper deformed at high strain rate using a Split Hopkinson Pressure Bar. It further explains the use of this data for obtaining material strength parameters for the Johnson-Cook strength model. The chapter also reports on different experimental measurements, such as neutron diffraction, for detailed characterisation of the specimens. Finally, it compares MD results for the activation of slip directions with experimental measurements.

Chapter 8 presents the conclusions and future scope of the present study.