MONTE CARLO SIMULATION

OF UNIAXIAL TENSION

By

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Chapter 1

Introduction

Semiconductor industry requires exact characterization of mechanical properties of materials at the microscale. This involves sample preparation, miniaturization or fabrication of new equipment setup, calibration, analysis and validation of the data. Micro Electro Mechanical Systems (MEMS) have been devised since 1957 to cater the needs of the semiconductor industry. The accuracy and reliability of the data has gained significant importance due to the tremendous growth of the semiconductor industry.

1.1 Introduction to Micro Electro Mechanical Systems (MEMS)

The development of semiconductor industry has given new impetus to microscale material testing due to the importance of thin films. The performance of a transistor might be compromised by a shift of threshold voltage if the residual stress in the deposited film is high. Residual stress in a dielectric thin film coated over a wafer surface may even cause cracking of the film or warping of the substrate wafer. So it is imperative to know the basic mechanical properties of the materials used like the Young's modulus, the fracture strength and the yield stress to manufacture mechanical elements form thin

films. The measurement of these properties was conducted as a part of development of a specific device and its characterization. As a result, simple structures and simple analysis were used to evaluate properties even though the property to be found could not be isolated from other unknown properties. Also the effect of element size and fabrication process made the interpretation of the results very difficult. So with the development of the semiconductor industry, the need for reliable material data increased tremendously.

One of the earliest and simplest methodologies is to miniaturize the common tension testing apparatus and measuring the tension force applied to micro-sample and its elongation. The micro-sample and the testing apparatus were made together by common micromachining steps to avoid the problems of measuring micro-samples with the macroscopic test system. This resulted in questionable calibration and reliability of the setup.

One of the main efforts in improving the reliability of the micro-sample testing methods is to design the apparatus and specimen to avoid the problems of preparation of the sample, fixing the sample, alignment of the sample and the setup, and measurement of the elongation of the gauge length.

Pearson et al. (1957) determined the mechanical properties of silicon whiskers (20μm dia.) using a bending test. Bending test offers the advantage of needing smaller force compared to tensile test while offering a deformation large enough to be measured by optical microscopy. Since the specimen is pushed instead of being pulled, the gripping

problem is eliminated. This method is also not affected by slight misalignments in the loading directions, so the samples can be prepared without major concern of accommodating the loading.

Tsuchiya et al (1998) also used the bending test method to evaluate the structural strength, fracture strength and fatigue damage of single crystalline silicon using a bridge configuration with a mass in the middle. Johansson et al (1988) measured the fracture strength of single –crystalline silicon (75 –240 μm wide, 8-16 μm thick and 75 – 500 μm long) using the bending test in a SEM chamber. Jones et al (1996) used the bending test to measure fracture strain of polycrystalline silicon (3 μm in width and 1.75 μm in thickness. The authors developed an analytical model for accommodating the nonlinearity in the bending to analyze the deformed shape.

The major disadvantage of the bending test is due to the analysis of the data. The large nonlinear deformation and stress concentrations at the boundary are the major contributors to the difference of the results. Johansson et al reported a strain value of 2% for the fracture strain of single crystalline silicon while with the same specimen size and similar conditions Wilson and Beck et al (1996) reported a value of 0.8%. The major difference in the above values was attributed to the consideration of stress concentration.

Taechung and Chang-Jin Kim (1999) integrated the sample and loading of the direct tension system at microscopic level for measurement of mechanical properties. Direct tension test at the micro level, although the most reliable for measurement of mechanical

properties, is difficult to accomplish due to requirements of proper sample alignment and deflection measurement. Typically these tests are performed in SEM chamber to preserve the surface from contamination and oxidation. This causes further problem since the entire setup has to be miniaturized to fit a SEM chamber. Tsuchiya used strain gauges for force and displacement measurements. They overcame the problem of sample holding by using the electrostatic attraction force. Greek and Johansson (1997) used an optical encoder for displacement measurement instead of strain gauges. The finite stiffness of the loading setup was taken care of by statistical means. Chasiotis and Knauss (1998) used an atomic force microscope to obtain the topology of the sample while stretching it uniaxially. They used digital image-correlation of the surface roughness data to validate the results from the AFM.

Advantages and Disadvantages of MEMS

MEMS has several advantages and some limitations over the conventional material testing process as tabulated by Taechung and Chang-Jin Kim (1999)

1.2 Advantages of MEMS:

- Bending tests and standard tension test methods using MEMS are accurate and repeatable.
- Non destructive testing possible
- With the integration of sample preparation and experimental setup, the human error factor is greatly reduced

- Contamination and oxidation are vastly reduced by the use of vacuum chamber in the SEM

1.3 Limitations of MEMS:

- The experimental setup and sample preparation at the microscale is somewhat difficult and time consuming.
- The cost of the setup can be significantly high and can be performed only in sophisticated laboratory conditions.
- The accuracy and the interpretation of the results from the experiments are based on the analytical or statistical models.

In order to overcome some of these limitations and utilize this precise technology, it is imperative to devise alternative technology for material testing for a better understanding of the mechanical properties at the nano and micro level. Computer simulation is a handy tool to investigate and characterize the mechanical properties of materials.

Observation of a scientific system, formulation of a hypothesis, prediction of the system behavior based on a mathematical model, and validation of the hypothesis forms the four pillars of any scientific research. In the case of manufacturing process, especially at the nanoscale or micro scale, this philosophy not only is costly but also not feasible at times. In such times, we turn to the other alternative of simulation. Simulation overcomes many shortcomings of the conventional research process. Complex system interactions of the system, effects of parameter changes and simplification of the system and the associated

processes can be effectively studied without the associated costs. MD falls under the category of dynamic simulation, which is time dependent. Monte Carlo simulation is a stochastic simulation, which depends on the probability density function of the governing system.

Molecular Dynamics Simulation

Molecular Dynamics simulations have been used to study phenomena at nano-meter scale that cannot be attained in continuum analysis. MD simulations can give atomistic level details of the system, which can be a compromise between the analytical and experimental solutions. MD simulation involves calculation of the trajectory of every atom in the material bulk by solving the partial differential equations of all the atoms in the bulk using an empirical inter-atomic force model. The results of the MD simulations have been sufficiently validated by various literatures on studies of ultra precision machining using MD.

Molecular Dynamics, by virtue of its theory has enjoyed many advantages over FEM and continuum mechanics. The distances between the nodes in MD are fixed by the lattice constant and are not arbitrary. By higher temporal and space resolution, the size effects are properly accounted for.

MD techniques do not require complicated and expensive machine tools. By virtue MD simulation can provide theoretical limits of any machining process. The various process parameters in machining can be effectively studied without expensive setup costs. MD

can also effectively characterize voids, discontinuities and impure metals with the use of proper potential functions.

However the limitations of the MD technique imposes certain constraints on the implementation and interpretation of the MD data. . The simulation time is still a constraint even with the fastest computers available today. The major constraint is the number of atoms that can be considered is directly related to the computational time. Since 6N equations are to be solved for each trajectory calculation, this imposes a severe constraint on the applicability of MD to large systems. This can be overcome with the use of faster computers, but is still a long ways from the practical speeds of operation. Due to non-availability of proper potential model, MD is limited to pure elements with maybe defects, grain boundaries and voids. The depth of cut that can be studied in MD is in the nanometer range. The cutting speeds in the order of 500m/s, due to long processing times required otherwise, attract criticism. A proper dissimilar atom interaction potential model is required to study tool work interactions. This can be overcome with the use of infinitely hard tool but with the compromise of not being able to study the tool-work interactions, tool wear etc.

Monte Carlo Simulation

Numerical methods that are known as Monte Carlo methods can be loosely described as statistical simulation methods, where statistical simulation is defined in quite general terms to be any method that utilizes sequences of random numbers to perform the simulation. Monte Carlo methods have been used for centuries, but only in the past several decades has the technique gained the status of a full-fledged numerical method

capable of addressing the most complex applications. The name ``Monte Carlo" was coined by Metropolis during the Manhattan Project of World War II, because of the similarity of statistical simulation to games of chance, and because the capital of Monaco was a center for gambling and similar pursuits. Figure 1 illustrates the idea of Monte Carlo, or statistical, simulation as applied to an arbitrary physical system. Assuming that the evolution of the physical system can be described by probability density functions (probability density function's), then the Monte Carlo simulation can proceed by sampling from these probability density function's, which necessitates a fast and effective way to generate random numbers uniformly distributed on the interval [0,1]. The outcomes of the random samplings or trials must be accumulated or tallied in an appropriate manner to produce the desired result. In contrast, a conventional numerical solution approach would start with the mathematical model of the physical system, discretizing the differential equations and then solving a set of algebraic equations for the unknown state of the system.

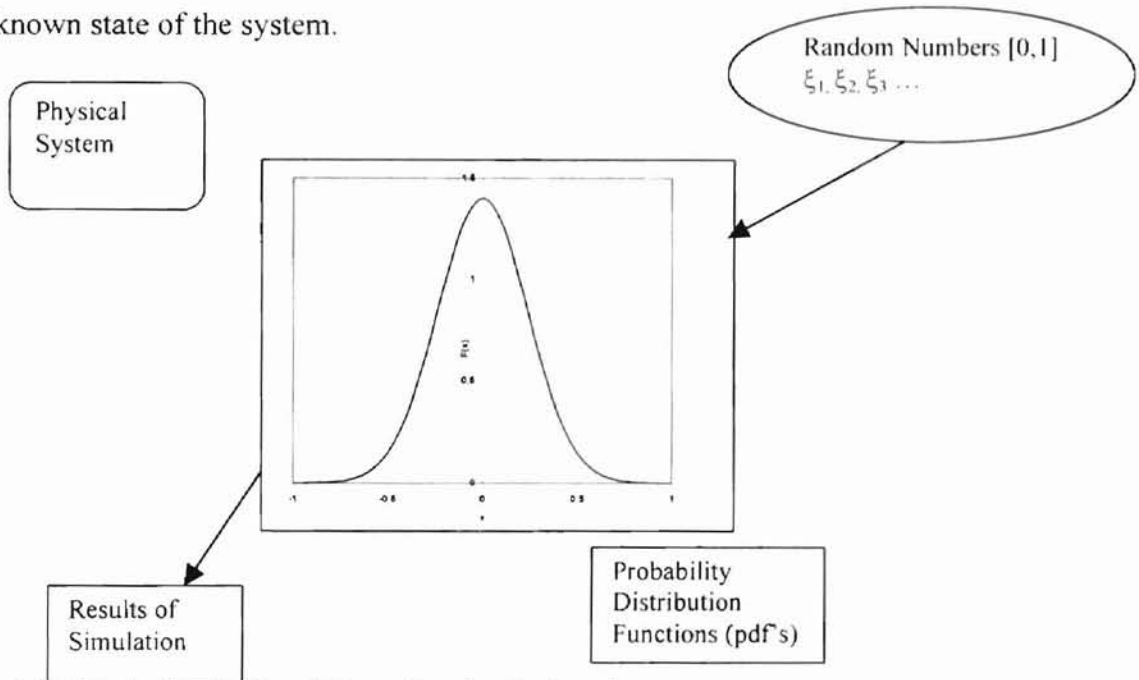

Fig 1.1: Monte Carlo Simulation of a physical system

It should be kept in mind though that this general description of Monte Carlo methods might not directly apply to some applications. It is natural to think that Monte Carlo methods are used to simulate random, or stochastic, processes, since these can be described by probability density function. However, this coupling is actually too restrictive because many Monte Carlo applications have no apparent stochastic content, such as the evaluation of a definite integral or the inversion of a system of linear equations. However, in these cases and others, one can pose the desired solution in terms of probability density function. This step allows the system to be treated as a stochastic process for the purpose of simulation and hence Monte Carlo methods can be applied to simulate the system. Therefore, one should take a broad view of the definition of Monte Carlo methods and include in the Monte Carlo rubric all methods that involve statistical simulation of some underlying system, whether or not the system represents a real physical process. This wide diversity of methods is the reason that ``Monte Carlo is not Monte Carlo is not Monte Carlo." – Hall (1873)

In Chapter 1, a brief description of the MEMS technology, its application in the semiconductor industry is detailed.

In Chapter 2, a discussion on the works reported in the literature on MSEM and studies of tension tests using molecular simulation is presented. Chapter 3 gives a description of the problem statement of this investigation. In Chapter 4, a brief description of the Monte Carlo theory for molecular dynamics simulation for uniaxial tension test is presented. The basic Monte Carlo algorithm for molecular dynamics is described.

In Chapter 5, the procedure used in the simulation of the tension test is described in detail. In this method, the computational time for the simulation is shown to be reduced considerably by the use random moves to calculate the relative position of the atoms at various stages of the simulation as compared to the solving of Hamiltonian equations in the conventional method.

Chapter 6 deals with the results obtained from the Uniaxial tension test. The results are compared to the conventional molecular dynamics simulations and the theoretical results from the handbook [21]. The yield strength of the tested material was found to increase with the decrease in the ductility and the value of the strain at fracture was found to increase with the increase in ductility of the material.

Chapter 2

Literature review

Manifestation of the scale effect is abundant in nature. Biologists have reported by empirical observation of nature that surface force becomes important than body or muscle force in the world below 1mm, the domain which, was not realized before the advent of MSEM. The advancements in the fields of medicine, information technology, ultra precision machining, and semiconductor applications has directed the research community to device advanced technology to manufacture components in the micro to nano scale. Only a better understanding of the material properties at the nanometer level can facilitate this.

2.1 Literature on Microscale Material Testing

The earliest tension test on a micrometer scale is attributed to Eisner (1955). He passed current through diphenyl carbazide to grip the ends of a silicon whisker of 1-micrometer in diameter. The whisker is sucked into the melt pool of the diphenyl carbazide and a force of the order of one hundredth of a gram is applied and controlled using a micromanipulator. The fractured whiskers are then mounted on an electron microscope for determining the diameters. The accuracy of the sample preparation and diameter measurement was cited as the limitations of the process.

Petersen and Guarnieri (1979) of IBM Research Laboratory described a measurement technique for studying the Young's modulus of a wide variety of thin films. This process, the author claims overcomes the problems due to the extreme fragility of the samples, concomitant difficulties in sample preparation and film wrinkling due to strains between the film and the substrate. They used very small cantilever beams fabricated from insulating films deposited on silicon by selectively etching the silicon out from under the insulating layer in a controlled manner. The beams are then vibrated electrostatically and the Young's modulus is measured from the mechanical resonance frequency. The chemicals used during etching and processing temperatures of over 1000 deg C would affect the mechanical properties of the material. The limitations of this process are claimed to be the calibration of the mechanical resonator, the accuracy of the etching apparatus and the theoretical model used for determining the Young's modulus from the resonance frequency.

Johansson and Schweitz (1988) performed *in situ* fracture testing of silicon cantilever beams (10-20 μ thick) in a SEM. They designed an apparatus for the testing purpose, which could be fitted inside the vacuum chamber of the SEM. The measured data was compared with the analytical fracture model for the fundamental fracture parameters such as Young's modulus, fracture limit, fracture strength and fracture strains. They reported good agreement of their experimental results with the analytical results.

Yi and Kim (1999) measured the Young's modulus of single crystal silicon in three major directions by direct uniaxial tension tests using a microscale beam specimen of 10 μm thick and 50 –100 μm wide. The samples were custom manufactured from NRF at the University of California. The stack actuators used for the elongation of the specimen had the capability of maximum output of 150 μm with sub-micrometer increments. The setup designed was calibrated for 4με resolution of strain measurement. The strain was measured using an optical interferometry technique thereby avoiding physical contact with the specimen. A data acquisition system was used for data analysis. The authors concluded that since the deviation of the Young's modulus was found to be low in the [110] direction, the testing procedure was reproducible and reliable. Also the measured values were found to be closer to the handbook values, within reasonable error bounds. They supplemented this work with testing for etchant effect, used in the preparation of the samples, on the tensile strength.

Tsuchiya et al. (1998) devised a tensile tester using an electrostatic-force grip to evaluate the tensile strength and the reliability of thin-film materials. The apparatus was located inside a scanning electron microscope (SEM) chamber for *in situ* observation. The apparatus was used for tensile testing of polycrystalline silicon (poly-Si) thin films with dimensions of 30-300 μm long, 2-5 μm wide and 2 μm thick. A mean tensile strength of 2.0-2.8 and 2.0-2.7 GPa was reported for nondoped and P-doped poly-Si respectively, depending on the length of the specimens, irrespective of the specimen width. Statistical analysis of these size effects on the tensile strength predicted that the location of the fracture origin was on the edge of the specimen, which was identified by the SEM

observation of the fracture surface of the thin films. The authors also described sample preparation, setup of the apparatus in the SEM chamber and the validation of the results using a theoretical model as possible limitations of the process.

2.2 Literature on Molecular Dynamics Simulation techniques

Several methods and advancements have been made to facilitate MD simulation such as the book keeping technique, linked-list method, Area Restricted Molecular Dynamics (ARMD) and Length Restricted Molecular Dynamics (LRMD). These basically aim at achieving higher computational speed, better memory management, and getting MD closer to conventional speeds and sizes. These have been achieved partly by the availability of faster computers and better methodologies. Each of the methodologies has their own advantages and limitations.

2.2.1 Book – Keeping Technique:

In the book keeping technique (Rentsch et al. 1994), a list of neighboring atoms for each atom is created. This is based on an empirical parameter called the cutoff radius, which is dependent on the material property. This limits the interaction of an atom to only those neighboring atoms that are within the specified cutoff radius. This formulation saves a considerable computation time as the interaction of an atom with all other atoms are neglected since their contribution to the result is insignificant. When the neighbor list of this process has to be updated, the complete system is cheeked for neighboring atoms of

each atom. This is the actual over head involved in this technique. Since in a cutting operation with each time step the position of the atoms changes, the corresponding changes in the neighbor atom list has to be updated for each atom. This is a process, which can be characterized by a time complexity of the order of O (N^2). Since this process is just a sub process of the computational process, the time complexity of the overall process is far greater that O (N^2). However, this method is generally adopted in all MD simulation studies.

2.2.2 Linked – List Method

This method is an optimization of the book keeping technique to overcome the computational time involved in updating of the neighbor list by the use of a structured simulation space (Rentsch et al. 1994). In this technique, the simulation space is divided into small volumes and neighboring volumes are tabulated. Only the volumes associated with a particular space has to be refreshed at each time step. Several implementation of this approach have been used in MD simulations (Allen and Tildeseley 1991).

In this method, the atom space is divided into cellular volumes or regions. A general approximation for the region size is twice the maximum cutoff radius of any atom pair in the simulation model. The cell to which an atom belongs is determined and is associated with that particular atom. This information contains two sets of data i.e. which cell an atom belongs to and which atoms are in a particular cell. When generation of the bond list for any particular atom, only a particular cell is to be checked for bonds with the atoms in the same cell or cells which are in the cut off radius. This process, reduces the

generation of the bond list to a process with a time complexity of the order of O (N) compared to O (N^2) for the Book- Keeping process. With this implementation, the computation time for generation of the bond list is insignificant compared to the trajectory calculation time. This is a significant improvement since the bond list generation time dominates the computations in the Book Keeping method. This also ensures that as the size of the system increases the gain on the computational time is significant.

2.2.3 Area Restricted Molecular Dynamics

Maekawa et al. (1995) introduced the concept of Area Restricted Molecular Dynamics (ARMD). In this method, the simulation is carried out in a region near the tool nose with a radius of 7.3 nm. This restricted area moves along with the tool in the direction of cut. A thermostat placed next to the moving atoms, which are surrounded by a fixed boundary, dissipates the heat generated in the restricted area. The disadvantage with this method is that the area is based on the cutting conditions and tool geometry. This necessitates a comparison with conventional MD simulation. So this method warrants a conventional simulation to be executed before selecting the area for the ARMD simulation.

Computation of forces and potential however is restricted to the region within the cutoff radius in the restricted region where the atoms are affected by the tool movement. This process reduces the overall computation time by a factor of three. But this gain is offset by the necessity to run a conventional simulation and this process also does not address

the memory requirement since all the atoms in the system, even those that do not participate in the cutting process is stored in the memory.

Also the relaxation time in this process is not adequate for the system to recover sufficiently. This results in the system carrying more defects.

2.2.4 Length Restricted Molecular Dynamics

The length of the work piece is maintained constant throughout the experiment (Naga and Komanduri 1997). But, its position is made to shift along the direction of the cut, i.e. the atoms from the machined part of the work material that are not going to affect the simulation results significantly are discarded but their memory positions are retained. These memory positions are used to add new atoms to the work material. This ensures a reduction in the number of atoms considered in the simulation. Also, with a small initial work piece, it is possible to simulate cutting action to any distances.

The basic assumption in the LRMD method is that once the tool has advanced into the work material through a small distance, the work material atom will exert minimum influence on the future simulation results since, their interaction with the too atoms will be negligible. Consequently, those atoms can be ignored for future computations. These atoms which are not participating in further computations are either ignored or retained. In the LRMD process these atoms are added to the leading edge of the work piece at the peripheral zone.

The number of layers of the atoms to be discarded are chosen and initialized and is executed each time the exchange procedure is executed. In principle, atoms from any part of the workpiece can be stored for the exchange process with the constraint that the number of layers stored for the exchange process should be same as the number of layers to be replaced.

Molecular Dynamics of Tension

MD simulation has been extensively used for tensile testing process. Lynden-Bell (1992) [7-9] conducted MD MC simulation of uniaxial tension test on platinum, gold, rhodium and silver at various temperatures They reported failure due to void formation, void growth and nano cracks. They reported an increase of stress to a maximum followed by a decrease. This they attributed to structural rearrangements of the crystal. Ductile materials were reported to have local regions of disorder even at the beginning of the simulation compared to the less ductile materials where the region of disorder was relatively less and formed at a later stage.

Rentsch and Inasaki (1995) conducted uniaxial tension tests of silicon using MD simulation to verify material representation of silicon in fracture. They reported a linear increase of stress-strain relationship followed by a failure. They also computed the value of Young's modulus and specific surface energy. The failure was observed to be sudden and they also observed an anisotropic deformation in the structure.

Doyama (1995) conducted MD simulation of uniaxial tension for copper and iron single crystal in [111] and [001] orientations with free boundaries. They suggested a notch to be the source of stress concentration and cause for failure. The initial deformation was attributed to dislocations on different slip planes followed by crossage between dislocations and dislocations and inhomogeneous deformation.

Heino et al. (1998) conducted simulation of tension on copper using molecular dynamics. They used manybody potentials for the inter-atomic interactions and calculated the tensile and shear modulii of copper. The differences in the simulation results to the handbook values were attributed to unaccounted boundary effects.

The Monte Carlo method proposed in this investigation overcomes these limitations. It can perform simulations on larger systems with reduced computation time, less memory space requirements and also eliminates the necessity of high velocity of operations.

2.3 Literature review on Monte Carlo Method

Even though Monte Carlo methods have been in use since the World War II, their application to the field of molecular simulation has gained significance only in the last few years. Monte Carlo has found applications in many fields ranging from nuclear physics to Bingo Games. There are many flavors of Monte Carlo available and chronicled by Kennedy (1999). He has also explored the possibility of Monte Carlo process being parallelized to use multiple processors to gain computational time advantage. Monte

Carlo process by the very nature of it formulation is an ideal candidate for parallel processing.

Monte Carlo is ideal for evaluating any kind of infinite-dimensional integral (A.D.Kennedy 1999) of the form

$$<\Omega>=\frac{1}{Z}\int[d\phi]e^{-s(\phi)}\Omega(\phi)$$ where the action is S and the measure is $d\phi$.

The partition function Z is chosen such that <1> = 1. The field configurations (ϕ_1, ϕ_2, ...ϕ_N) each chosen from the probability function

$$P(\phi_i)[d\phi_i]=\frac{1}{Z}e^{-s(\phi)}[d\phi_i]$$

The measure of the operator Ω on each configuration is formulated and the average is computed as follows

$$\bar{\Omega}\equiv\frac{1}{N}\sum\Omega(\phi_i)$$

As the probability reaches unity, the configuration of the average value of the operator tends to the expectation value of N.

$$<\Omega>=\lim_{N->\infty}\bar{\Omega}$$

If the probability distribution has finite moments the configuration average is a gaussian distributed with the expectation value <Ω> as its mean and with a standard deviation which falls as inverse of the square root of N.

$$<\Omega>\approx\bar{\Omega}+O(\sqrt{\frac{C_2}{N}}) \qquad N\longrightarrow\infty$$

Where $C_2 = <(\Omega - <\Omega>)^2>$ is the average variance of Ω.

The Markov process defines the process of generation of a sequence of configuration. The Markov process is based on the fact that the new configuration is based only on the predecessor and is ergodic if

$$\alpha \equiv \inf_{\phi_i \phi_f} P(\phi_i \longrightarrow \phi_f) > 0$$

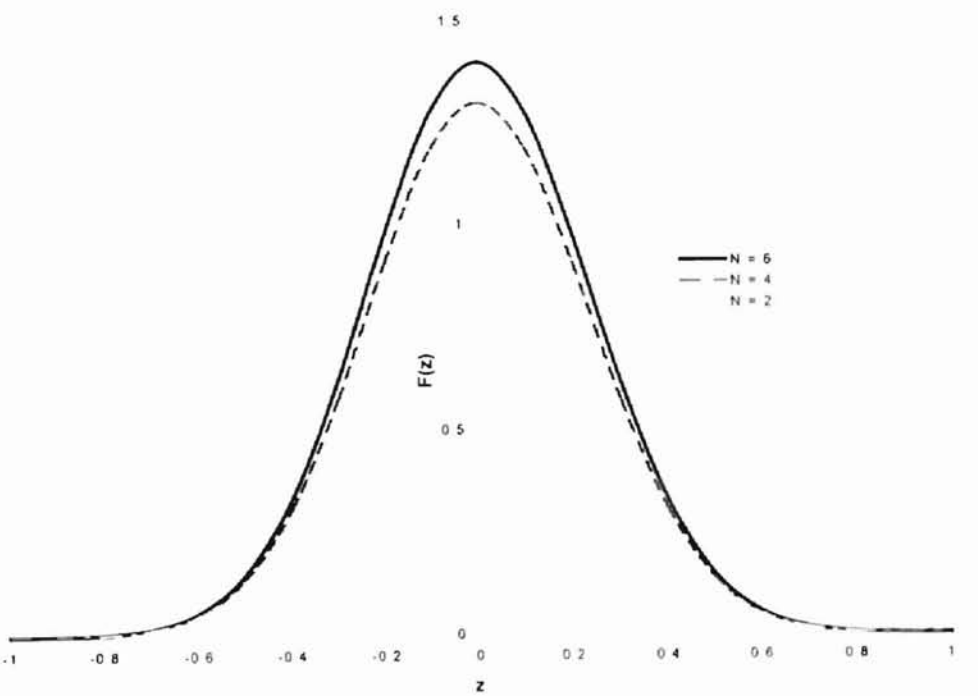

Fig 2.3.1: The approach of the probability function f (z) to a Gaussian distribution.

The Markov process is made to satisfy the detailed balance of the form given below.

$$[d\phi_i]Q(\phi_i)P(\phi_i - \phi_f) = [d\phi_f]Q(\phi_f)P(\phi_f - \phi_i)$$

From this balance, the Metropolis algorithm is derived as

$P(\phi_i \longrightarrow \phi_f) = \min\left[1, \frac{Q(\phi_f)}{Q(\phi_i)}\right]$ This satisfies the balance equation.

Kennedy describes a molecular dynamics Monte Carlo process which, consists of three components: MD trajectory, a momentum flip and an acceptance step. MD is an approximate integration of the Hamilton's equations on phase space,

$$U(\tau) : (\phi, \pi) \longrightarrow (\phi', \pi')$$

The above equation is area preserving given by the below and reversible

$$\det U_{\cdot} = \det\left[\frac{\partial(\phi', \pi')}{\partial(\phi, \pi)}\right] = 1$$

The momentum flip changes the sign of the fictitious momenta and a metropolis accept reject test to obtain the desired distribution. The composition of the MDMC is given by the equation below

$$\begin{pmatrix} \phi' \\ \pi' \end{pmatrix} = \left[F o U(\tau) \upsilon(e^{-\delta H} - y) + \iota\upsilon(e^{-\delta H} - y)\right]\begin{pmatrix} \phi \\ \pi \end{pmatrix}$$

This procedure involves a forward and backward integration of the Hamiltonian equations This is a highly computer intensive computational process. The Monte Carlo process described in this investigation uses the metropolis accept reject criteria but uses a Markov random walk instead of the MD trajectory described by Kennedy.

Uhlherr (2000) performed MC simulations on bulk atomistic polymer systems. He formulated a design to vary the degrees of freedom on the torsional angles about all atoms in a manner, which maintains the chemical connectivity, and the composition of the material. This method combines the elements of ConRot (Dodd et. al. 1993) and CB methods proposed by Leontidis et al (1994). It is a concept similar to the HOLE method of Escobedo and de Pablo (1995), which is restricted to fully flexible molecules. The ConRot method or the CB methods individually have some limitations. These algorithms have restriction in sampling of the molecular space due to their inherent formulations. These have been successfully over come by the Hybrid Monte Carlo method proposed by Uhlherr [5].

In a concerted rotation (ConRot) algorithm, a selected driver torsion angle within a polymer backbone is varied and a geometric solution is determined for the sequence of six adjacent torsion angles, such that only a localized section of the chain is displaced. In a configuration bias Monte Carlo (CB) method, a bond in a selected chain is removed and regrown such that each successive atom is given an energetically biased new position.

The basic technique used by Uhlherr is a generalization of the CB method where each move consists of a randomly selected region of material, removing all the atoms inside the region, then replacing them one at a time in energetically biased new locations within the specified region. The ratio of the original statistical weight to the generated new configuration is used for the metropolis accept-reject criterion. The author reports a drop in accept-reject ratio for individual chains in the simulation.

Spath and Raff used a Monte Carlo method for modeling diffusion – controlled bi-molecular reactions in matrices. Monte Carlo method was used by Spath and Raff to simplify the treatment of matrix reactions at the cost of explicit temporal reactions. After preparation of the initial state, Monte Carlo moves are made at equally spaced, arbitrary time intervals on each A molecule and AB pair in the system. At every move, every A molecule is permitted to diffuse randomly to any adjacent matrix site with a specific probability, which is chosen randomly from the distribution characteristics of the particular zone in which the A molecule resides. AB pairs are permitted to undergo reaction with a constant probability at each Monte Carlo move. This procedure is continued until at least 75 % of the initial A has reacted. The plot obtained by this simulation was used to determine the kinetics of the system. The authors report consistency of the Monte Carlo results with the results generated by calculation and established the feasibility for the use of Monte Carlo method for the process.

The authors also have successfully used Monte Carlo method to study hydrogen and oxygen atom diffusion through imperfect xenon and argon matrices at cryogenic temperatures (Pan and Raff 1993). The oxygen atom diffusion into Ar and Xe matrices were computed by the authors by using classical variational transition theory which employs Markov random walk and damped trajectory procedure to effect convergence. The MC procedure in this investigation also employs a Markov random walk and damped trajectory combination to simulate the uniaxial tension test as described by Raff. et al [6].

Chapter 3

Problem Statement

It can be seen, from the earlier MD simulation works in 2D and 3D, that the computational time is highly prohibitive. It was overcome by using cutting speeds far higher, of the order of 100-500 m/s, than the conventional range of 1-5 m/s. In addition, the simulation was confined to a few thousand atoms. To take the process of molecular dynamics simulation to practical scale, these issues has to be addressed – the speed of the operation, the computation time and the number of atoms in the simulation has to be increased. One approach is to use faster computers. But even with the fastest computers available today, due to inherent complexity of the simulation process, the computational speeds have not shown significant improvement. Also, due to computational complexity, the speed of operation is still far from the conventional speeds in practice. Alternative methodologies have to be devised to overcome the above problems. Monte Carlo lends itself as a methodology to circumvent the problem of computational complexity and due to its inherent formulation can take the simulation to the speeds used in practice. Since

the computational time is small compared to the conventional MD simulation, the number of atoms in the simulation can be considerably increased.

Molecular modeling and simulation of nanometric tension tests using Monte Carlo method involves understanding of the science, mathematics and probability. Understanding the inter-atomic potentials requires knowledge of physical chemistry. Solving the equations of motion requires knowledge of mathematics and an understanding of probability and statistics is required for handling the Monte Carlo process. Programming the process involves knowledge of computer science and to study and analyze the simulation data requires a strong fundamental engineering background.

The objectives of this investigation are as follows,

1. To develop the Monte Carlo method that can be used to simulate tension test using a 3D model. The process should enable a reduction in the computer time and memory space requirements. The simulation is based on the assumption that at every stage of the simulation, the specimen tries to achieve a minimum energy state. Consequently, Monte Carlo moves are designed to take the structure to a minimum potential. By generating the bond list for only those atoms that are participating in a Monte Carlo move and computing the potential of only those atoms, a significant reduction in the computer time is expected
2. To validate the results of this technique by comparing the simulation data with the conventional MD process and the data from hand books.

3. To characterize the time complexity of the process and compare it with the conventional MD processes.
4. To apply the Monte Carlo technique to simulate specimens with several of thousand atoms and evaluate the simulation.

Chapter 4

Theory of Monte Carlo Simulation

4.1 Introduction

Monte Carlo methods have been used for centuries but only in the past several decades has the technique gained the status of a full-fledged numerical method capable of addressing the most complex applications. The name ``Monte Carlo'' was coined as a code name by Metropolis, for this secret Manhattan Project during the World War II, because of the similarity of statistical simulation to games of chance, and because the Capital of Monaco was a center for gambling and similar pursuits. Monte Carlo is now used routinely in many diverse fields, from the simulation of complex physical phenomena, such as radiation transport in the earth's atmosphere and the simulation of subnuclear processes in high-energy physics experiments, to the mundane, such as the simulation of a Bingo game

Monte Carlo method has been shown to be effective in reducing the total computational time from O (N^2) to the order of O (N log N), where N is the number of atoms used in the

model. Also, with the use of MC method the concept of velocity, that has been a significant source of criticism in the MD technique, is eliminated.

The expression "Monte Carlo method" is very general. Monte Carlo (MC) methods are stochastic techniques--meaning they are based on the use of random numbers and probability statistics to investigate problems. MC methods are used in everything from economics to nuclear physics to regulating the flow of traffic. Of course the way they are applied varies widely from field to field, and there are dozens of subsets of MC even within each sphere of application. But, broadly, "Monte Carlo" experiment is one, which uses random numbers to examine some problem.

The use of MC methods to model physical problems facilitates the examination of more complex systems which were infeasible earlier. Solving equations, which describe the interactions between two atoms, may be fairly simple but solving the same equations for hundreds or thousands of atoms is computationally intensive. With MC methods, a large system can be sampled in a number of random configurations, and that data can be used to describe the system as a whole.

Statistical simulation methods may be contrasted to conventional numerical discretization methods, which typically are applied to ordinary or partial differential equations that describe some underlying physical or mathematical system. In many applications of Monte Carlo, the physical process is simulated directly, and there is no need to even write down the differential equations that describe the behavior of the system. The only

requirement is that the physical (or mathematical) system be described by probability density functions (probability density functions).

The essential principle of the MC method, applied to a mechanical process involves reaching the minimum potential in every stage. The equilibrium position of the atoms in the system is obtained by random moves at every stage. The computational time associated with numerical integration of the classical Newtonian equations of motion for the interacting particles over a certain period of time during very every time step is obviated. The benefits of this methodology are twofold – the computational time is reduced and the velocity parameter as used in the MD simulation is not necessary since the position of the atom at every stage is not computed but is based on the random Monte Carlo move. The only overhead is the repetitive computation of the potential of the system. This can be significant, if the system is very large.

In the MC process, the random Monte Carlo moves are made on 'n' number of atoms from the system comprising of 'N' number of atoms. Here 'n' is very small compared to the total number of atom (N) in the system. In a typical simulation, 'n' is of the order of 4-10 if the total number of atoms in the system, N, is of the order of a few thousand. So, by computing the change in the potential of only these participating atoms in any Monte Carlo move, we can estimate the direction of the potential change in the entire system. This effectively means that if the time complexity overhead for the computation of potential is of the order of O (N^2) in the case of the entire system, the time complexity for the selected atoms is O (N). This reduction coupled with the computer time saved by not

calculating the trajectory can result in a manifold increase in the size of the system that can be simulated. This in effect means that the simulation can theoretically be stretched on to macro level compared from the nanometer scale of MD.

4.2 Formulation of the MC Model

The essential principle of Monte Carlo simulation for the tension test is the random moves made on the selected group of atom to reach the most minimum potential for the entire system over every stage of the system from an initial condition to the final desired state. The workpiece is represented as an ensemble of N atoms arranged in a configuration characteristic of the crystal system of the material under consideration. Thus silver, copper, nickel and aluminum are characterized by a FCC structure . Only FCC metals are considered as the pairwise Morse potential used in this investigation, is found t be more appropriate for this class material (Komanduri et. al. 2000).

The atoms in the workpiece are composed of Newtonian atoms and boundary atoms. The Newtonian atoms are the ones that are selected for the random moves during any Monte Carlo move. The top and the boundary layer of the structure are defined as the boundary layer. The boundary atoms are the rigid bases, which are not affected during the moves. Thus the positions of the boundary atoms with respect to each other will not change during the entire simulation.

A 'pull' in the Monte Carlo method comprises of moving the boundary layer by a specific distance followed by a series of Monte Carlo moves and a damped trajectory. The tension process is assumed to be an isothermal process and the room temperature of

298 K is used for the thermal constraint based on Maxwell-Boltzmann distribution for the metropolis accept-reject criteria. The interatomic potentials of the workpiece atoms are used to rearrange the atoms into a minimum potential configuration during each pull.

In a typical Monte Carlo move, a small set of 'n' atoms is selected randomly from the structure. The potential due to these selected atoms with respect to the structure is calculated. The selected atoms are moved by small distances Δx, Δy and Δz, which are generated randomly, in the x, y and z directions. The value of Δx, Δy and Δz should be between 0 and the maximum pull executed in that particular move.The change in the potential is calculated after the move. If the change is negative then the move is accepted. If the change is positive, a thermal constraint based on the Maxwell-Boltzmann distribution is imposed to determine the acceptance. This process is cycled through the entire gamut of the moving atoms.

The atoms can be selected either randomly or cyclically to ensure that all the atoms are selected. Also an acceptance-rejection ratio of 0.5 is maintained. Once the Monte Carlo moves are completed, the damped trajectory is executed to ensure that the system is indeed in the minimum possible potential.

This entire process of Monte Carlo pull – boundary pull, Monte Carlo moves and damped trajectory are repeated till the tension specimen breaks.

Chapter 5

Uniaxial Tension Test by Monte Carlo Method

5.1 Tension Model

A FCC structure comprising of N atoms is setup with the top and the bottom layers defined as the boundary layers. The structure is divided into a number of layers prior to making any Monte Carlo moves as shown in fig 5.1.1.

A Monte Carlo pull is initiated by pulling the all the atoms by a small value $\xi\Delta L$. The value of ξ is proportional to the position of the atom with respect to the boundary. The top boundary is pulled in the positive direction and the bottom boundary is pulled in the negative direction. A small number of atoms from the layer one is selected and the potential due to the selected atom is computed (V_{old}).

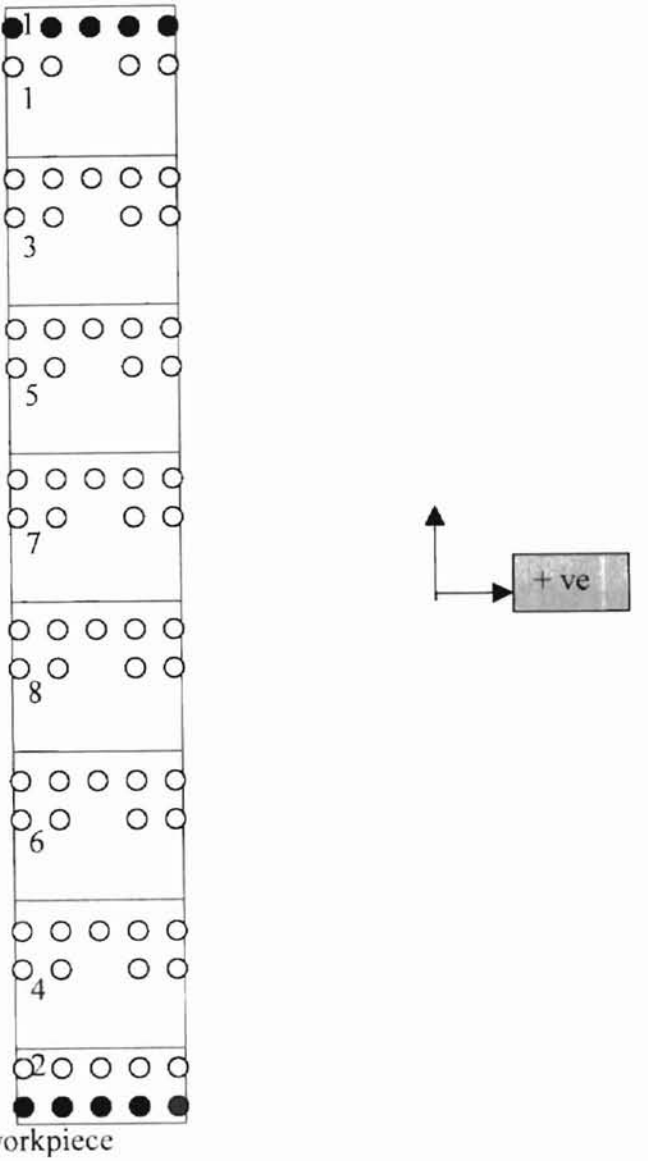

Fig 5.1.1: Schematic of the tension workpiece

The empirical potential used for the simulation was a pair-wise sum of Morse Potential governed by

$$V(r_{ij}) = D\{\exp.(-2\alpha(r_{ij} - r_e) - 2\exp(-\alpha(r_{ij} - r_e))\}$$

Where r_{ij} and r_e are instantaneous and equilibrium distances between the atoms i and j respectively. D and α are numerical constants depending on the material properties.

$$V_{old} = \sum_{MovingAtoms} V(r_{ij})$$

Three random numbers ξ_1, ξ_2, ξ_3 are generated between 0 and 1 for the Markov random walk and the new position of the selected atoms are computed as follows.

$$X_i^{new} = X_i^{old} + \Delta x \xi_1$$

$$Y_i^{new} = Y_i^{old} + \Delta y \xi_2$$

$$Z_i^{new} = Z_i^{old} + \Delta z \xi_3$$

The changed potential, due to the selected atoms, of the system is computed considering the new position of the moved atoms (V_{new}). The change in the potential of the system due to the move is given by:

$$\Delta V = (V_{old}) - (V_{new})$$

If the changed potential, ΔV is less than zero, the system is moving towards a lower potential and hence the move is acceptable. If the change in potential is positive, the Maxwell-Boltzmann distribution is applied to determine the acceptance as the basis for metropolis accept reject criteria The Maxwell-Boltzmann distribution is given by

$$X = e^{(-\Delta V/RT)}$$

Another random number ξ_4 is generated between zero and one and is compared with the value of X. If X is greater than ξ_4 then the move accepted. Otherwise the move is rejected. A new set of atoms is selected within the first layer and a Monte Carlo move is made. Once all the atoms in layer 1 has been effected, layer 10 is selected and similar moves are made. The sequence for Monte Carlo moves is one layer from the top half, followed by a layer from the bottom half. This is done to ensure that the atoms affecting

the potential of the structure are aware of the change in the position of the boundary. The moves are percolated from the boundary towards the center of the structure. Since, the trajectories are not calculated, the atoms in the center, which are atomistically far from the boundary are not aware of the change in the position and may not cause a positive change in the potential.

Any given set of atoms in three-dimensional space, have six degrees of freedom and they can be moved many number of ways. In this simulation a combination of x, y, z change in directions is considered. The other possible combinations are not considered. As a result the potential of the system may not be the most minimum. After the Monte Carlo moves are cycled through the entire set of atoms in the structure, a damped trajectory is executed. A damped trajectory ensures that the system reaches the minimum potential for the given configuration. This comprises of a Monte Carlo pull.

The forces are computed using the relation

$Fx_i(t) = - \delta Vi(t)/ \delta x$

Where Vi (t) is the potential of an atom i at time t and Fx is the force in the x direction. Similarly the forces in the y and z directions are computed and are used to relate the potential energy to the forces.

The Monte Carlo pulls are executed successively till the specimen undergoes fracture.

All simulations were conducted on a Digital Alfa workstation with a clock speed of 500 MHz.

5.2 Monte Carlo Algorithm for Uniaxial Tension

The following is the step by step description of the uniaxial tension test by Monte Carlo method using damped trajectory and Monte Carlo moves with Morse potential for inter-atomic interactions:

a) Set up the coordinates of the atoms in atomic units in terms of x, y, and z coordinates in a FCC structure. The unit typically is in angstroms. The workpiece is typically divided into three zones, namely, the moving zone, the peripheral zone, and the boundary zone.

b) The inter-atomic potential is defined for the setup and a look-up table is created for the potential at various distances. This is done to reduce the computational time involved in the calculation of the potential.

c) The Morse potential is of the form

$$V(r_{ij}) = D\{\exp.(-2\alpha(r_{ij}- r_e) - 2\exp(-\alpha(r_{ij}- r_e))\}$$

Where r_{ij} and r_e are instantaneous and equilibrium distances between the atoms j and i respectively. D and α are numerical constants depending on the physical properties of the material. The table below lists the potential parameters used in the simulation.

Material	Structure	Lattice Const	α parameter	Equilibrium radius	D parameter
		in nm	in nm^{-1}	γ in nm	In eV
Aluminum	FCC	0.405	11.646	0.3253	0.2703
Copper	FCC	0.362	13.588	0.2866	0.3429
Silver	FCC	0.409	13.69	0.3115	0.3323
Nickel	FCC	0.352	14.199	0.278	0.4205

Table 5.2.1 Morse parameters used in the simulation

d) Relax the Structure: When the atoms are placed in the lattice structure, they are at an energy state higher than their minimum especially at the corners and edges. This is a process that iterates over the entire set of atoms till they reach a minimum energy configuration. Since the atoms are close to their minimum-energy state when they are setup, the time taken for this process is very small.

e) The next step is to determine the bond list of the atoms. The cut off radius is used to determine which of the atoms are bonded to which others. Any atom farther than the cutoff radius causes negligible changes in the potential and is ignored.

f) A Runge-Kutta procedure is then performed to implement the effect of bonds. This involves calculating the average forces experienced over a time step by calculating the forces at four different locations. This is basically a simultaneous solutions approach with the final behavior based more on the mid point calculations. Since there are 4N positions to be calculated at every time step, where N are the number of atoms, this is computationally intensive.

g) A damped trajectory consists of repeated calls to the relaxation routine and the Runge-Kutta procedure to ensure that the structure is indeed in the minimum potential state at that particular configuration.

h) In the above processes discussed, the most time consuming routines are the calculation of the cutoff and the potential of the system. In the case of Monte Carlo simulation, it is sufficient to calculate only the potential of the system only due to selected atoms and hence it would suffice to create a bond list of only those selected atoms. This reduces the time complexity from O (N^2) to O (N).

i) Once the structure is relaxed, the Monte Carlo loop is executed till the specimen breaks. A typical loop consists of a pull, layer setting, randomizing the atom list, randomly selecting the atoms, calculating the potential due to the selected atoms, moving of the atoms by a Markov random walk, calculating the changed potential and changing the configuration of the structure based on the acceptance of the move.

j) In the pull routine, all the atoms in the specimen are moved by a specific distance. The distance that an atom is moved to is proportional to the relative distance from the center of the structure. The underlying principle is that in a tension test, the atoms closest to the point of application of pull experiences the maximum force and the atoms further from the point of application of the force experiences the least force.

k) After pulling the atoms, the structure is divided into ten layers. The layering is again based on the position of the atom in the structure. The numbering of the layers is done in the top-bottom method i.e. the topmost layer is followed by the bottom most layer. This is done so that when the atoms closer to the boundary are moved first. This ensures that the atoms far away from the boundary are aware of the change in the position of the boundary atoms.

l) After the layers are set, the bond list is randomized and their indexes are stored in an array. This is to ensure that the atoms are not selected sequentially.

m) Once the atoms are layered and randomized, the Monte Carlo move is executed. A Monte Carlo move consists of selecting a few atoms in the specimen, calculating the potential of the specimen due to the selected atoms, and moving the atoms by a random distance by a Markov random walk. The random distance generated for the

movement of the atom is based on the time seed. The distance is between the range of 0 and 1.

n) The random walks are controlled using the following rules:

i) If the position of the atom is in the positive z direction the movement is allowed only in the positive z direction and vice versa.

ii) If the position of the atom is in the negative x directions, the atoms are allowed to move only in the positive x direction and vice versa.

iii) If the position if the atom is in the positive y direction, the atoms are allowed to move only in the negative y direction and vice versa.

These rules are set up to ensure a better Metropolis acceptance rejection ratio based on Maxwell-Boltzmann distribution.

o) Once the atoms are moved to the new position, the changed potential of the system due to the new configuration is calculated after creating the new bond list.

p) If the new potential is less than the old potential then the move is accepted and the positions of the atoms are permanently changed. If the move is rejected then the Maxwell-Boltzmann distribution criteria of acceptance is checked for. If the move is still rejected, the old positions of the specimen are restored.

q) The steps m through p is looped over the entire set of atom in the structure.

r) The forces and the potential energy of the system are computed.

s) The energy of the system increases after the pull is executed and decreases after the execution of Monte Carlo moves and damped trajectory

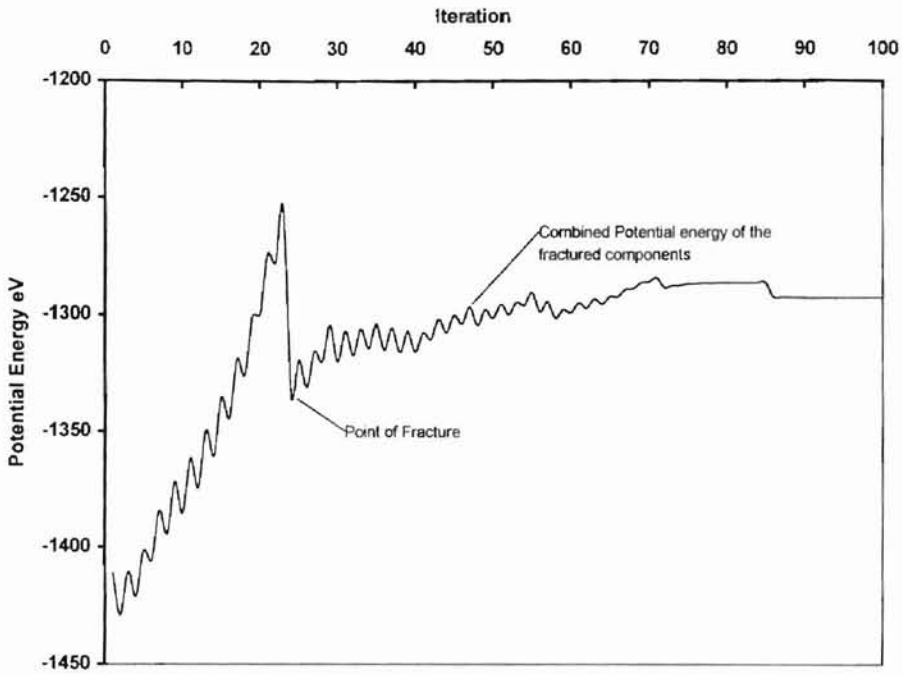

Fig 5.2.1: The variation of Potential energy through Monte Carlo Iterations

t) Once the Monte Carlo move is completed, the system is closer to the minimum potential for that configuration. Now the damped trajectory is executed to take the system to the most minimum potential at that state.

u) The steps j through r are executed till the specimen breaks.

Chapter 6

MC Simulation of Uniaxial Tension – Results and Discussion

Uniaxial tension loading was conducted for copper nickel, aluminum and silver using the Monte Carlo method. The programming was done in 'C'. A Digital alfa workstation, Model 500 au with a clock speed of 533 MHz was used for the simulation.

The Morse potential parameters for the work materials are given in table 5.2.1. The work material dimension was based on 1:4 ratio namely the length is four times the width that is conventionally used in tension tests. Similar experiments using the conventional MD process for the same configurations of the work piece were conducted on the same Digital alfa workstation. Table 6.1 gives the details of the workpiece sizes and the simulation time.

Material	x (A)	y(A)	z(A)	Number of atoms	Time in min for MC	Time in min for MD
Copper	5	5	5	666	28.6	251.85
Aluminum	5	5	5	666	28.6	251.85
Nickel	5	5	5	666	28.6	251.85
Copper	5	5	10	1271	87.95	544.4
Aluminum	5	5	10	1271	87.95	544.4
Nickel	5	5	10	1271	87.95	544.4
Copper	5	5	20	2481	233.17	1726.6
Aluminum	5	5	20	2481	233.17	1726.6
Nickel	5	5	20	2481	233.17	1726.6
Silver	5	5	20	2481	233.17	1726.6

Table 6.1: Details of the work material configurations used in the simulation.

The plot of the time versus the number of atoms comparing the time taken by the Monte Carlo simulation and the conventional MD simulations are shown in fig 6.1

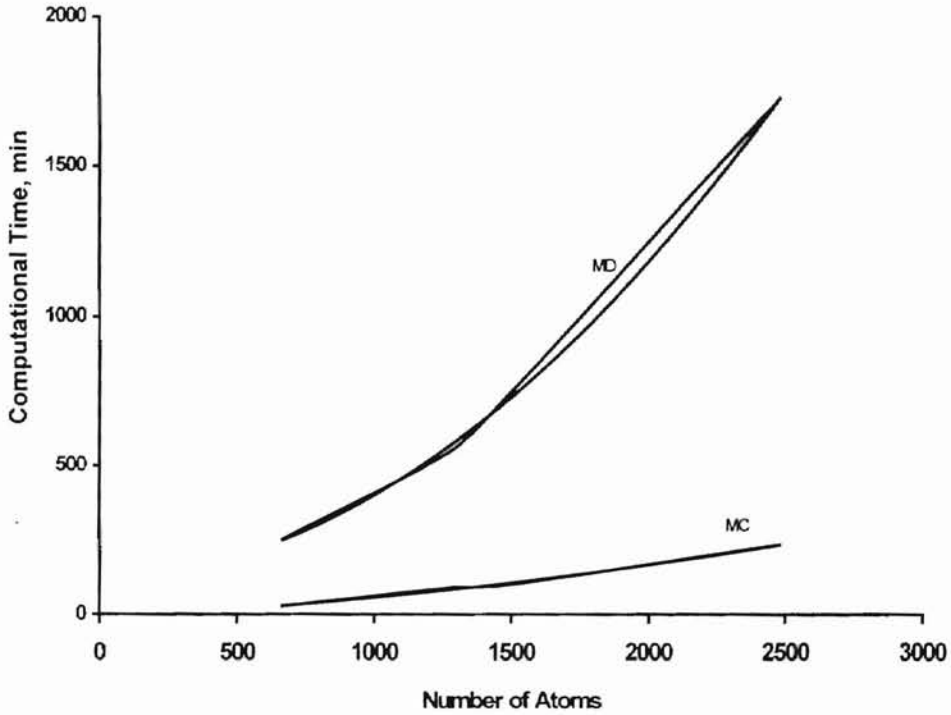

Fig 6.1 Plot of computational time vs. number of atoms

The computer time for the simulation shows a linear relationship for the Monte Carlo process confirming a time complexity of O (N) where N is the number of atoms. The time comparison clearly shows the obvious advantage of the MC process over MD simulation, especially as the number of atoms increases.

The MC simulation of the gauge sections is shown in fig 6.2 – 6.5 and the comparison of the stress-strain relation for the tested materials are shown in fig 6.6.

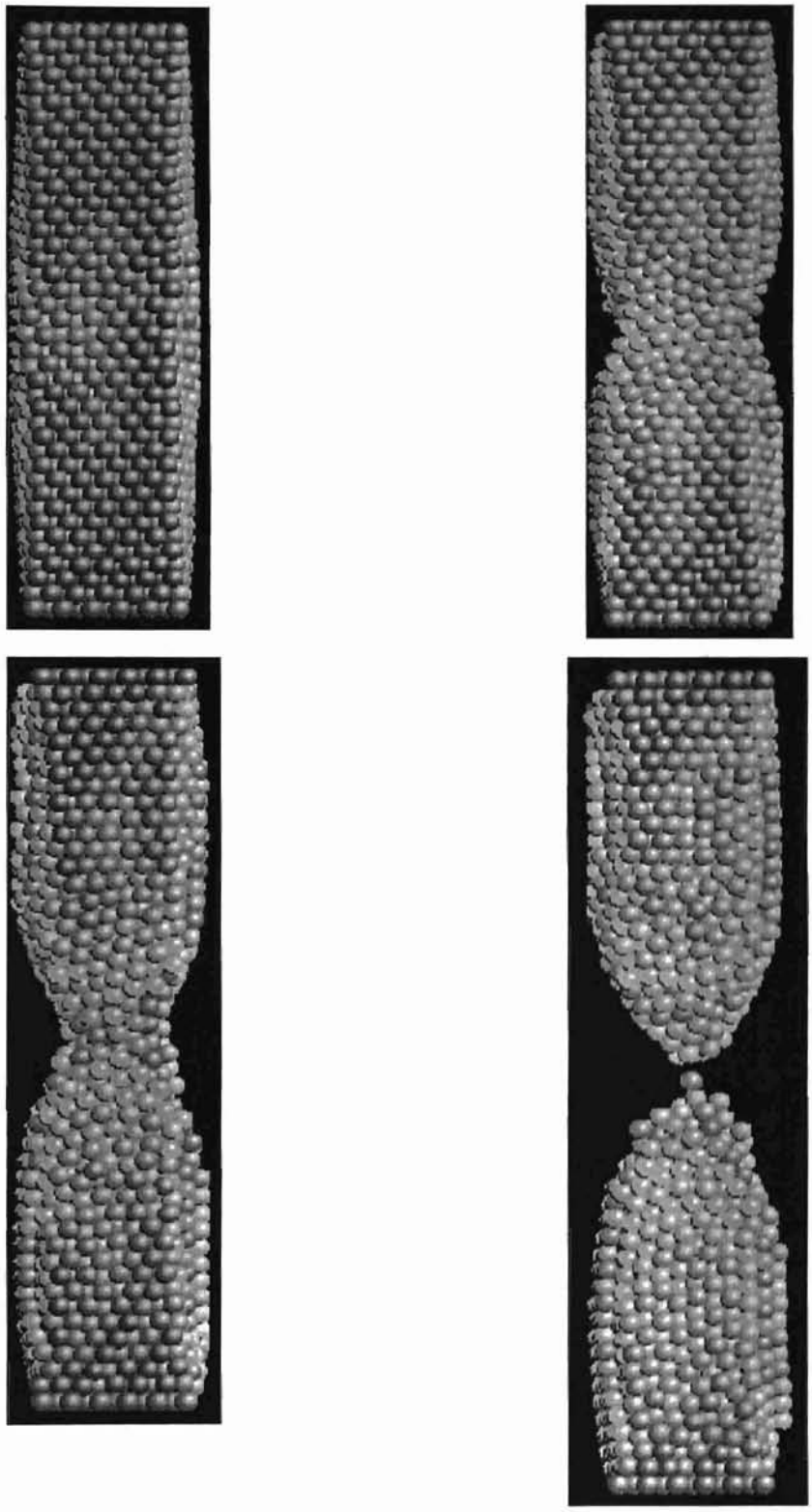

Fig 6.2: Plot of gage section of MC simulation for tensile loading of copper (5x5x20)

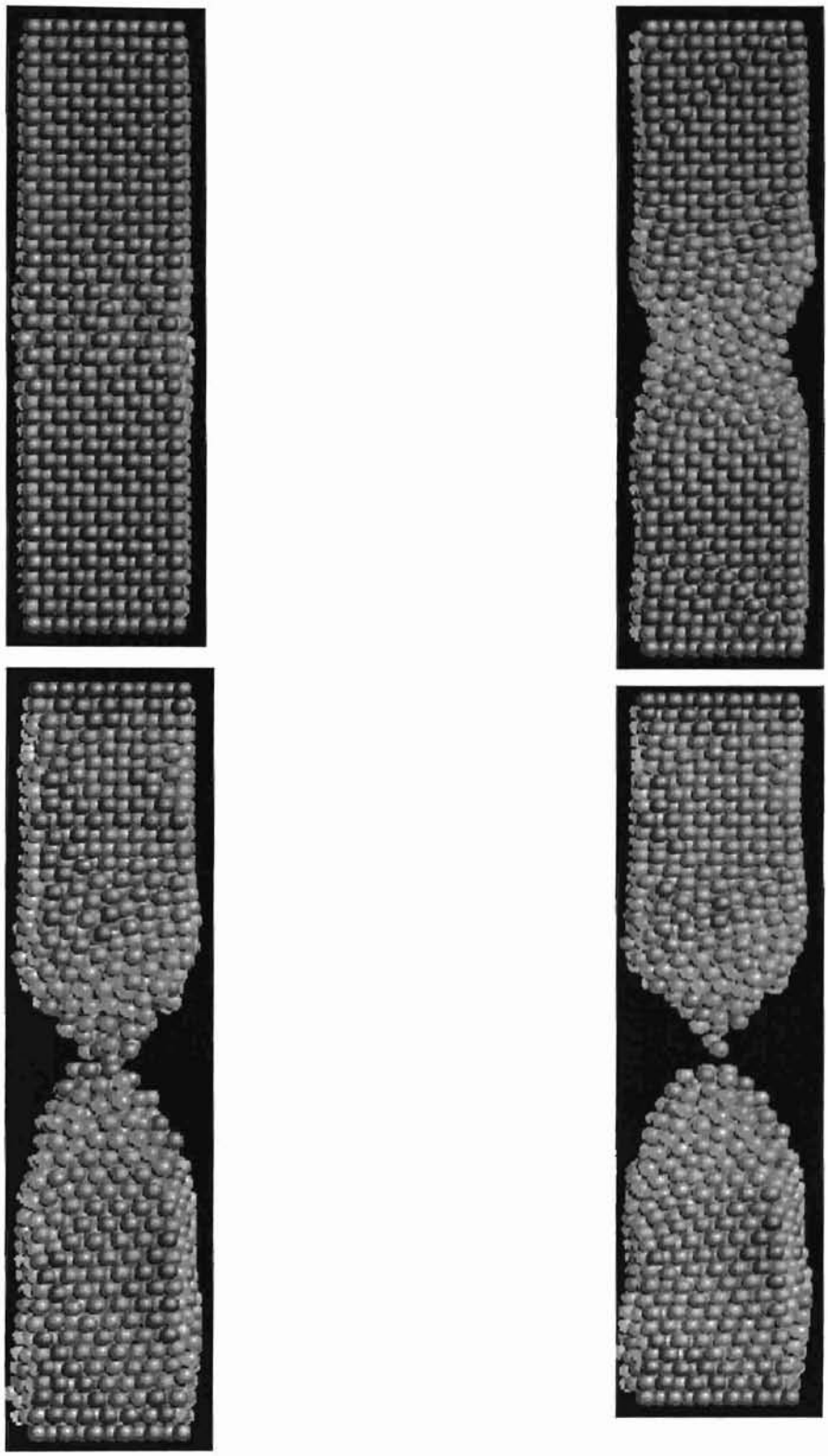

Fig 6.3: Plot of gage section of MC simulation for tensile loading of Aluminum (5x5x20)

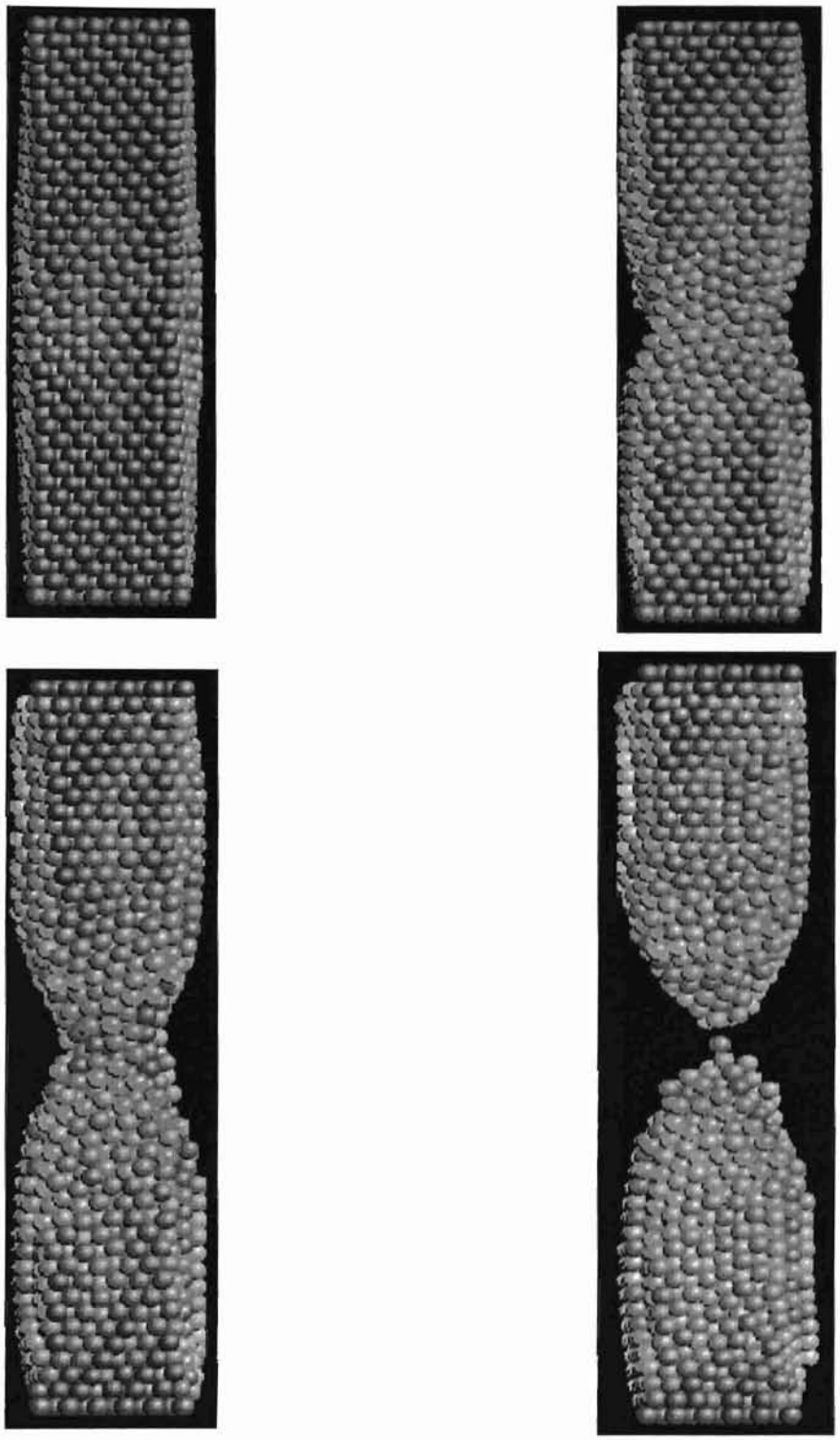

Fig 6.4: Plot of gage section of MC simulation for tensile loading of Nickel (5x5x20)

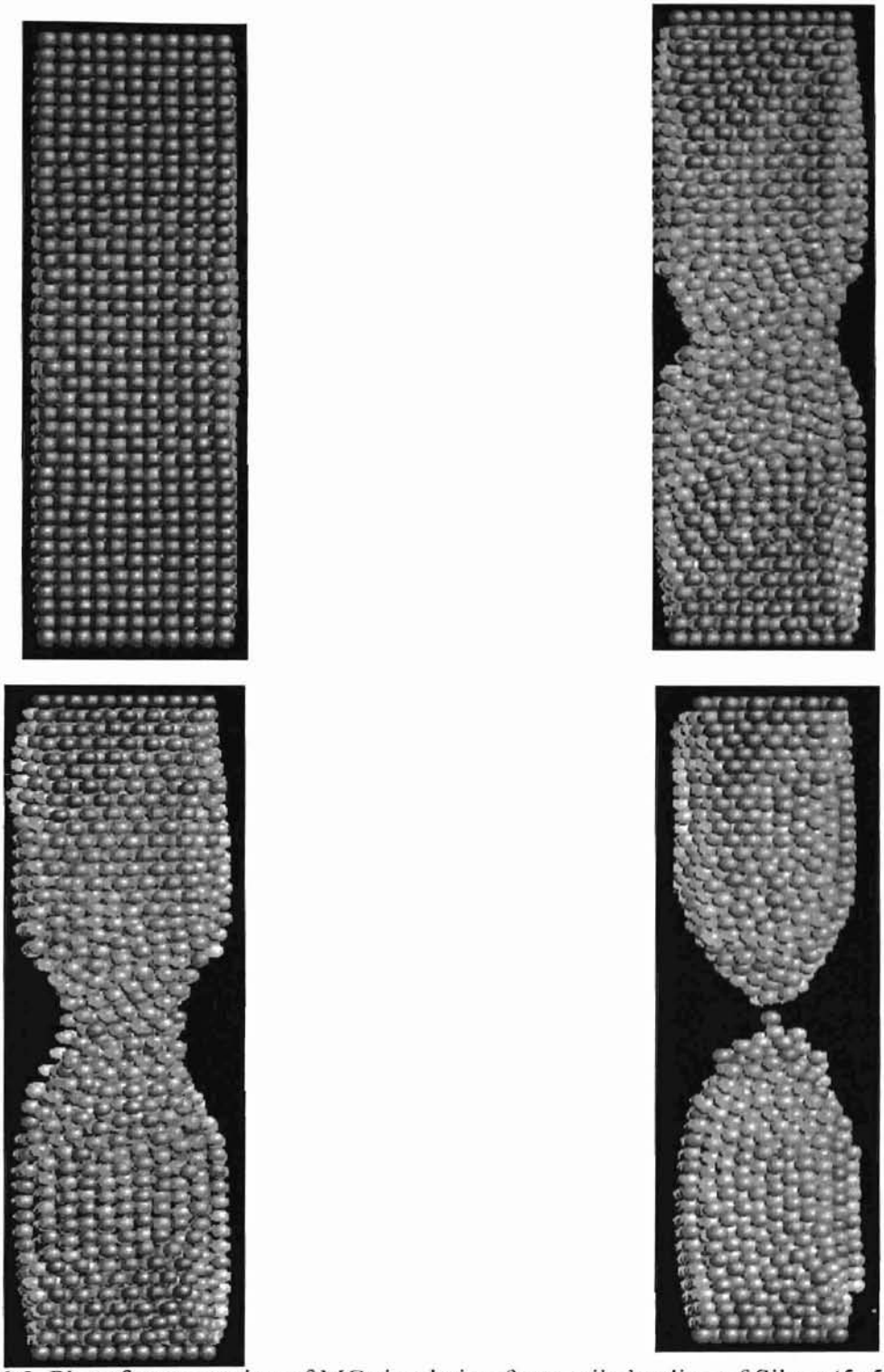

Fig 6.5: Plot of gage section of MC simulation for tensile loading of Silver (5x5x20)

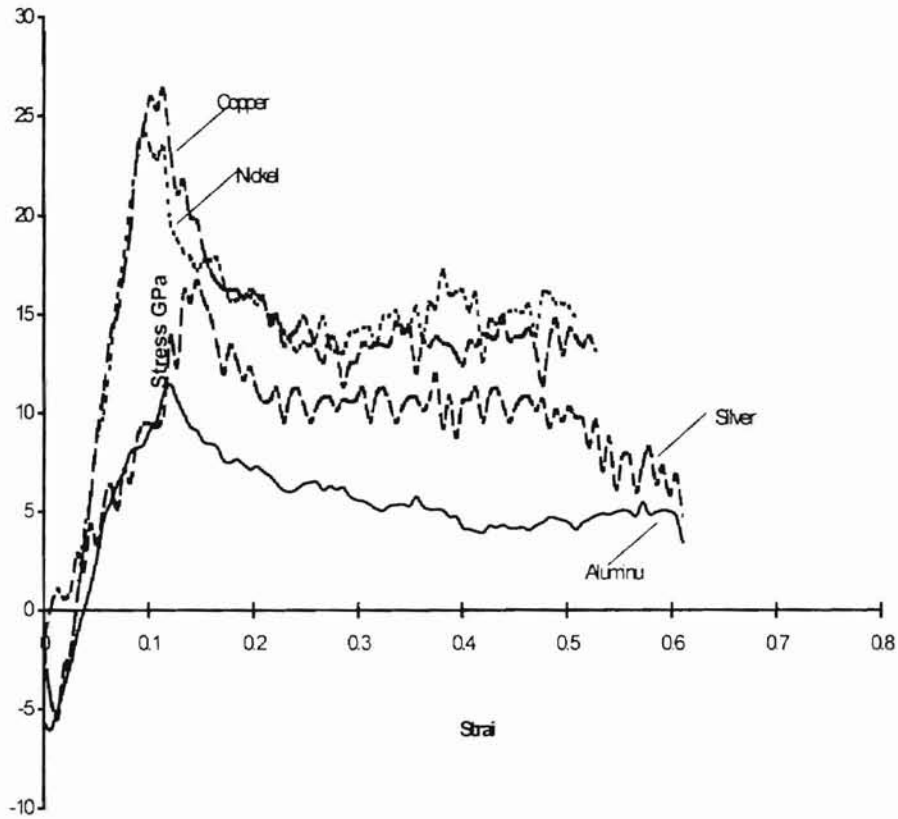

Fig 6.6: Plot of stress vs. strain for Silver, Copper, Nickel and Aluminum

Figures 6.2, 6.3, 6.4 and 6.5 are for FCC material copper, aluminum, silver and nickel respectively. The discussion of the plots is based on both the data obtained from the MC simulation as well as the animation based on the software developed by Stewart (1998).

Initially the specimens for all the FCC materials were found to be slightly under compression. This may be attributed to the structure trying to attain a minimum surface energy. Since a sphere has the minimum volume to surface ratio, the structure tries to attain a spherical structure. But due to the presence of the boundary layer, which restricts the mobility of the moving atoms, the bulge is observed.

Considerable distortion of the structure and disorder is noticed even at the very early stages of loading, as observed from the simulation for all the FCC materials tested. As the simulation continues, the specimen is pulled apart. A neck is observed bridging the top and bottom part of the crystal. For aluminum, the necking is observed for a prolonged duration as compared to nickel. For copper and nickel, this necking is longer than aluminum and silver. Since aluminum is highly ductile, the atoms are held together for a longer duration resulting in a longer neck. The length and the duration of the neck were found to decrease with the decrease in the ductility of the material.

As the elongation proceeds, the neck elongates terminating in a failure. The strain value at which the failure occurs increases with increase in the ductility of the material. Nickel is observed to break far earlier than the other three materials. Aluminum exhibited the

maximum necking. This can be attributed to the increase in the ductility from nickel to aluminum.

Based on the animation and the plots of stress-strain relations, the strain to fracture was observed to be lower for nickel compared to aluminum, copper or silver. Aluminum, being very ductile, has a higher strain to fracture value. Thus the strain to fracture observed to decrease with decrease in the ductility of the material. The radius and the length of the neck were found to be different for different materials. As can be observed from Figures 6.2-6.5. The radius of the neck at fracture for aluminum was the least and nickel had the maximum radius. The length of the neck was maximum for aluminum and the least for nickel since nickel is more brittle compared to aluminum. The void volume for aluminum, copper, silver and nickel were more distributed throughout the structure. As a result the atoms in the FCC materials were held together for a longer duration effecting a longer neck. In the cases where there is a concentration of void volume near the center of the structure and the neck was relatively shorter, the specimen failed earlier.

The engineering stress-strain from the MC simulation for the FCC metals is plotted in Figure 6.6. The stress is found to increase to a maximum tensile strength of the specimen under consideration followed by a gradual drop. The specimen was observed to break at a positive stress value. The stress value starts at a negative value for all the specimens. This is due to the initial compression discussed earlier. The slope of the stress strain curve was measured and given in Table 6.2 for computing the value of the Young's modulus (See Table 6.2).

Material	Elastic Modulus GPa by MC	Maximum Tensile Strength GPa by MC	Maximum Tensile Strength MPa from Handbook	Elastic Modulus GPa from handbook
Aluminum	91	11.5	76	69
Copper	147	26.4	107	115
Nickel	184	24.2	217	207
Silver	97	16.7	80	71

Table 6.2: Material properties computed form the simulation plot compared with the values from the handbook

As can be observed from plots, copper exhibits the maximum tensile strength and aluminum exhibits lower tensile strength. The computed value of the elastic modulus also shows the same trend. The strength as expected decreases with the increasing disorder in the work material or increase in the ductility as reported by Heino et al. (1998) and Lynden – Bell (1995).

Chapter 7

Conclusions and Future work

Micro-Electro Mechanical Systems (MEMS) are currently being used today for characterizing the material properties of thin films of the order of few microns. However, sample preparation, miniaturization of the experimental apparatus, fitting of the specimen to the apparatus without inducing initial stresses, calibration of the apparatus, prevention of contamination of the specimen and analysis of the data obtained from these experiments are a subject to interpretation. Since the specimen size used in MEMS are of the order of few microns, MC simulation can be used as an alternate approach to the experimentation.

7.1 Monte Carlo Simulation

The Monte Carlo method using Markov random walk technique and a metropolis accept reject criteria was developed for the simulation of uniaxial tensile loading. A code was written in C programming language for the implementation of the Monte Carlo method and the results were compared with the conventional MD simulation process.

1. Monte Carlo simulation of uniaxial tension has been conducted on single-crystal materials e.g. aluminum, copper, nickel and silver to investigate the relative advantage in terms of time complexity with respect to the MD simulation.
2. Failure of the work materials, preceded by void formation and necking is observed to be similar to their behavior at microscale.
3. The FCC materials had considerable necking and high strain at fracture.
4. Nickel had the highest of maximum tensile strength amongst aluminum, copper and silver as is expected.
5. The radius and the length of necking was observed to increase with the ductility of the material
6. The engineering stress-strain plot showed a clear necking region, a maximum tensile strength and a positive value for fracture stress.
7. The strain at fracture was observed to decrease with the decrease in ductility of the material

7.2 Future Work

There are some scopes for optimization of the Monte Carlo process. This process involves repeated calls to the damped trajectory routine, which involves computation of the bond list of the interacting atoms of the entire structure. This can be optimized using the linked cell method proposed by Stewart (1998).

The initial bulging of the specimen can be alternately explained by the wave theory. The time duration of the bulge can be studied and analyzed using the analytical models available in the field of shock wave propagation.

Alternate the possibility of decreasing the computation time for the damped trajectory computation using methods like the steepest-descent method conjugate-gradient method and other suitable methods can be explored.

The Monte Carlo method developed for the tension test can be extended to the cutting process. The procedure would involve movement of the tool by a small distance at every stage, execute the Monte Carlo move followed by damped trajectory to obtain the minimum potential position for that particular stage.

By repeated random walk and damped trajectory, the minimum potential state at every stage of the tool movement can be determined. The point of consideration would be the velocity effect. Monte Carlo method involves only a change in the velocity and not the velocity by itself. Also, time is not an explicit variable in the MC method. The speed in a cutting process affects the temperature of the machined surface. So, the velocity can be implemented indirectly as a function of temperature.

One possible solution would be to characterize the temperature as a function of the cutting parameters using the conventional MD simulation and using the trends observed

as a functional input to the MC method. However, this would involve the problem of using very high cutting speeds.

Alternately, a mathematical formulation involving forward and reverse integration of the Hamiltonian equations proposed by A.D.Kennedy (1999) can be used at conventional speeds for temperature characterization. The resulting functional form can be incorporated as an accept-reject criterion in the MC method.

Also MC method can be extended to micro scale and facilitate the characterization of thin films of a variety of materials ranging from conventional metals to silicon. The MC method can eliminate the necessity of complex and costly apparatus required by Micro Electro mechanical systems (MEMS).

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