Abstract

Linking material property acquisition and modeling in the nanometric scale with those on the macro-scale is currently one of the most challenging fields of research in material science in general and in micromachining in particular. Due to computational limitations it is presently impossible to inflate atomic level models and simulations to the macro sized components we work with daily. This knowledge of material behaviour will provide insight into process development, modeling and the optimization of critical ultra-precision machining processes.

Key words


Introduction

The investigation of ultra-precision machining is vital for developing new materials, tooling and processes. In the past extensive cutting tests were carried out to understand and optimize critical process parameters. This procedure is often costly and time consuming [Komanduri, 1993]. An alternate approach is to make use of detailed physics based models like Finite Element Analysis (FEA), Finite Difference Method (FDM), and Molecular Dynamic (MD) techniques. Through the use of FEA and FDM techniques, a wide range of problems in traditional machining applications have been investigated, such as determining the temperature and stress distribution in the cutting zone, residual stress and chip formation [Li et al, 1995]. FEA and FDM use continuum mechanics approaches to address metal cutting problems. In these techniques the workpiece material is looked at as a continuous structure where the micro-constituents such as crystal structure, grain sizes, and inter-atomic distances are neglected. In MD simulations the nodes, which define the resolution of the model, are selected based on the atomic structure of the material where the inter-nodal spacing relates to inter-atomic distances [Komanduri and Raff, 2001]. In this case detailed information related to material behavior is captured. Unfortunately the depths of cut and cutting speed, which can be investigated using MD, are not currently at levels commonly practiced in ultra-precision machining.

Calibrating the required material properties necessary to run the FEA models with experimental data is a significant challenge. As the size of the sample under study decreases the challenge increases due to the complexity of handling the workpieces and measuring the parameters under the required conditions of workpiece size, high stress and high strain rate. However, atomic based simulations like MD provide a means of acquiring new data that can assist in calibrating the material properties for use in an FEA model.

Thus this paper presents a new methodology to provide an FEA model with relevant material properties for ultra-precision machining. The approach used is based on the MD simulation of a uniaxial tension test configuration from which key material properties are extracted. In this way the nanometric scale information required for two dimensional FEA simulations evaluating the cutting force can be obtained. Ultra precision single point turning operations were performed and the cutting forces were measured using a high frequency, high resolution dynamometer. This was done to validate the forces obtained from the FEA model and to demonstrate the effectiveness and usefulness of the proposed technique.

Molecular Dynamic Simulation Model

Extensive experimental work has been carried out in metal cutting to develop, describe, and optimize cutting conditions and processes. This procedure is typically costly and time consuming. This has motivated the search for alternatives to expand our understanding of these processes while minimizing the experimental effort required. The molecular dynamic simulation approach was introduced in the early 1990’s to model nanometric cutting processes [Stowers et al, 1991; Belak et al, 1993; Li et al, 1995].
In this work, MD is used to acquire material properties at the nanometric level by conducting simulations of tension tests under nanometric scales as shown in figure 1.

The potential function used to describe the interatomic relations between the silicon atoms in this work is the Tersoff potential energy in the form:

\[ V = \sum_{i \neq j} \phi(r_{ij}) \]

Where:

\[ \phi(r_{ij}) = F_r(r_{ij}) + b_{ij}F_a(r_{ij}) \]

Where \( b_{ij} \) is a function of the cut-off radius and the angles between the atomic bonds. \( F_r(r_{ij}) \) & \( F_a(r_{ij}) \) are the repulsive and attractive forces between atoms \( i \) and \( j \) and can be represented as:

\[ F_r(r_{ij}) = Ae^{(-\lambda r_{ij})} \quad F_a(r_{ij}) = -Be^{(-\mu r_{ij})} \]

Some of the silicon properties and the computational parameters used in the MD model are listed in Table 1. MD simulations were carried out at different loading rates (20-500 m/s) to investigate the effect of strain rate on the material behaviour and mechanical properties. It was concluded that atomic rearrangements were slightly different with no obvious change in material behaviour. Figures (2-3) show the formation of the necking phenomena with 100 atoms at 0.5\( r_0 \) tensile load.

### Table 1: Parametric values and Silicon properties used in MD simulation

<table>
<thead>
<tr>
<th>Potential Energy function</th>
<th>Tersoff potential</th>
</tr>
</thead>
<tbody>
<tr>
<td>Configuration</td>
<td>2D</td>
</tr>
<tr>
<td>( A )</td>
<td>1830 eV</td>
</tr>
<tr>
<td>( B )</td>
<td>471 eV</td>
</tr>
<tr>
<td>( \mu )</td>
<td>1.7322 Å(^{-1})</td>
</tr>
<tr>
<td>( \lambda )</td>
<td>2.48 Å(^{-1})</td>
</tr>
<tr>
<td>Tension test</td>
<td>Uniaxial</td>
</tr>
<tr>
<td>Lattice structure</td>
<td>Diamond cubic</td>
</tr>
<tr>
<td>Lattice constant (( r_0 ))</td>
<td>5.43 Å</td>
</tr>
<tr>
<td>WP dimensions</td>
<td>16( r_0 ) x 4( r_0 )</td>
</tr>
<tr>
<td>Crystal orientation</td>
<td>[001]</td>
</tr>
<tr>
<td>Density</td>
<td>2328 kg/m(^3)</td>
</tr>
<tr>
<td>Temperature</td>
<td>300 K</td>
</tr>
<tr>
<td>Melting temperature</td>
<td>1410 °C</td>
</tr>
</tbody>
</table>

**Fig.2:** Initial atomic position for the tension test specimen

**Fig.3:** Simulation test for 100 atoms structure with 0.5\( r_0 \) stretch

**MD simulation results**

A different set of parameters was used to test and validate the proposed techniques performance under variable loading rates. Table 2 presents the corresponding values of the simulation results of key material properties. The stress-strain relation curves at
different loading rates for silicon are provided in figure 4.

Table 2: MD simulation results for Si

<table>
<thead>
<tr>
<th>$\sigma_{ut}$ (GPa)</th>
<th>$\varepsilon_{max}$ Stress</th>
<th>E (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td>0.25</td>
<td>165</td>
</tr>
</tbody>
</table>

Finite Element Model

Finite element analysis (FEA) is a simulation technique that can provide useful information and address a wide range of machining problems. It uses continuum mechanics approaches to address metal cutting problems where the workpiece material is considered a continuous structure where the micro-constituents such as crystal structure, grain sizes, inter-atomic distances…etc. are neglected. In this method, distances between nodes and number of nodes are selected based on the level of detail expected from the simulation. An orthogonal cutting test was then simulated using FEA. The model is developed using ABAQUS/Explicit Finite element solver (v.6.4). The workpiece and tool are constructed as 2D deformable shell structures. The cutting is performed using a diamond tool at 5 m/s constant cutting speed with a 10 micrometer depth of cut. The rake and clearance angles are both set to be of 10 degrees. The cutting was simulated under dry conditions. Figure 5 shows the simulation setup with the tool/workpiece arrangement.

The linear elastic as well as the nonlinear plastic behaviour of the workpiece material is introduced to the FEA model from the data acquired through the MD simulation model. The crack propagation criterion is based on the plastic strain failure inequality described as follows:

$$\varepsilon_{pl} \geq \varepsilon_{pl}^f$$

Where $\varepsilon_{pl}^f$ is the current plastic strain on each element of the model and $\varepsilon_{pl}^f$ is the maximum allowable plastic strain before failure.

The FEA model presented provides the necessary link between the MD simulation model and the experimental work. It gives the means required to validate both the MD and the FEA models by comparing their combined results (figure 6) to the experimental ones obtained in the lab for the prediction of the forces during the cutting process.

Experimental Setup

Experimental validation of the MD simulation model and FEA model were conducted on a Precitech machine with nanometric position accuracy using a
diamond tool for a 10 micron depth of cut and a 10\(\mu\)m/rev feed rate. Figure 8 shows the arrangement setup between the silicon wafer on the vacuum chuck and the tool holder setting on the Kistler Mini-Dynamometer for the force measurement using Lab view software.

![Image](image.png)

**Fig.7: Experimental setup on the Precitech machine**

**Experimental Results**

Cutting forces were measured with the Kistler MiniDyn through Lab view software. Figure 8 shows the variation of the cutting forces with time. Comparing figure 6 and 8, we can conclude that there is a good agreement between the theoretical values calculated using the hybrid MD-FEA model and the experimental values measured in the micro-cutting lab. Cutting forces were found to be in the order of 15-20 Newton for a 10\(\mu\)m depth of cut.

![Image](image.png)

**Fig.8: Cutting forces from experimental test**

**Conclusion**

In this work, we introduced the use of molecular dynamics and dislocation theory as a link between nano-scale and meso-scale modules with the finite element method calculations serving as a bridge between the modules. The purpose of this work is to fill the void between the nanometric scale information required to model micro-cutting and the known macro-scale mechanical behaviour of materials in metal cutting. The proposed study suggests several future perspectives for the use of alternative modules aiming to further our knowledge of material behaviour modeling related to manufacturing processes.

**References**


