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Prediction of cutting forces in the micro-machining of silicon using a "hybrid molecular dynamic-finite element analysis" force model

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Abstract

The study and development of micro-machining technology has been an area of ongoing focus for numerous researchers. Interest in this topic has been increasing over the past decade due to the trend towards higher accuracy, smaller-sized components. Linking material property acquisition and modelling in the nanometric scale with those on the micro-scale is a considerable challenge in material science in general and in micro-machining in particular. Due to computational limitations it is presently extremely difficult to inflate atomic level models and simulations to the micro-sized component dimensions. This detailed knowledge of material behaviour will provide the necessary insight to support process development, modelling and the optimization of critical ultra-precision machining processes. This paper presents a new methodology of providing a finite element model of the micro-cutting process with relevant material properties acquired from a newly developed molecular dynamics simulation model of a uniaxial tension test performed on silicon. Material properties such as yield stress, ultimate stress and modulus of elasticity are extracted from the stress–strain curve produced by the molecular dynamics model and automatically fed to the finite element model to evaluate the cutting forces required to machine a silicon wafer using different cutting parameters.

Keywords: Ultra-precision machining; Micro-machining brittle materials; Cutting forces prediction; Molecular dynamic simulation; Nanometric material properties; Finite element analysis

1. Introduction

The investigation of micro-machining is fundamental to the development of ultra precision processes involving new materials and tooling. In the past, extensive cutting tests were carried out to understand and optimize different process parameters. These procedures are often costly and time consuming [1]. An alternative 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, as well as residual stress and chip formation [2]. 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. Conversely, 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 [3]. In this case detailed information related to material behaviour 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.

The calibration of the required material properties necessary to run the FEA models with experimental data is a significant challenge. As the size of the specimen under study decreases the challenge increases due to the complexity of handling the specimen and measuring the parameters under the required conditions of workpiece

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Nomenclature

r_{ij}	interatomic distance between atoms i and j (Å)
$\phi(r_{ij})$	potential energy function (J)
θ_{jik}	angle centred on atom I (deg)
θ_{ijk}	bond angle between bonds ij and ik (deg)
$F_r(r_{ij})$	repulsive force between atoms i and j (N)
$F_a(r_{ij})$	attractive force between atoms i and j (N)
$R_c(r_{ij})$	cutoff radius function (Å)
q_i^{old}	old atoms' coordinates (Å)
q_i^{new}	new atoms' coordinates (Å)
Δq	Markov step size
ξ_i	randomly generated numbers from a uniform distribution interval [0,1]
ξ_k	random number from the kth Markov step
$\Delta\phi$	potential energy change of the system for the kth Markov step (J)
$\Delta\phi_{min}$	proximity error factor (J)
G	material shear modulus (GPa)
η	material viscosity coefficient
τ	relaxation time (s)
T	material temperature (K)
U	activation energy of the regrouping process (J)
K_B	Boltzmann constant ($1.38 \times 10–23$ J/K)
ω	damage parameter for the finite element model
m	strain rate sensitivity index
$\dot{\varepsilon}_0$	reference strain rate (s^{-1})
$\bar{\dot{\varepsilon}}_{pl}$	equivalent plastic strain rate (s^{-1})
$\Delta\bar{\varepsilon}_{pl}$	equivalent plastic strain increment (s^{-1})
$\Delta\bar{\varepsilon}_{pl}^{f}$	maximum allowable plastic strain before failure (s^{-1})
$\bar{\sigma}$	yield stress at non zero strain rate (GPa)
τ_{max}	maximum shear stress (GPa)
p	Material pressure stress (GPa)
q	Von Misses stress (GPa)
θ	current material temperature (K)
θ_{melt}	material melting temperature (K)
$\theta_{transition}$	temperature at or below which no temperature dependence on yield stress expansion (K)
$\hat{\theta}$	non-dimensional temperature
R_a	surface roughness (μm)

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.

Extensive experimental work has been carried out in metal cutting to develop, describe, and optimize cutting conditions and processes. Presently material properties are often determined using tensile, shear, compression, and indentation tests. Performing tensile tests on extremely small workpieces and collecting meaningful nano-indentation results is very challenging. They require procedures that are extremely difficult, time consuming and the use of sophisticated equipment that is typically quite costly. Also, the production of a realistic workpiece samples in the form of a tensile specimen or nano-indentation sample is very difficult and requires special preparation methods so as to not to alter the properties and structure of the material.

Some experimental studies were conducted at the micro-level inside a scanning electron microscope as well as an atomic force microscope with a scanning tunnelling microscope [4,5]. Silicon specimens were prepared by etching to the shape of a tensile test specimen with lengths varying from 30 to 300 μm and a width of 2–5 and 2 μm thick. It was found that the etching procedure used for the production of these test specimens affected the measured properties. One of the major problems was with the difficulty in calibrating the micro-actuators used to deliver the uniaxial force required for measurement. In this study an atomic force microscope was used to observe the elongation of the specimen while it was being pulled in uniaxial tension. It has been observed that there was an order of magnitude difference between the experimental sizes in micro-metres to the nanometric sizes required for determining the material properties at the nanometric scale.

This has motivated the search for alternatives to expand our understanding of these processes while minimizing the experimental effort required. To this end the authors' effort has been focused on implementing a molecular dynamic model to assist in understanding material properties on this scale.

The molecular dynamic simulation approach was introduced in the early 1990s to model nanometric cutting processes [2,6,7]. Presently the MD simulation of nanometric level cutting process simulations has been carried out at very high cutting velocities; i.e. on the order of 200–500 m/s. This is done to save on computation time by bringing the cutting speed closer to the atomic movement speed. This compromise allows one to model the cutting process but the results are unrealistic when compared to practical cutting operations typically involving cutting speeds of 2–10 m/s. These simulations were also applied on single crystal cubic metals such as Al, Cu, Ni for face centered cubic metals (FCC) and Fe and Cr for body centered cubic (BCC) metals, to investigate the mechanism of deformation and fracture. Failure of the workpiece due to nanometric cracks and void formation were then compared to the macro-scale processes [4]. In these tests the loading rates were found to affect the estimation of the material properties such as the strain at failure. This was found to be estimated at higher values than the ones reported at the macro-scale level. The stress–strain relationship obtained from such simulations show the same trend of behaviour as compared to the normal scale but with a different order of magnitude [1]. Studies have shown that the radius of the neck formed in the middle section of