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Oluwajobi, Akinjide O. and Chen, Xun

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Simulation of Abrasive Machining Using Molecular Dynamics

A.O. Oluwajobi and X. Chen

Centre for Precision Technologies, University of Huddersfield, Queensgate, Huddersfield HD1 3DH, UK

Introduction

The development of ultra-precision processes which can achieve excellent surface finish and tolerance at nanometre level is now a critical requirement for many applications in medical, electronics and energy industry. Presently, it is very difficult to observe the diverse microscopic physical phenomena occurring in nanometric machining through experiments. The use of Molecular Dynamics (MD) simulation has proved to be an effective tool for the prediction and the analysis of these processes at the nanometre scale. The complexity and the cost of experimental investigation have made this approach even more suitable as simulation results sometimes point interesting directions for experimentation.

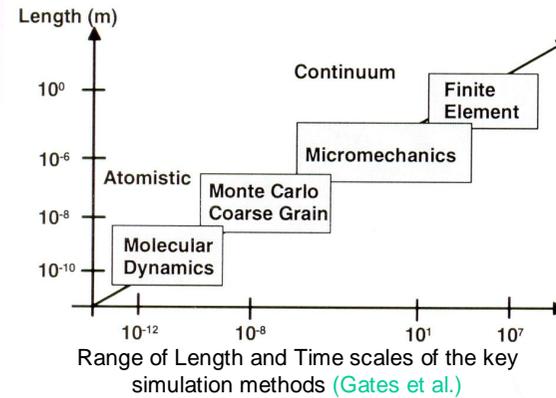
Objective

To model abrasive machining using the Molecular Dynamics (MD)

Methodology

The outline of the MD simulation is as follows:

- Choose the model, choose an appropriate interatomic potential and the means of calculating the equations of motion
- Initialize the model
- Relax the model from its initial state to its dynamically equilibrium condition
- Run the simulation and analyze the results



Equations

Newton's Law

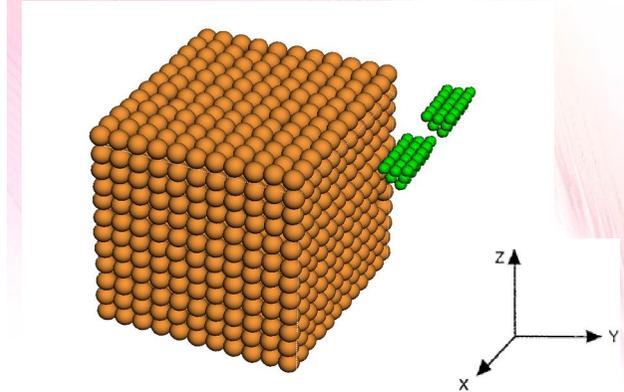
$$F_i = - \frac{\partial}{\partial r_i} V(r_i, \dots, r_N) \quad \dots\dots(1)$$

L-J Potentials

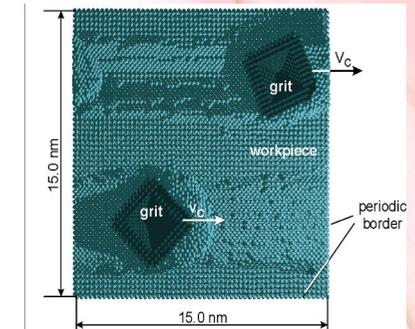
$$V_{ij} = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad \dots\dots(2)$$

Basic Verlet Algorithm

$$r(t + \Delta t) = 2r(t) - r(t - \Delta t) + a(t)\Delta t^2 \dots(3)$$



Schematic of the MD Simulation



Modelling of two abrasives that cut through a workpiece over its whole length at 100m/s using MD Groove Scratching with 2 Grits (top view - 360 000 time steps, 144 ps) (Brinksmeier et al 2006)

Conclusions

The MD simulation provides details of the abrasive machining at the atomistic level.