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MODELLING ABRASIVE MACHINING TECHNIQUES USING MOLECULAR DYNAMICS

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ABSTRACT

The development of ultra-precision processes which can achieve nanometre surface finishes and tolerances 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 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. A review of the MD was undertaken, as this method can improve our understanding of nanometric processes and subsequently minimize experimental efforts.

Keywords abrasive machining, molecular dynamics, modelling

1 INTRODUCTION

Although abrasive machining is a century-old technology, it still plays an important role in industry today. In fact the need for high accuracy and high efficiency machining of difficult-to-machine materials is making the application of abrasive technologies increasingly important. Also, the abrasive machining has an advantage that the failure of one cutting edge doesn't affect the process unlike other machining processes, because machining is performed with a large number of cutting edges (Inasaki et al 1993). Conventionally, the finite element method has been used to model processes and deformation at the macro and micro levels, but it was found to be difficult to apply to micromachining processes around 1nm (Inamura et al 1993). The MD can readily be used to solve such problems, as it is an effective microscopic approach for analysis from the atomistic viewpoint. The MD method was initiated in the late 1950s at Lawrence Radiation Laboratory in the US by Alder and Wainwright in the study of statistical mechanics (Alder and Wainwright 1959). Since then, the use of the simulation method has spread from Physics to Materials Science and now to Mechanical Engineering. In the field of nanometric cutting, Belak pioneered work on the study of cutting copper with a diamond tool (Belak and Stowers 1990). Initially, the method was used extensively to model indentation and cutting (see figures 1 and 2). In 1991, Belak and Stowers first applied the MD to abrasive processes (Belak and Stowers 1991) and Rentsch and Inasaki's study later presented the first results of simulations targeted on the pile-up phenomenon in abrasive machining (Rentsch and Inasaki 1994). Relatively, not many studies have been carried out on abrasive machining, and this may likely be due to difficulties in developing suitable models in terms of the micro topography and in terms of the required potential functions for the material and interactions of interest. Also, MD studies have been restricted to single or few grits interfering with a work piece (Brinksmeier et al 2006). All these call for more studies on abrasive machining MD simulations.

2 THE MOLECULAR DYNAMICS METHOD

Molecular dynamics (MD) is a computer simulation technique used in the study of the motions of a set of particles – atoms. The technique works by following the time evolution of a set of interacting atoms while integrating their equations of motion. The method is based on statistical mechanics – a way to obtain a set of configurations distributed according to some statistical distribution function (Ercolessi 1997).

The simulation consists of the numerical, step-by-step, solution of the classical equations of motion. For a set of N atoms,

$$F_i = m_i a_i \quad (1)$$

Where m_i is the mass of atom i, $a_i = \frac{d^2 r_i}{dt^2}$, the acceleration of the atom i and F_i is the force acting on atom i. (The forces are usually obtained as the gradient of a potential energy function, see equation 2).

The outline of the MD simulation is as follows:

- Choose the model, choose an appropriate molecular 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

2.1 Choose the model, choose an appropriate molecular potential and the means of calculating the equations of motion

The major task in a MD simulation is the selection of the potential. This is a function, $V(r_1, \dots, r_N)$ of the position of the nuclei which represents the potential energy of the system. Where (r_1, \dots, r_N) represents the complete co-ordinate position of the atoms. Then forces are derived from it as,

$$F_i = -\frac{\partial}{\partial r_i} V(r_1, \dots, r_N) \quad (2)$$

Strictly speaking, the problem of modelling a material is that of finding a potential function for that material. If the potential function doesn't model the behaviour of the atoms correctly, the results produced from the simulation would be wrong. As examples, the following are potentials and are adequate for the following materials – indicated below, viz; Lennard-Jones, Morse, Tersoff, Born-Meyer and Embedded-Atom potentials (Komanduri and Raff 2001).

Lennard-Jones Potential:

$$V_{ij} = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad (3)$$

Where σ is a constant which is dependent on the physical properties of the material. This potential is suitable for rare gases (argon, krypton).

Morse Potential:

$$V_{ij} = D \{ \exp[-2\alpha(r_{ij} - r_e)] - 2 \exp[-\alpha(r_{ij} - r_e)] \} \quad (4)$$

Where,

r_{ij} and r_e are instantaneous and equilibrium distances between atoms i and j respectively
 α and D are constants determined on the basis of the physical properties of the material

The Morse potential is suitable for cubic metals.

Tersoff Potential:

$$V_{ij} = V_r(r_{ij}) - B_{ij} V_a(r_{ij}) \quad (5)$$

Where V_r and V_a are the potentials due to repulsive and attractive forces between atoms i and j and B_{ij} is a parameter that provides the information for the direction and the length of the bond. The Tersoff potential is used for covalently bonded materials like silicon atoms.

Born-Meyer Potential:

$$V_{ij} = A \{ \exp[-2\alpha(r_{ij} - r_0)] \} \quad (6)$$

Where A and r_0 are constants dependent on the material.

This potential is used for ceramics.

Embedded-Atom Potential:

$$V_{ij}(R) = U_{ij}(R) + 2G'_i(\bar{\rho}_i)\rho_j^a(R) + G''_i(\bar{\rho}_i)(\rho_j^a(R))^2 \quad (7)$$

Where U_{ij} is an electrostatic interaction between two atoms, G is the embedding energy, $\bar{\rho}$ is a constant background density, ρ^a is the average atomic electron density of atom and R is the separation of the atoms.

The i and j depict the interacting atoms, G' and G'' are the derivatives of G . The embedded-atom potential was developed for a wider range of metals. It incorporates an approximation for the many-atom interactions neglected by the pair-potential scheme.

The list of the potentials is not exhaustive; and there are other potentials which are modified forms of the ones already discussed.

Generally, the most commonly used interaction model is the Lennard-Jones (LJ) pair potential. It is the standard potential to use for all the investigations where the focus is on the fundamental issues, and not studying the properties of a specific material.

After the choice of the potential, the next step is to select an appropriate algorithm for the integration of the equations of motion. This is the main kernel of the simulation program. The MD simulation is based on Newton's second law of motion. The time integration algorithms for the solution of these equations are based on finite difference methods. It is important to note that this is so because the collisions between atoms are not instantaneous, but they are strong repulsive and attractive interactions that occur over a finite duration. Examples of these methods are Verlet and predictor-corrector algorithms.

The Verlet algorithm is of three types, namely; the basic (position) Verlet, the Verlet Leapfrog and the velocity Verlet algorithms. The basic Verlet algorithm uses two, third order Taylor expansions, and calculates the positions at the next time step from the positions at the previous and current time steps. The predictor-corrector algorithm, on the other hand consists of three steps. The first step is to predict (by Taylor expansion) positions and their time derivatives at time, $t + \Delta t$, from values known at a time t . The second step is to compute the force by taking the potential at the predicted positions, and comparing the resulting acceleration, with the predicted acceleration. The last step is to correct the positions and their derivatives by using the difference between the computed and the predicted acceleration (known as the error signal). The predictor-corrector algorithm gives more accurate results, but it is computationally expensive and requires large storage.

2.2 Initialize the model

To initialize the simulation, the MD 'box' (the control volume) must be defined and initial positions and velocities of the atoms must be assigned – this is a kind of initial randomization.

Positions of the atoms can be defined, by assuming certain crystal structure and the initial velocities can be randomly assigned.

2.3 Relax the model from its initial state to its dynamically equilibrium condition

The model of having atoms positioned and assigned velocities as above implies that additional potential energy between atoms has been artificially applied to the system. This is not the case in real solids, where atoms are actually vibrating around their equilibrium positions. So, it is necessary to relax this initial model from its artificially assigned initial conditions to its natural, dynamically equilibrium condition.

2.4 Run the simulation and analyze the results

The simulation is then run and the results analyzed. See figures 3 and 4. Using the MD, the effect of such variables as edge effect, cut depth et cetera can be defined and the simulations conducted accordingly. It is also easy to vary the properties of the work materials and the cutting tools in MD simulations (Komanduri and Raff 2001).

3 EXAMPLES OF MD SIMULATION OF ABRASIVE MACHINING

(Rentsch and Inasaki 1994) modelled a copper work material and a diamond tool for their study. They used the Lennard-Jones potential function for the copper atom interactions, but kept the boundaries and the tool stiff. A total of 11476 atoms in 13 horizontal (1,1,1) – layers of fcc-lattice were used for the copper, and the tool was shaped from a diamond lattice block by clearing on the four (1,1,1) –planes. Using a cutting speed of 100m/s, they observed a pronounced build-up phenomenon after 25000 time steps (see figure 3).

The MD simulation of nanometric cutting was carried out with a range of negative-rake tools to simulate the Ultra-Precision Grinding (UPG) process by (Komanduri et al 1999). A copper work material and an infinitely hard tool (tungsten) were used in the simulations. A pairwise sum of Morse potential was used for the study, in which they concluded that simulation tests can facilitate a better understanding of the process without the need for expensive and time consuming machining or grinding experimental work.

The investigation of the fundamental atomistic processes in chemical mechanical polishing of copper was carried out by (Ye et al 2002). They simulated the nanoscale polishing of a copper surface by a single abrasive particle, using the embedded atom method potential. They focused on the mechanical abrasion aspect of material removal and found that dislocations and atomically rough planarized surface were formed.

(Lin et al 2003) used the MD method to survey the features of grinding energy dissipation, grinding stress, strain state and grinding temperature in the atomic space. The workpiece and the tool materials were assumed to be monocrystalline silicon with a covalent bond and diamond respectively. A Tersoff potential function, suited to a multibody system was employed for the simulation. They found out that as the abrasive grain cut into the workpiece continuously, the value of the grinding force increased gradually in a repeated fluctuation manner. Also, it was observed that atoms of the crystal lattice were reconstituted and parts of the non-crystal atoms were piled up on the front of the abrasive grain.

To be more realistic, (Rentsch and Inasaki 2006) extended the state-of-the-art MD material modelling to consider fluids like coolants. They considered the impact of such fluids on the surface generation and the tribological contact conditions. The fluid-fluid interactions were calculated on the basis of the Lennard-Jones potential function and the embedded potential function was used for the inner workpiece reactions (the internal tool dynamics were ignored). They observed an intensive self-diffusion of the fluid atoms, and these filled the whole free space above the workpiece. No impact on the stress distribution was observed, but the whole fluid-tool/workpiece contact was heated up in a narrow range.

Rentsch and Brinksmeier obtained a 3-D MD simulation of the grinding process (Brinksmeier et al 2006). Using the embedded atom method potential and 100000 atoms, they modelled two abrasives that cut through a workpiece over its whole length at 100m/s (see figure 4). They found that the periodic borders in the horizontal plane led to complete groove formation in the cutting direction.

The MD simulations of nanoindentation followed by scratching at constant depth on the Si-terminated (0 0 1) surface of 3CSiC was carried out by (Noreyan and Amar 2008). They investigated the dependence of the friction coefficient, scratch hardness, and wear on scratching depth, velocity, direction, and indenter size and shape. The workpiece was assumed to have the 3C SiC cubic crystal structure, and a diamond tip was used. Both were modelled using the Tersoff potential. They found that the friction coefficient and the scratch hardness increased with indentation depth but decreased with increasing scratching velocity. They also noted that the direction dependence of the friction coefficient is weaker at high scratching velocity.

In most of the MD simulations, the representation of the abrasives have been simplified to a block, pyramid, or shell of stiff atoms with sharp or rounded edges that have no dynamics themselves (Brinksmeier et al 2006). There is need for more studies on the dynamics within the abrasives.

4 CONCLUSION

The MD simulation is a powerful tool for the understanding of the abrasive process. It can be used to obtain information on cutting force, grinding force, friction coefficient, the result of the chip removal process, and also to predict deformation conditions which cannot be easily duplicated experimentally. Such information could open up a huge potential to improve abrasive machining performance at the nano-scale. It can be seen that most current MD analyses are theoretical simulation. Little information is available on experimental validation. This may suggest that a lot of work has to be done before MD could be applied to actual practical works.

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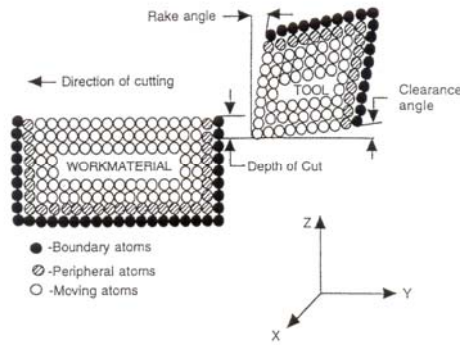


Figure 1: Schematic of the MD Simulation of Nanometric Cutting (2D) (Komanduri and Raff 2001)

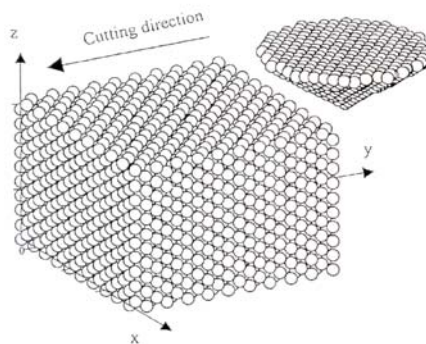


Figure 2: Schematic of the MD Simulation of Nanometric Cutting (3D)(Fang and Weng 2000)

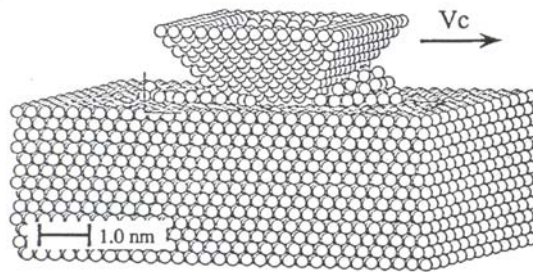


Figure 3: Advanced MD Simulation with Straight Aligned Tool (Rentsch and Inasaki 1994)

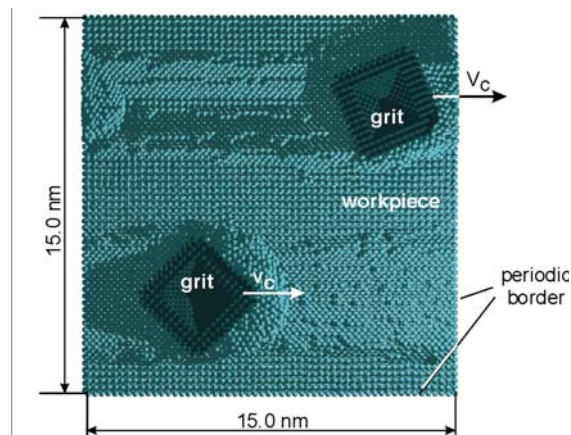


Figure 4: - Groove Scratching with 2 Grits (top view - 360 000 time steps, 144 ps) (Brinksmeier et al 2006)