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The Effect of Interatomic Potentials on Nanometric Abrasive Machining

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Abstract— **One of the major tasks in a Molecular Dynamics (MD) simulation is the selection of adequate potential functions, and if the potentials don't model the behaviour of the atoms correctly, the results produced from the simulation would be useless. Three popular potentials namely; Embedded- Atom Potential (EAM), Morse and the Lennand-Jones, were employed to model copper workpiece and diamond tool in nanometric abrasive machining. From the simulation results and further analysis, the EAM potential was found to be the most reliable because it best describes the metallic bonding of the copper atoms and it demonstrated the lowest cutting force variation. More pile of atoms is observed during the phenomenon of ploughing and the potential and total energies are more stable with the EAM.**

Keywords- Interatomic Potentials; Molecular Dynamics; Abrasive Machining

I. INTRODUCTION

Abrasive machining is one of the oldest technologies that human beings had applied, but it still plays an important role in industry today. The need of high accuracy and high efficiency machining for difficult-to-machine materials makes the application of abrasive machining technology increasingly important. Further, abrasive machining has an advantage that the failure of one cutting edge does not affect the process unlike other machining processes, because the abrasive machining is performed by a large number of cutting edges [1]. The development of ultra–precision processes which can achieve excellent surface finish at nanometre level is now a critical requirement for many applications in medical, electronics and energy industry. Currently, it is very difficult to observe the diverse microscopic physical phenomena occurring in nanometric machining through experiments. The use of Molecular Dynamics (MD) simulation may prove to be an effective tool for the analysis and prediction of machining 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 the right directions for experimentation.

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 [2]. Since then, the use of the simulation method has spread from Physics to Materials Science and now to Mechanical Engineering. The major task in a MD simulation is the selection of an adequate potential function, and if the potential doesn't model the behaviour of the atoms correctly, the results produced from the simulation would be useless. This is very important as the MD method can improve our understanding of nanometric processes and subsequently give helpful insights into phenomena that are otherwise intractable to investigate experimentally.

In the field of nanometric cutting, Belak pioneered work on the study of cutting copper with a diamond tool [3]. Initially, the method was used extensively to model indentation and cutting (see Figs. 1 and 2).

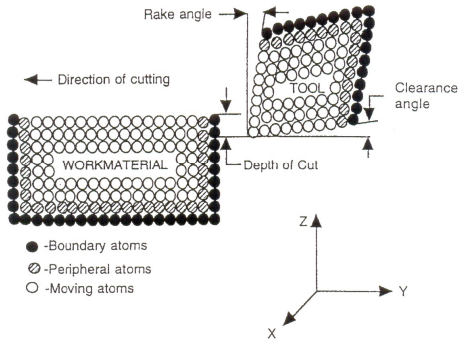

Figure 1. Schematic of the MD Simulation of Nanometric Cutting (2D) [4]

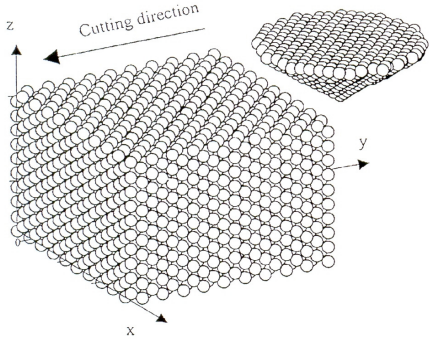

Figure 2. Schematic of the MD Simulation of Nanometric Cutting (3D) [5]

In 1991, Belak and Stowers first applied the MD to abrasive processes [6] and Rentsch and Inasaki's study later presented the first results of simulations targeted on the pile-up phenomenon in abrasive machining [7]. 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 selection of potential functions for the material and interactions of interest. Also, MD studies have been restricted to single or few grits interfering with a workpiece [8]. All these call for more studies on abrasive machining MD simulations.

II. FUNDAMENTALS OF MD AND EXAMPLES OF MD SIMULATIONS OF ABRASIVE MACHINING

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 the equations of their motion. The MD is deterministic. Once the positions, velocities and accelerations of the particles are known, the state of the system can be predicted. The method is based on statistical mechanics – a way to obtain a set of configurations distributed according to some statistical distribution functions [9].

The MD simulation is based on Newton's second law of motion. It consists of the numerical step-by-step solution of the classical equations of motion. For a set of N atoms,

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

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).

Rentsch and Inasaki [7] modelled a copper workpiece and a diamond tool using the Lennard-Jones potential function for the copper atom interactions, but kept the boundaries and the tool stiff. They observed a pronounced build-up phenomenon after 25000 time steps (See Fig. 3).

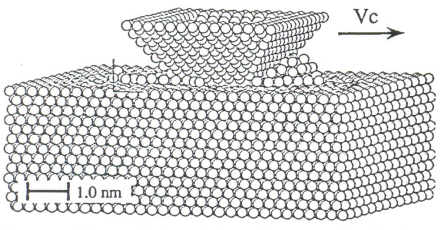

Figure 3. Advanced MD Simulation with Straight Aligned Tool [7]

Komanduri et al [10] used copper workpiece and an infinitely hard tungsten tool for their simulation. They used Morse potentials and a cutting speed of 500m/s. Ye et al [11] investigated the chemical mechanical polishing of copper by a single abrasive particle, using the EAM potential. Lin et al [12] surveyed the features of grinding energy dissipation, grinding stress, strain state and grinding temperature in the atomic space. They used silicon as the workpiece and the tool materials, using the Tersoff potential function. Rentsch and Brinksmeimier obtained a 3-D MD simulation of the grinding process [8]. Using the EAM potential and 100000 atoms, they modelled two abrasives that cut through a workpiece over its whole length at 100m/s (See Fig. 4).

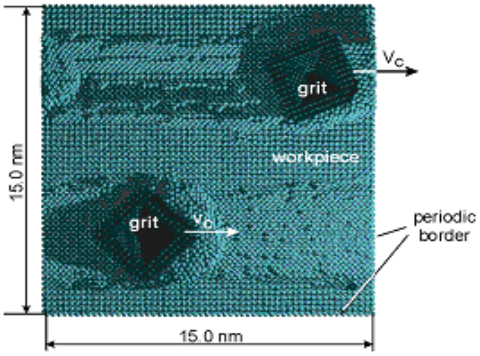

Figure 4. Groove Scratching with 2 Grits (top view - 360 000 time steps, 144 ps) [8]

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 [8]. Pei et al [13] and Promyoo el [14] carried out MD simulations of the nanometric cutting of copper with diamond tool. They both studied the effects of the tool rake angle and the interatomic potentials (Morse and EAM) on the process. Pei et al [13] found out that there is no big difference in the simulated chip formation, but Morse potential results in about 5-70% higher cutting forces than the EAM potential. They both found EAM to be better than Morse potential for the simulations. Their studies were based on 2-D models, but the performance of 3-D simulations remains unknown.

III. INTERATOMIC POTENTIALS FOR MD

A material is made up of atoms, which are bound by chemical reactions, and these reactions are interactions between electrons and nuclei. The exact prediction of the correlation between the micro/nano-structure and properties of materials requires a solution of the time dependent Schrödinger wave equation (See equation 3) for about 10^{23} nuclei and electrons in a real material, with a Hamiltonian describing the entire particle interactions involved in the problem [15].

$$i\hbar \frac{\partial}{\partial t}\Psi(r,t) = -\frac{\hbar^2}{2m}\nabla^2\Psi(r,t) + V(r)\Psi(r,t) \qquad (3)$$

This is extremely computationally demanding, and it is not currently feasible. To overcome this limitation, near-first-principles ab initio calculations/methods are used.

The energy of N interacting particles can be written as [16,17]

$$E = \sum_i V_1(r_i) + \sum_{i<j} V_2(r_i, r_j) + \sum_{i<j<k} V_3(r_i r_j r_k) + ... \quad (4)$$

Where r_n is the position of the nth particle and the functions V_1, V_2, V_3 are the m-body potentials.
So, it follows that the potential of a system $V(r_1, r_2, ...r_N)$ can be assumed to be the sum of the effective pair potentials $V(r_{ij})$ as,

$$V = \sum_i \sum_{j>i} V(r_{ij}) \quad (5)$$

Where r_{ij} is the distance between particles i and j.

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. Morse is also an example of a pair potential which is suitable for modelling cubic metals. The EAM is a many-body potential, which is used for a wider range of metals.

A. Lennard-Jones Potential [18]

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

Where σ is a constant which is dependent on the physical property of the materials.

B. Morse Potential [19]

$$V_{ij} = D\{\exp[-2\alpha(r_{ij} - r_e)] - 2\exp[-\alpha(r_{ij} - r_e]\} \quad (7)$$

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

C. Embedded-Atom Potential (EAM) [20, 21]

$$E_{tot} = \sum_i G_i(\rho_{h,i}) + \frac{1}{2}\sum_{i,j} V_{ij}(r_{ij}) \quad (8)$$

Where $\rho_{h,i}$ is the total electron density at atom i due to the rest of the atoms in the system.

G_i is the embedding energy for placing an atom into the electron density
$V_{i,j}$ is the short range pair interaction representing the core-core repulsion
r_{ij} is the separation of atoms i and j

TABLE 1. MD SIMULATION PARAMETERS

Parameters	**Values**
Bulk Temperature	*293 K*
Cutting Direction	*[100]- Along the x-axis*
Cutting Speed	*150m/s*
Cutting Depth	*1.0nm*
Time Step	*0.3fs*
Run	*100000steps*

Table 1 shows the simulation conditions applied in this research. The workpiece consists of 16000 copper atoms with perfect FCC lattice. It includes 3 kinds of atoms namely; boundary atoms, thermostat atoms and Newtonian atoms. The boundary atoms are kept fixed to reduce edge effects. The thermostat atoms conduct the heat generated during the cutting process out of the workpiece and the Newtonian atoms obey the Newton's equation of motion. The cutting tool consists of 912 carbon atoms with perfect diamond lattice structure. The cutting tool is pointed shaped and it is modelled as a rigid body.
The atomic interactions in the simulation are the following, namely;
Cu-Cu : interactions between copper atoms
Cu-C : interactions between copper atoms and diamond atoms
C-C : interactions between the diamond atoms (treated as rigid)
The LAMMPS MD software [22] was used for the simulations.

D.. Modelling with Lennard-Jones (LJ) Potential

Equation (6) is used, where σ and ε are constants which are dependent on the physical property of the material. The LJ parameters used for the atom interactions are σ = 2.2277 Angstroms and ε = 0.415eV [23], which apply to both the Cu-Cu and the Cu-C interactions.

The simulation and the cutting forces are shown in Figs. 5a and 5b. The potential energy and the total energy for the LJ modelling are given in Fig. 6 and the temperature variation is shown in Fig. 7.

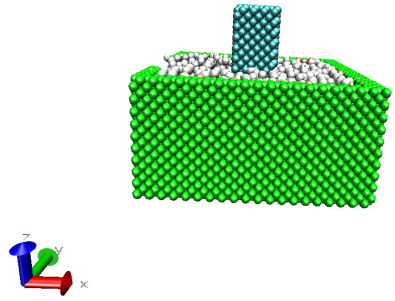

Figure 5a: Simulation with LJ Potential

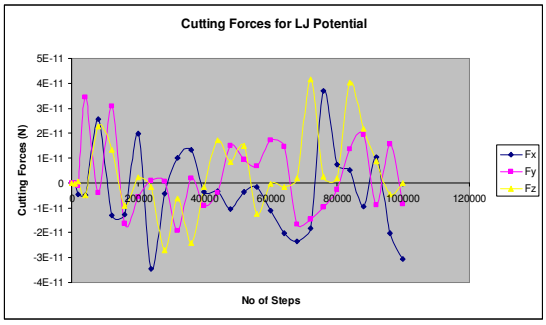

Figure 5b: Cutting Forces for LJ Potential

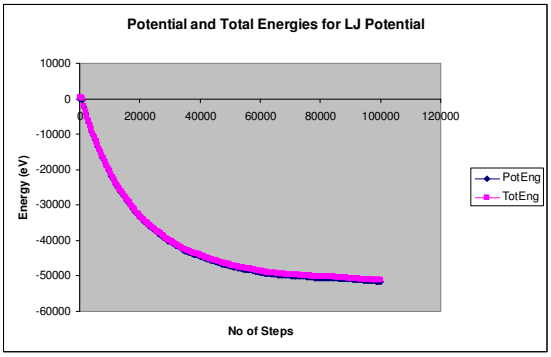

Figure 6: Potential and Total Energies for LJ Potential

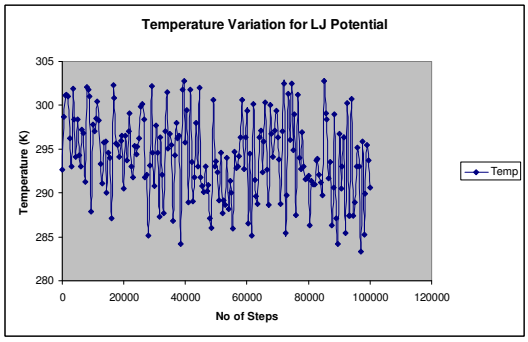

Figure 7: Temperature Variation for LJ Potential

E. Modelling with Morse Potential

Equation (7) is used;

For Cu-Cu interactions: [24, 13]

$D = 0.3429eV,\ \alpha = 0.13588(nm)^{-1},\ r_e = 0.2866nm$

For Cu-C interactions: [23]

$D = 0.087eV,\ \alpha = 0.17(nm)^{-1},\ r_e = 0.22nm$

Cut-off distance was 0.64nm (that is, the interactions between atoms separated by more than this distance are neglected).

The simulation and the cutting forces are shown in Figs. 8a and 8b. The potential energy and the total energy for the Morse modelling are given in Fig. 9 and the temperature variation is shown in Fig. 10.

F. Modelling with EAM Potential

Equation (8) is used, (the parameters used for the Cu-Cu interactions are from the file - Cu_u3.eam in LAMMPS and [19]). These parameters were also used for Cu-C interactions. (Ideally, this should not be the case, but the errors should be negligible, because the tool edge is treated as rigid).

The simulation and the cutting forces are shown in Figs. 11a and 11b. The potential energy and the total energy for the EAM modelling are given in Fig. 12 and the temperature variation is shown in Fig. 13.

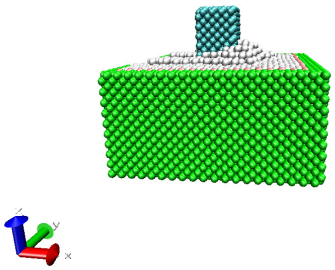

Figure 8a. Simulation with Morse Potential

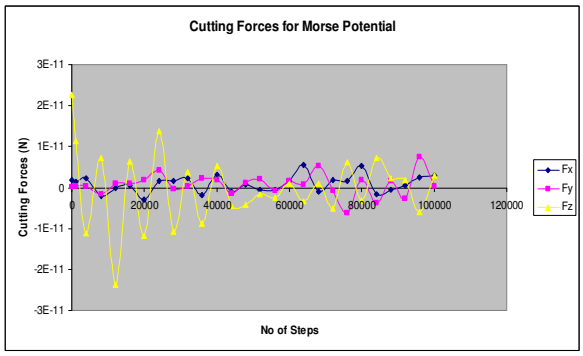

Figure 8b. Cutting Forces for Morse Potential

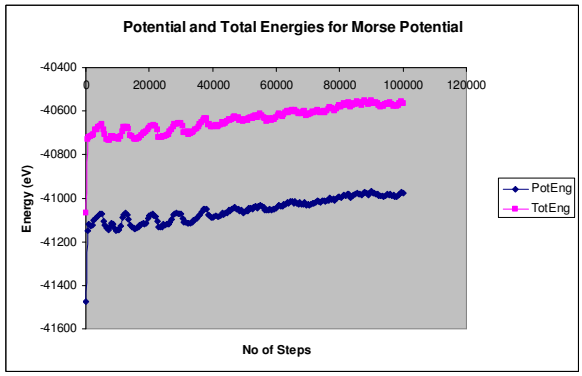

Figure 9. Potential and Total Energies for Morse Potential

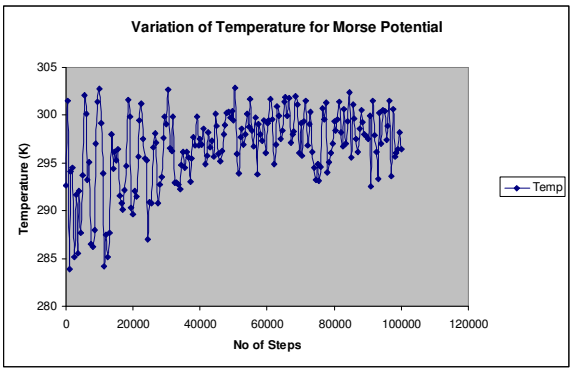

Figure 10. Temperature Variation for Morse Potential

G. Modelling with EAM Potential

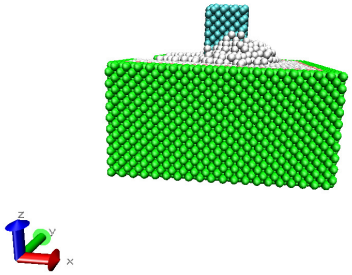

Figure 11a. Simulation with EAM Potential

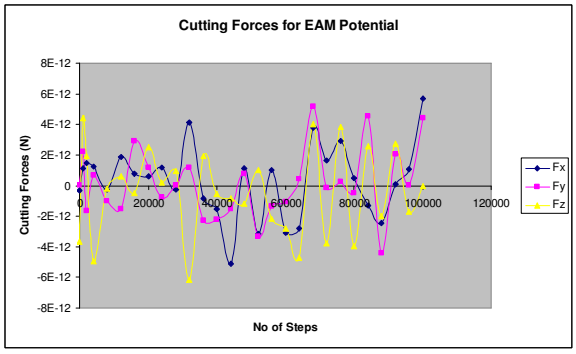

Figure 11b. Cutting Forces for EAM Potential

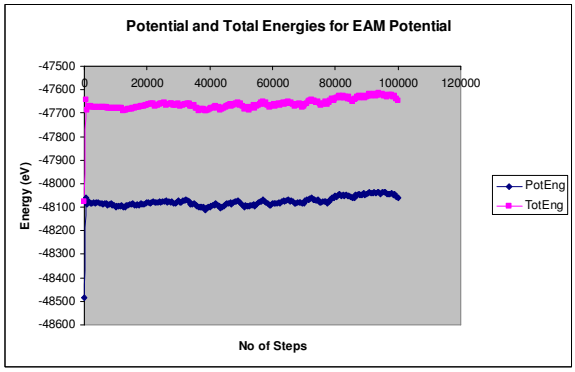

Figure 12: Potential and Total Energies for EAM Potential

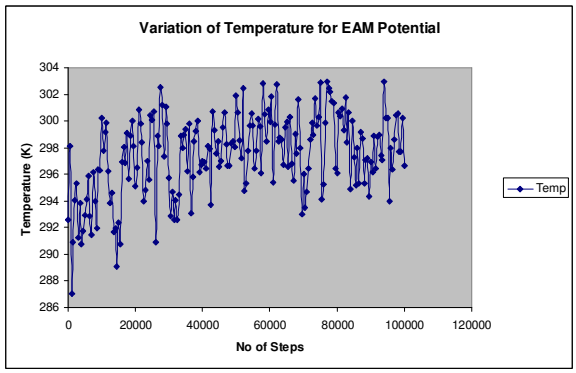

Figure 13: Temperature Variation for EAM Potential

RESULTS AND DISCUSSION

For the LJ model, the cutting forces varied in the range from around -3.5E-11N to 4.0E-11N; the phenomenon of ploughing was not observed; and the potential energy and total energy were initially unstable, but stabilizing after 60000steps. As observed in Fig. 5a, the copper atoms behave more like gases than solids, as they don't show the cohesiveness in solids. The temperature variation shows a slight average decrease with the increase in the number of simulation steps. For the Morse model: the cutting forces were in the range from around -2.5E-11N to 2.3E-11N; the phenomenon of ploughing was observed with pile-up of 4 layers of atoms; and the potential energy and total energy fluctuate initially and stabilize after 80000steps. The temperature variation shows a slight average increase with the increase in the number of simulation steps. For the EAM model: the cutting forces were in the range from around -6.2E-12N to 6.0E-12N; the phenomenon of ploughing was observed, with pile-up of 5 layers of atoms; and the potential energy and total energy are relatively stable. The temperature variation shows a slight average increase with the increase in the number of simulation steps. The results of the EAM model confirm those of [13, 14], that the EAM potential best describes the metallic bonding in the copper atoms.

CONCLUSION

The EAM potential is the most suitable of the 3 potentials used for the modelling of abrasive machining of copper atoms work piece with diamond tool. This is because tbe EAM potential provides the best description of the metallic bonding in the workpiece, also, the cutting forces variation is smallest, more pile of atoms is observed in ploughing and the potential and total energies are more stable for the depth of cut considered. Therefore the EAM potential should be used for the modelling of copper atoms and other fcc metals in MD simulations of abrasive machining.

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