International Journal of Hybrid Information Technology
Vol.9, No.3 (2016), pp. 407-414
http://dx.doi.org/10.14257/ijhit.2016.9.3.38

Simulation Analysis of the Effects of Tool Rake Angle for Workpiece Temperature in Single Crystal Copper Nanometric Cutting Process

Ge Jiang-hua[1], Zhang Chun-tao[1], Wang Ya-ping[1], Sui Xiu-lin[1] and Guo Yong-bo[2]

[1]School of Mechanical Engineering, Harbin University of Science and Technology, Harbin, 150080, China

[2]Precision Research Engineering Institute, Harbin Institute of Technology, Harbin, 150001, China

gejianghua@sina.com

Abstract

When the accuracy of the machined workpiece reaches to the nanometer scale, the atomic state in the cutting region、cutting force and the temperature of the workpiece newton layer must be analyzed from the atomic or molecular scale. Experiments will be difficult and time-consuming because the severe requirements of experiment for ultra-precision machine tool、resolution of detecting instrument and tool geometry, it becomes very difficult to study the effects of tool rake angle for nanometric cutting process and especially the workpiece temperature. Molecular dynamics simulation was used to carry out molecular dynamics modeling、simulation and analysis for diamond tools with different rake angle in single crystal copper surface nanometric cutting process, first of all, three-dimensional molecular dynamics simulation model of the workpiece and the tools with different rake angle were established; secondly, tools with different rake angle were used to machine the single crystal copper workpiece and calculated the CNA value of the workpiece atoms、the cutting force and the temperature of the workpiece newton; at last, the effect law of different tool rake angle for the atomic state in cutting region、cutting force variation and temperature of the workpiece newton in single crystal copper nanometric cutting process were analyzed. It was shown that when the rake angle value is negative, the increasing of temperature of workpiece newton with the increasing of the rake angle; when the rake angle value is positive, the decreasing of temperature of workpiece newton with the increasing of the rake angle.

***Keywords**: nanometric cutting, tool rake angle, molecular dynamics, cutting force, workpiece temperature*

1. Introduction

In recent years, with the development of micro electro mechanical system and nano electro mechanical system, the device tends to miniaturization, the scale and processing precision of the machined device reached to nanometer scale. In the process of nano-machining, machining occurs in a very small area, which contains only a few atoms layers or hundred of atomic layers. Material is considered as a collection of atoms or molecules, the removal of material is essentially a discrete process, the machining phenomenon in nature is to cut off the coalescent of chemical bonds between atomics, to achieve the removal of atoms or molecules. When the characteristic size of the grain is in the nanometer scale, it has the characteristics of small grain size, high defect density and large volume fraction occupied by grain boundary, showing out many characteristic different from macro material. Therefore，using cutting theory based on the traditional continuous medium mechanics to explain the cutting process is questionable, so, it must study the atomic state in cutting region、cutting force and workpiece temperature in the process of nanometric cutting from the perspective of the molecule and atom. Molecular dynamics (MD) method has a function of communicating macroscopic properties with microstructure and it has been proved to be an effective method to study the nanometric machining [1-4].

In the nanometric machining process which has only a few atomic layers, the influence of tool geometry for the machining process has been much higher than that of the traditional machining [5], and it especially has an important influence for the chip shape、cutting force and workpiece temperature in the machining process. Tool rake angle plays an important role in tool geometry, the change of the tool rake angle will inevitably lead to the variation of the chip shape and the fluctuation of the cutting force in the workpiece machining process, then cause the change of the workpiece surface temperature, and ultimately affect the machining surface quality of the workpiece.

Many scholars use molecular dynamics simulation method to study the mechanism of nanometric machining, some typical work has Komanduri [6] simulated the nametric cutting process of using diamond tool in combinations of different crystal orientation and different cutting direction, the influence rule of crystal orientation for cutting force、the ratio of thrust to cutting force and the specific energy were investigated, and it is found that the bigger the tool rake angle, the smaller influence of crystal orientation for the cutting force、the ratio of thrust to cutting force and the specific energy. Tanaka and Shimada [7] studied the process of diamond tool cutting mono-crystalline silicon in different machining parameter by molecular dynamics method, results showed that crack extension during ductile-mode machining can be avoided by using tool with much bigger negative rake angle to generate compressive stress field around cutting region, and it is an effective ductile-mode machining brittle material. Pei [8] studied the influence of tool geometry in nanometric machining process by molecular dynamics simulation method, it is found that it is easy to machining high-quality surface when the tool rake angle in the range form -45° to 45°, and cutting force and the ratio of thrust to cutting force decreasing with the change of tool rake angle. Promyoo [9] studied the chip formation mechanism with tool rake angle in nanometric cutting single crystal copper, it is found that cutting force、thrust force and the ratio of thrust to cutting force decreasing with the increasing of tool rake angle and the chip thickness decreased with the increase of the rake angle. Lai[10]studied the critical rake angle in nanometric cutting single crystal copper by molecular dynamics simulation method, results showed that the minimum effective rake angle for chip formation is -65º~ -70º,when the effective rake angle is -80 º,chip formation even pile-up formation does not occur in nanometric cutting.

The previous work mainly focused on the influence rule of tool rake angle for cutting force、the ratio of thrust to cutting force, the specific energy and chip formation, little work has been done for the investigation of tool rake angle for workpiece temperature in nanometric cutting process, however, temperature has an important influence for workpiece machining accuracy and machined surface quality, so it has an important significance to study the influence of tool rake angle for the workpiece temperature in the nanometric cutting process. This thesis based on molecular dynamics simulation method, establishing the three-dimensional molecular dynamics simulation mode of nanometric cutting single crystal copper, analysing the influence of different tool rake angle for the atomic state in cutting region and cutting force in single crystal copper nanometric cutting process, then analysing the influence of different tool rake angle for the workpiece temperature in nanometric cutting process.

2. Molecular Dynamics Simulation Mode and Computational Method

Molecular dynamics simulation mode of single crystal copper nanometric cutting as shown in figure 1.The simulation mode includes single crystal copper workpiece with face centered cubic structure and a diamond tool. The workpiece is divided into three different kinds, namely, boundary atoms, thermostat atoms and newton atoms, respectively. The boundary atoms are fixed in positions to reduce the edge effects and maintain the proper symmetry of lattice, without participating in calculation. The motions of newton and thermostat atoms obey newton's second law Hamiltonian equations of motion using the Velocity-Verlet algorithm. The initial velocity of copper atoms is assigned based in Maxwell distribution.

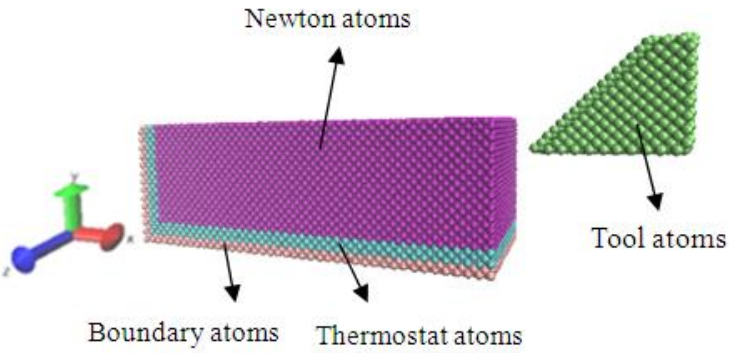

Figure 1. Molecular Dynamics Model of Nanometric Cutting Single Crystal Copper

Calculation parameters used in molecular dynamics simulation as shown in table 1. Due to the computing power limitations, the copper workpiece size is set as 15nm×5nm×6nm. The three- dimensional orientation of copper workpiece is x-[1 0 0], y-[0 1 0], z-[0 0 1]. Cutting is conducted along the $[\bar{1}\ 0\ 0]$ orientation on the top surface of work piece (1 0 0) plane. The time step is set as 1 fs. The initial temperature of the system is set as 300K, in order to maintain the constant temperature of thermostat in cutting process，the velocities of thermostat atoms are rescaled when the temperature departs more than 10K of the specified temperature, and this algorithm allows heat energy transfer from the machined region into the workpiece interior. Periodic boundary condition is imposed in Z direction to reduce the effect of simulation sale and edge. Surfaces are assumed to be passivated, so physisorption and chemisorption of surfaces are not considered. Diamond tool is filled with carbon atom of diamond structure. Tool rake angle is -60°、-45°、-30°、-15°、0°、15°、30°、45°、60°, respectively. The tool is set as rigid body because of the hardness of diamond is much bigger than copper in simulation. In the initial stage, tool is positioned 1nm on the right of workpiece in order to avoid the effect of long-range attractive force between the workpiece and the diamond cutting tool. The system is thermally equilibrated to 300K for 10ps using a Nose-Hoover thermostat. The system simulation has two stages: initial relaxation and tool cutting.

Table 1. Molecular Dynamic Simulation Parameters

Material	workpiece：single crystal copper	tool：diamond
Workpiece dimensions	15nm×5nm×6nm	rake angle： -60°、 -45°、
Atom number	40000	-30°、-15°、0°、15°、

MD time step	1fs	30°、45°、60°
Initial temperature	300K	
Cutting speed	300m/s	
Cutting depth	1.0nm	
Cutting distance	0-11nm	
Cutting orientation	[-1 0 0] orientation,(1 0 0)plane	

The interatomic actions includes between copper atoms (Cu-Cu)、between copper atoms and diamond atoms(Cu-C) and between diamond atoms(C-C) in system. The interatomic action of C-C is not considered because of regarding tool as rigid body. Among，The Cu-Cu interactions between copper atoms are described by the EAM potential [11]. The total atomic potential energy of a system is expressed as

$$U = \sum_{i} F_i(\rho_i) + \frac{1}{2}\sum_{i,j}^{i\neq j}\phi_{ij}(r_{ij}) \quad (1)$$

Where, ϕ_{ij} is the pair-interaction energy between atom i and j, F_i is the embedding energy of atom i, ρ_i is the host electron density at site i induced by all other atoms in the system, which is given by

$$\rho_i = \sum_{j\neq i}\rho_j(r_{ij}) \quad (2)$$

For the Cu-C interactions between workpiece and tool atoms, Morse potential is used [12], the Morse potential is written as

$$\phi(\gamma_{ij}) = D\left[\exp(-2a(r-r_0)) - 2\exp(-a(r-r_0))\right] \quad (3)$$

Where, D, a and r is the cohesion energy、the elastic modulus and the equilibrium distance between atom i and j, respectively. According to literature [13]，the cohesion energy $D = 0.087eV$, the elastic modulus $\alpha = 0.514nm^{-1}$, the equilibrium distance $r = 0.205nm$.

The conversion between kinetic energy and temperature of each atom can be computed at each time step, as the follows equation

$$\frac{1}{2}\sum_{i} m_i v_i^2 = \frac{3}{2} n k_B T_i \quad (4)$$

Where, n is the number of atoms, v_i represents the instantaneous velocity of atom i, k_B is Boltzmann constant, T_i is the temperature of atom i, m_i is the mass of atom i.

The thesis uses Large-scale Atomic/Molecular Massively Parallel simulator (LAMMPS) [14] to carry out molecular dynamics simulation, using Visual Molecular Dynamics (VMD) [15] and Atomeye [16] to visualize the computing result of molecular dynamics, adopting Common Neighbor Analysis (CNA) [17] to identify the characteristic of each atom from start to finish in nanometric cutting process and distinguish intrinsic stacking fault and dislocation nucleation.

3. Simulation Results and Discussion

Atoms state in material interior after cutting single crystal copper with tool rake angle from -60° to 60° as shown in Figure 2(a)—(i), atoms are colored according to the computed CNA value. Among, red atoms are Other atoms which is in workpiece surface or dislocation defect circumstances, blue atoms represents HCP atoms which is in intrinsic stacking fault or twin boundary. The FCC copper atoms that have no deformation are not showed. It is found that tool rake angle has an important influence for chip shape and dislocation motion, with the increasing of tool rake angle, the increasing of chip volume piled-up front of cutting tool. When the rake angle value is negative, the chip is mainly extruded by tool. Workpiece material below the tool is underwent bigger stress and the chip become small because of the big plastic deformation in workpiece. At the same time, machined surfaces generate elastic recovery, the chip move along rake face of tool and tool flank and more dislocation generate in cutting region; when the tool rake angle value is positive, the chip mainly is sheared by tool, the chip move along the rake face of tool, almost without chip moving along tool flank; when the tool rake angle is zero, the chip is underwent shearing and extruding at the same time. Compared with negative rake angle and positive rake angle, the difference is that also generating many dislocations in front and down left of tool. The average temperature change of workpiece newton layer under different tool rank angle as shown in Figure 3. It is found that when the tools rake angle value is negative, with the increasing of tool rake angle, the rising of the average temperature of workpiece newton layer; when the tool rake angle value is positive, with the increasing of tool rake angle, the reducing of the average temperature of workpiece newton layer. The reason above-mentioned phenomenon is that the chip will take the most heat away in nanometric cutting process, with the increasing of tool rake angle, the increasing chip volume of piled-up front tool, then the increasing of chip taking heat with the increasing of tool rake angle. It is still found that the reducing of workpiece newton layer average temperature negative rake angle than positive rake angle after cutting. This reason is that the friction heat generated by extruding between negative rake angle tool and chip is more than that generated by shearing between positive rake angle tool and chip.

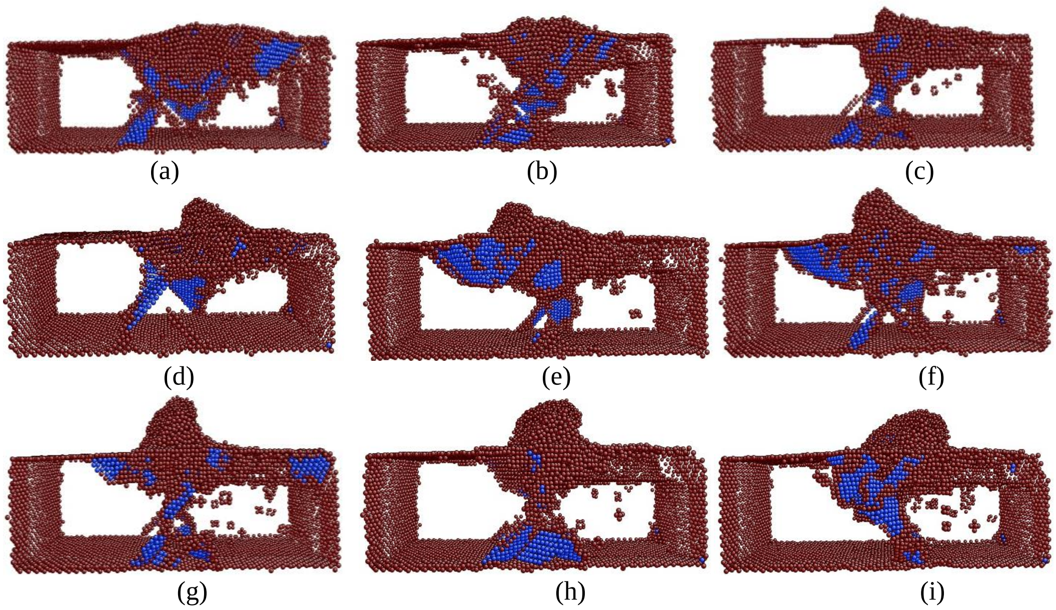

Figure 2. The Atom Coloring Snapshots of CNA under Different Tool Rake Angle in the Cutting Distance of 8nm

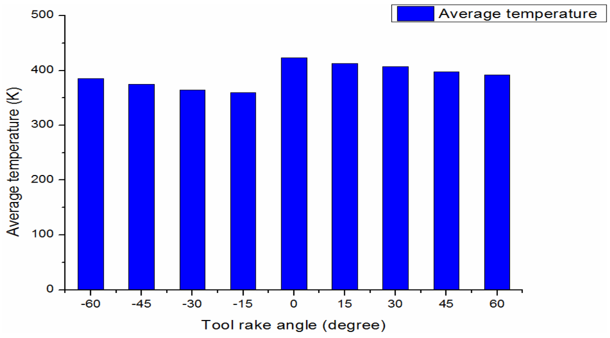

Figure 3. The Average Temperature of Workpiece Newton Atoms Under Different Tool Rake Angle

The curve of cutting force-cutting distance under different tool rake angle in the cutting thickness of 1nm as shown in Figure 4. It is found that tool rake angle has an important influence for cutting force. For the negative rake angle tool, with the decreasing of tool rake angle, the cutting force appears slowly, the reason is that when the initial distance between tool and workpiece is same, the smaller of tool rake angle, the slower of contacting between tool rake face and workpiece; for zero and positive rake angle tool, when the cutting distance is 1nm, the cutting force rises obviously, when the cutting distance reaches to 4nm, the cutting force maintain fluctuating steadily. The fluctuation is mainly owing to dislocation generation and evolution in workpiece interior during cutting process. The strain energy clustered together in single crystal copper lattice exceed its critical value of combination bond, the lattice is destroyed and the strain energy is released, then causing the instantaneous fluctuation of cutting force.

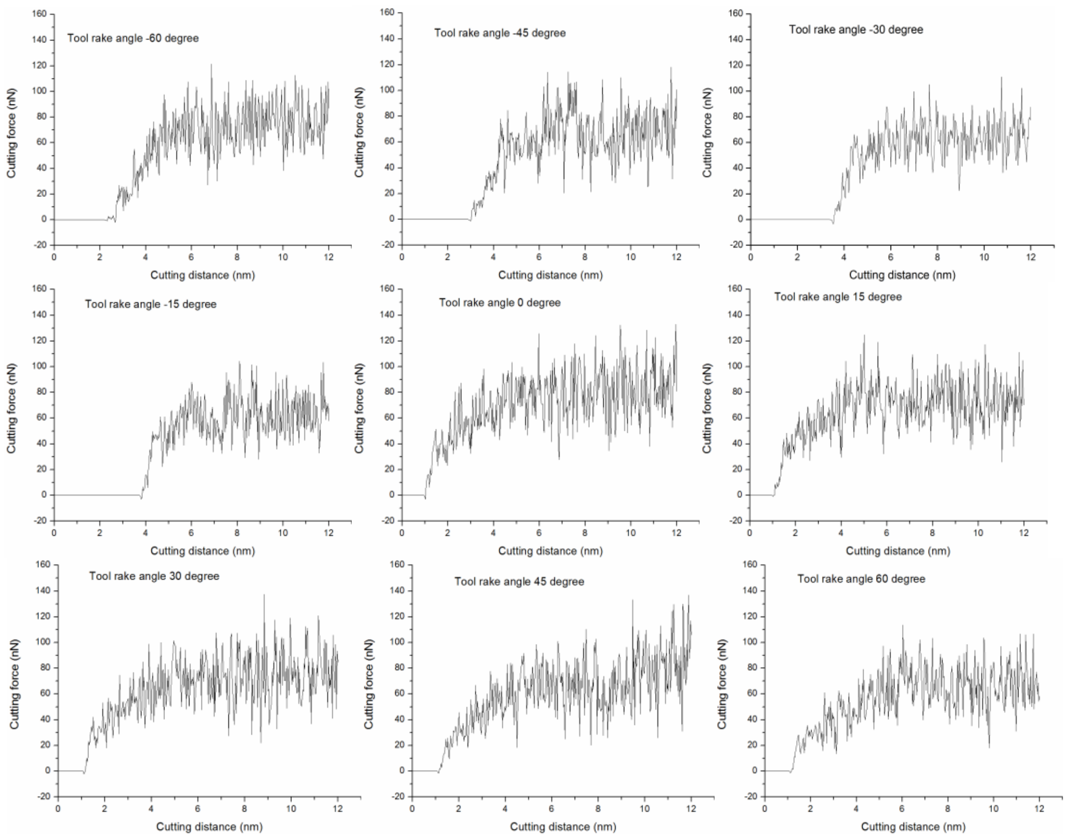

Figure 4. The Curve of Cutting Force-cutting Distance under Different Tool Rake Angle in the Cutting Thickness of 1nm

In order to compare the influence of tool rake angle for cutting force, calculating the average value of cutting force under different tool rake angle, as shown in figure 5. Tool rake angle has an important influence for average cutting force, when the tool rake angle value is negative, with the increasing of tool rake angle, the increasing of average cutting force which is received by workpiece; when tool rake angle value is positive, with the increasing of tool rake angle, the decreasing of average cutting force which is received by workpiece. The temperature variation curve of workpiece newton layer under different tool rake angle as shown in Figure 6. Corresponding to Figure 5, it is can be found that the temperature of workpiece newton layer and the average cutting force that workpiece received exist linear relationship, namely, the bigger of average cutting force of workpiece received, the higher of temperature of workpiece newton layer. Then, it indirectly shows that when tool rake angle value is negative, with the increasing of tool rake angle, the temperature of workpiece newton layer rising; when the tool rake angle value is positive, with the increasing of tool rake angle, the temperature of workpiece newton layer decreasing. In Figure 5, it is still found that when tool rake angle value is zero, the average cutting force that workpiece received is the biggest, so it should use tool with some certain rake angle in actual nanometric cutting process.

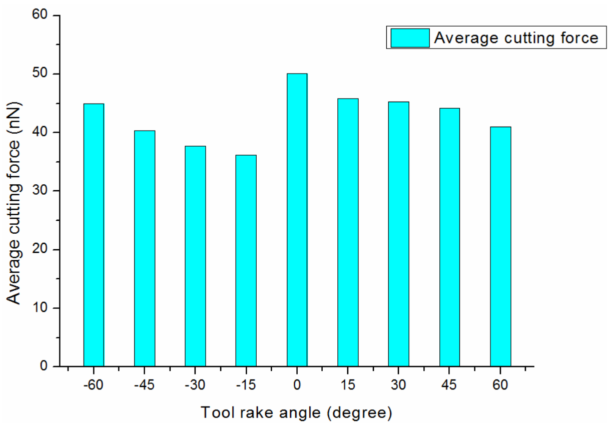

Figure 5. The Mean Cutting Force under Different Tool Rake Angle

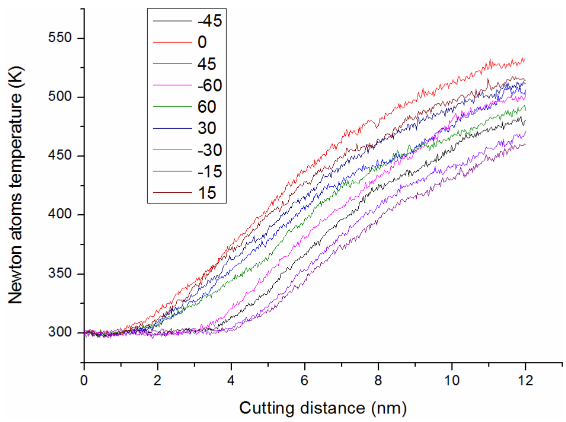

Figure 6. The Temperature Variation Curve of Newton Atoms under Different Tool Rake Angle

4. Conclusions

Molecular dynamics simulation was used to carry out molecular dynamics modeling、simulation and analysis for diamond tools with different rake angle in single crystal copper surface nanometric cutting process, the results achieved as follow:

(1) Tool rake angle has an important influence for chip shape in nanometric cutting process, with the increasing of tool rake angle, the increasing of chip volume piled-up in front of tool, the average temperature decreasing of workpiece newton layer with the increasing of chip volume.

(2) The temperature of workpiece newton layer and the average cutting force that workpiece received exist linear relationship, namely, the bigger of average cutting force of workpiece received, the higher of temperature of workpiece newton layer.

(3) Tool rake angle has an important influence for the temperature of workpiece newton layer, when tool rake angle value is negative, with the increasing of tool rake angle, the temperature of workpiece newton layer rising; when the tool rake angle value is positive, with the increasing of tool rake angle, the temperature of workpiece newton layer decreasing.

Acknowledgements

This research is supported by the National Natural Science Fund for Young Scholars of China (Project No.51405111). The authors would like to express their sincere thanks to the anonymous reviewers for their helpful comments and valuable suggestions on the paper.

References

[1] F. Z. Fang, H. Wu and Y. C. Liu, “Modelling and experimental investigation on nanometric cutting of monocrystalline silicon”, J. International Journal of Machine Tools and Manufacture, vol. 45, no. 15, **(2005)**, pp. 1681-1686.

[2] K. Cheng, X. Luo and R. Ward, “Modeling and simulation of the tool wear in nanometric cutting”, J. Wear, vol. 255, no. 7, **(2003)**, pp. 1427-1432.

[3] Z. C. Lin and J. C. Huang, “A study of the estimation method of the cutting force for a conical tool under nanoscale depth of cut by molecular dynamics”, J. Nanotechnology, vol. 19, no. 11, **(2008)**, pp. 115701.

[4] G. Xiao, S. To and G. Zhang, “Molecular dynamics modelling of brittle–ductile cutting mode transition: Case study on silicon carbide”, J. International Journal of Machine Tools and Manufacture, vol. 88, **(2015)**, pp. 214-222.

[5] Z. Wensheng, Z. Feihu and D. Shen, “Some Analysises of Extra Thin Cutting”, J. Journal of Harbin university of science and technology, vol. 3, **(2003)**, pp. 55-58.

[6] R. Komanduri, N. Chandrasekaran and M L. Raff, “M. D. Simulation of nanometric cutting of single crystal aluminum–effect of crystal orientation and direction of cutting”, J. Wear, vol. 242, **(2000)**, pp. 60-88.

[7] H. Tanaka, S. Shimada and L. Anthony, “Requirements for ductile-mode machining based on deformation analysis of mono-crystalline silicon by molecular dynamics simulation”, J. CIRP Annals-Manufacturing Technology, vol. 56, no. 1, **(2007)**, pp. 53-56.

[8] Q. X. Pei, C. Lu and F. Z. Fang, “Nanometric cutting of copper: A molecular dynamics study”, J. Computational Materials Science, vol. 37, **(2006)**, pp. 434–441.

[9] P. Rapeepan, E.-M. Hazim and Y. Xiaoping, “Molecular Dynamics Simulation of nanometric cutting”, J. Machining Science and Technology, vol. 14, **(2010)**, pp. 423-439.

[10] M. Lai, X. D. Zhang and F. Z. Fang, “Study on critical rake angle in nanometric cutting”, J. Applied Physics A, vol. 108, no. 4, **(2012)**, pp. 809-818.

[11] M. S. Daw and M. I. Baskes, “Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals”, J. Phys Rev B, vol. 29, no. 12, **(1984)**, pp. 6443–6453.

[12] L. A. Girifalco and V. G. Weizer, “Application of the Morse potential function to cubic metals”, J. Phys Rev, vol. 114, no. 3, **(1959)**, pp. 687–690.

[13] L. Zhang and H. Tanaka, “Towards a deeper understanding of wear and friction on the atomic scale—a molecular dynamics analysis”, J. Wear, vol. 211, **(1997)**, pp. 44–53.

[14] S. Plimpton, “Fast parallel algorithms for short-range molecular dynamics”, J. Journal of Computational Physics, vol. 117, no. 1, **(1995)**, pp. 1-19.

[15] W. Humphrey, A. Dalke and K. Schulten, “VMD-visual molecular dynamics”, J. Journal of Molecular Graphics, vol. 14, no. 1, **(1996)**, pp. 33-38.

[16] J. Li, “Atomeye: an efficient atomistic configuration viewer”, J. Modelling and Simulation in Materials Science and Engineering, vol. 11, no. 2, **(2003)**, pp. 173-177.

[17] J. D. Honeycutt and H. C. Andersen, “Molecular dynamics study of melting and freezing of small lennard-ones clusters”, J. Journal of Physical Chemistry, vol. 91, **(1987)**, pp. 4950-4963.

