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Simulation of temperature field during nanoscale orthogonal cutting of single-crystal silicon by molecular statics method

Zone-Ching Lin *, Meng-Hua Lin, Ying-Chih Hsu

Department of Mechanical Engineering, National Taiwan University of Science and Technology, Taipei 10672, Taiwan, ROC

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ABSTRACT

A quasi-steady molecular statics nanoscale cutting model is used to carry out simulation of nanoscale orthogonal cutting of single-crystal silicon by the diamond tools with different edge shapes. Based on the simulation results, this paper analyzes the cutting force, equivalent stress and strain, and temperature field. When the diamond tool moves to cut the single-crystal silicon, displacement of atoms is caused due to the effects of Morse force on each other. After a small distance that each atom moves, the concept of force balance is used to directly calculate the trajectory of each atom. Hooke–Jeeves direct search method is also used to solve the force balance equation, and obtain the new movement position of each atom. When chip formation and the cutting forces during cutting are calculated, further analysis is made. After the position of an atom's displacement is acquired, the shape function concept of finite element is employed to obtain the atomic-level equivalent strain. The equivalent stress–strain curve of single-crystal silicon acquired from the reference is used to calculate the equivalent stress produced under the calculated equivalent strain. This paper further supposes that temperature rise during nanoscale orthogonal cutting the single-crystal silicon is mainly produced from two heat sources: plastic deformation heat and friction heat. Thus, this paper uses the acquired equivalent stress and strain to calculate plastic deformation heat. Besides, this paper additionally develops a method to calculate the numerical value of friction heat produced by the single-crystal silicon atoms on the tool face and the numerical value of temperature rise of silicon atoms around tool face. Finally, the temperature rise produced from the two heat sources is added up for calculation of temperature field of the single-crystal silicon workpiece during nanoscale orthogonal cutting, and for making analysis. A simulation temperature field result obtained by the proposed quasi-steady molecular statics nanocutting model is qualitatively verified with the temperature field obtained by molecular dynamics method in the reference.

1. Introduction

Shimada [1] used two-dimensional (2D) model and molecular dynamics to conduct dynamic simulation of single-crystal orthogonal cutting and explore the cause of formation of chips. Childs and Maewaka [2] and Belak and Stowers [3] employed molecular dynamics theory to conduct numerical simulation, but their model still lacked a complete quantitative calculation. Pei et al. [4] indicated that the rake angle of cutting tool had significant influence on formation of chips and workpiece surface. The chips under rake angle -45° would be less because the workpiece has greater plastic deformation. Besides, the chips under rake angle -45° would have greater rebounding. Inamura et al. [5] regarded atoms as nodes, and combined the Morse potential among atoms with the work of atoms in order to overturn finite element method of atomic model. Furthermore, the concept of weight function was imported to induce the relationship among the displacement, strain and stress between atomic model and continuum model, resulting in strain distribution and stress distribution of workpiece. Cai et al. [6] used the same cutting tool radius to explore different cutting depths on silicon workpiece, and make simulative comparison among different cutting depths and radii of cutting tools. They found that the radius of cutting had to be properly small so as for easier cutting. The 2D model of Shimada [7] used molecular dynamics to carry out dynamic simulation of single-crystal silicon orthogonal cutting, and explore the cause of formation of chips. Tanakal and Shimada [8] used different volumes to match with different cutting depths, and different radii and different rake angles of cutting tools to explore the change of ductility and brittleness of silicon material. It was found that production of cracks could be avoided, and the cutting tool with negative rake angle could be effectively applied to ductile cutting. Tang [9] used conic cutting tool at 3 nm to simulate cutting of silicon workpiece. Cai et al. [10] used round-edge cutting tools with different nose radii to conduct simulation of molecular dynamic cutting of silicon workpiece,

* Corresponding author. Tel.: +886 2 2737 6455; fax: +886 2 2737 6243.
E-mail address: zclin@mail.ntust.edu.tw (Z.-C. Lin).

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and compared the temperatures produced during fabrication by cutting tools with different parameters.

The existing literature used molecular dynamics model to simulate heat source temperature. But this paper develops the use of molecular statics to carry out cutting simulation, and then the use of Morse force and equivalent strain/equivalent stress acquired from simulation to calculate temperature rise of plastic deformation heat source and friction rise of friction heat source respectively, and find the temperature field. Furthermore, this paper analyzes the physical phenomenon in times of fabrication, and explores the sharp-edge tool and round-edge tool would cause effects on production of cutting force and temperature heat source of the material. Using round-edge cutting tool and employing the way of molecular statics orthogonal cutting simulation, the paper calculates the temperature field, makes qualitative verification comparison with the molecular dynamics simulation results obtained by Cai et al. [10], and analyzes the physical phenomenon.

2. The three dimensional quasi-steady molecular statics nanocutting model for calculating temperature field of silicon workpiece

2.1. Calculation of cutting force

Through molecular statics, this paper finds the quasi-steady force balance equation to calculate the motion displacement of each atom. This paper firstly employs components in X, Y and Z directions to establish the simultaneous solution of force balance. Since the feed of each step in the paper does not exceed 0.002 Å, and atoms cannot go through another atom easily to create much deformation, this paper supposes that each feed does not exceed a distance of 1/2 lattice constant during searching the most suitable position of force balance deformation displacement.

The quasi-steady molecular statics nanocutting model of this paper uses the adopts Morse potential energy of two-body potential energy as the basis for calculation of the action force between molecules. The equation of Morse potential energy [11] is expressed as follows:

$$\Phi(r_{ij}) = D\{e^{-2\alpha(r_{ij}-r_0)} - 2e^{-\alpha(r_{ij}-r_0)}\} \tag{1}$$

D is binding energy, α is material parameter, r_{ij} is distance between two atoms and r_0 is equilibrium distance.

For the Morse potential energy function, when the distance between two atoms is greater than a certain distance, the action force between atoms will decrease rapidly. Therefore, it defines the distance cut-off radius r_c, and when the distance exceeds r_c, the action force is very small so it does not need to be calculated. In this way, the calculation can be tremendously simplified. Therefore, the Morse potential energy of the distance between two atoms inside r_c and outside r_c can be further expressed as the following equation:

$$\begin{cases} \Phi(r_{ij}) = D\{e^{-2\alpha(r_{ij}-r_0)} - 2e^{-\alpha(r_{ij}-r_0)}\} & r \leqslant r_c \\ \Phi(r_{ij}) \cong 0 & r \geqslant r_c \end{cases} \tag{2}$$

Table 1
Morse potential energy function parameters between diamond cutter and atoms of silicon workpiece material.

	Si–Si [12]	Si–C [13]
D: bonding energy (eV)	3.302	0.4352
α: Material parameter (Å^{-1})	0.798	4.6487
r_0: Balanced distance between atoms (Å)	4.208	1.9475

This paper adopts Morse two-bodied potential energy function to explain the interaction force between Si–Si and Si–C atoms, and the relative parameters of Morse potential energy equation for Si–Si and Si–C are shown in Table 1.

According to the Morse potential energy used by this paper, the action force between two atoms can be expressed as the following equation:

$$F(r_{ij}) = -\frac{\partial \Phi(r_{ij})}{\partial(r_{ij})} = 2D\alpha\{e^{-2\alpha(r_{ij}-r_0)} - 2e^{-\alpha(r_{ij}-r_0)}\} \tag{3}$$

When $r_{ij} = r_0$, the action force between atoms is just situated at a balance between attraction force and repulsive force. Both the cutter and workpiece material are at the situation of no action force. When $r_{ij} < r_c$, the diamond cutter and silicon material will produce action force.

By using Eq. (3), it can infer that the action force between two atoms can be expressed as the following equation:

$$\vec{F}_i = \sum_{i=1}^{n} \vec{F}_{ij}(r_{ij}) \tag{4}$$

i is a number given to the carbon atom of cutter, J is a number given to the silicon atom in material, n is number of silicon atoms, and r_{ij} is distance between two atoms.

The action force between two atoms acquired from Eq. (3) can be further divided into the components of force in three axes, $\vec{F}x$, $\vec{F}y$ and $\vec{F}z$, as shown in the following equation:

$$\vec{F}_i = \vec{F}x_i + \vec{F}y_i + \vec{F}z_i \tag{5}$$

$\vec{F}x_i$ is component of force of the action force in X direction, $\vec{F}y_i$ is component of force of the action force in Y direction, $\vec{F}z_i$ is component of force of the action force in Z direction.

Of course, after cutting has proceeded for a certain period, there is not just one silicon workpiece atom influenced by the Morse force of the diamond cutter. Hence, the Morse force vector of each silicon atom of the silicon workpiece being affected by the Morse force of diamond cutter after having moved to the new position, as well as the Morse force of other silicon atoms inside the cut-off radius acted on by each atom after moving to the new position are used in sequential order to find the sum of Morse force vector of each silicon atom. The sum of Morse force vector are further resolved as the Morse force component F_X in the X direction as well as the Morse force component F_Y in Y direction and F_Z in Z direction. As mentioned above, let the sum of the Morse force components in the X, Y and the Z directions be zero respectively. Then the force equilibrium equation of the quasi-steady molecular statics nanocutting model is formed, as shown in the following equation:

$$\begin{cases} F_X = \sum_{i=1}^{m} \vec{F}_{ix}(r_{ij}) = \sum_{i=1}^{m}\sum_{j=1}^{n} F_X(r_{ij}) = 0 \\ F_Y = \sum_{i=1}^{m} \vec{F}_{iy}(r_{ij}) = \sum_{i=1}^{m}\sum_{j=1}^{n} F_y(r_{ij}) = 0 \\ F_Z = \sum_{i=1}^{m} \vec{F}_{iz}(r_{ij}) = \sum_{i=1}^{m}\sum_{j=1}^{n} F_z(r_{ij}) = 0 \end{cases} \tag{6}$$

i is numbers assigned to all the atoms of diamond cutters that affect the Morse force of a certain silicon atom, j is numbers assigned to other silicon atoms inside the cut-off radius other than a certain silicon atom affected by the Morse force of cutter, m is quantity of all the diamond cutter atoms when corresponding to a certain silicon atom affected by the Morse force of cutter, n is quantity of other silicon atoms inside the cut-off radius other than a certain silicon atom affected by the Morse force of cutter, is r_{ij} distance between