Establishment of a cutting force model and study of the stress–strain distribution in nano-scale copper material orthogonal cutting

Abstract This article focuses on the establishment of a cutting force calculation model in terms of nano-scale orthogonal cutting, and investigates the stress–strain distribution of single-crystal copper that occurs in terms of nano cutting. The cutting force that occurs during the nano-scale cutting of single-crystal copper, and also its changes under different situations, can be found in this study. The molecular dynamics (MD) model was proposed to evaluate the displacement components of the atom in any temporary situation on the nano-scale cutting. The atom and lattice were regarded as the node and element, respectively. The shape function concept of the finite element method (FEM) is used to calculate the equivalent strain of the nodal atom and element. The equivalent stress–strain relationship equation was acquired by nano-scale thin-film tensile simulation in this study, and was used to further calculate the equivalent stress that occurs under the equivalent strain. Subsequently, a stress–strain distribution during nano-scale orthogonal cutting can be acquired.

Keywords Molecular dynamics · Nano-scale cutting · Stress–strain distribution · Copper

1 Introduction

The metallic cutting process is a complicated technique. Understanding the basic action of how the materials can be gradually removed by a tool is a critical issue of producing well-formed components. As the industry focuses on lightness, thinness, and compactness nowadays, the critical sizes of components have been moving towards the nano-scale. In order to understand the properties and processing mechanism of nano-processing, theoretical analysis and investigation is a must. Nano-scale processing involves changes in only a few atomic layers at the surface of the material. At such a small governing length scale, the traditional macroscopic analysis of the problem becomes questionable. Accordingly, the approach of the molecular dynamics (MD) model is undoubtedly needed to trace the behavior of atoms at this short-range and short-time interaction.

However, its application to machining is only of recent origin. For instance, in 1990, Shimada et al. [1] used atomic 2D modeling and began to apply MD on the simulation of the movement of nano-scale cutting and investigated the formation of a relationship of the cutting. Childs and Maekewa [2] and Belak and Stowers [3] used MD theory to proceed with the value simulation of the microscopic metallic materials cutting process. But their model lacked complete quantitative calculation. Isono and Tanaka [4] carried out a 3D MD analysis of the effects of temperature and interatomic force on nickel metal during nano cutting. Ikawa et al. [5] studied the 2D nanometric cutting of copper with a diamond tool. From 1991 to 1992, Inamura et al. [6, 7] used the Morse potential between atoms to form the pairwise potential of atoms and they regarded the atom as the node and the pairwise atomic potential as elements. Taking this as a starting point, they introduce the finite element method (FEM) of the atomic model, and used two kinds of atomic Morse potential as simulative examples. Ultimately, they acquired the changing phenomenon of the formation of the cutting, its capability of cutting, and its potential energy side by side with the movement of the workpiece. In 1993, Inamua et al. [8] further demonstrated a method to transform the atomistic model to an equivalent 2D continuum FEM cutting mode. Their method was to put the continuum model on the corresponding atomistic model first. The displacement of the node of the continuum model was a weight average (weight function) surrounding the external atom of the node of the continuum model, deriving the transformation of displacement from the atomistic model to the continuum model, as well as the stress–strain relationship. The position of every workpiece atom was calculated from the viewpoint of the least energy
position in every temporary situation, and was then transformed to the displacement and stress–strain among continuum models. Finally, the distribution of the maximum principal stress, the maximum principal shear stress, and the effective strain of the workpiece were acquired. Inamura et al. [8] stated that, as for determining the proper shape of a weight function, the problem is still unsolved.

The combination of FEM and MD in the literature mostly divides the simulation space into three zones: one is the atomic-scale MD simulation zone, another is the FEM calculation zone of the macroscopic continuum model, and the last is the transition zone, i.e., the interface zone between the MD simulation zone and the FEM calculation zone. As proposed by Izumi et al. [9], an integration of FEM and MD could be applied to investigate the elastic deformation behavior of Si during the tensile condition. Their method was to divide the simulation space into four zones, and they suggested the corresponding data adjustment of the two-layer transformation (transition) zone between the FEM zone and the MD zone. Liu et al. [10] mentioned an atomistic and continuum concurrent model to study the stress distribution of the epitaxial island at an elastic stage. The epitaxial island was simulated by MD, whereas the substrate was simulated by FEM. There was an overlapping zone between them, so as for the atomistic and continuum models to exchange necessary material information. The deformed portion of the workpiece during nano cutting is plastic deformation in this study. Therefore, we can not directly apply the above mentioned combination of FEM and MD to analyze the equivalent stress and equivalent strain in the MD zone during nano-scale cutting.

Based on the theory of MD, Lin and Huang [11] improved the FEM of the equivalent continuum model suggested by Inamura et al. [8]. They directly regarded the atom as a node and the lattice as an element. Lin and Huang [11] suggested a way of combining the FEM shape function concept and MD techniques to calculate the equivalent stress and equivalent strain at the cross-section of the center of the single-crystal copper based on the plane strain condition caused by 3D nano-scale cutting. The atom displacements can be obtained by the MD simulation. The equivalent strain for the material deformation can be obtained by the concepts of shape functions of FEM during the nano-scale cutting. The equivalent stress was derived from the equivalent strain from the corresponding flow curve. The flow curve was obtained from the regression of the stress–strain curve of nano copper thin-film tension test simulation. Also, a mathematical model formed by the cutting atoms of unreasonable position has been induced, so that these atoms can move along the surface of the tool. Also, “a cutting and separation principle combining Morse potential energy function and rigid steel tool space restriction principle” is proposed to be the cutting and separation principle of nano-precision orthogonal cutting, so that a nano-scale cutting model combining MD with FEM can be developed.

In order to acquire an equivalent stress–strain relationship equation, this article also researches into nano thin-film tensile test simulation. In the area of nano thin-film tensile materials, Lutsko [12] redefined the atomistic stress tensor by using statistical mechanics. His work provided a convenient way of calculating MD and also the determination of Young’s modulus. Since Lutsko published his landmark study, his methodology has become a benchmark tool for almost all microscopic stress calculation. Schøtz et al. [13] were the first to study a nanowire’s mechanical property change originated from grain boundary defects as applications of nano-scale material became more widely used. Schøtz et al.’s work paved a new way for nanostructured mechanics research.

Soon after, Iwaki [14] was the second to apply MD on nanostructure mechanics calculation. He used an L-J-12 potential model to simulate both the stress and strain of a thin film when subjected to a tensile stress. He also discovered that, in order to be consistent with the findings based on continuum mechanics, the total number of particles within the stress calculation zone needs to be 130 or more. Miyazaki and Shiozaki [15] were the first to calculate the coefficient of thermal expansion of α-Fe, and, therefore, demonstrated the feasibility of using MD to calculate physical parameters that are difficult to obtain experimentally.

As Lin and Huang’s [11] work, which did not calculate the cutting force that occurred during nano cutting, based on Lin and Huang’s theory, the complete cutting force calculation model and stress–strain analytical model of metal copper during 3D nano-scale orthogonal cutting can be established in this study. Also, the cutting values acquired by the simulation of different materials are compared with Ikawa et al. [5], so as to prove whether the cutting values proposed here are reasonable or not.

In order to investigate the stress–strain distribution caused by the single-crystal copper workpiece in terms of nano cutting, this article adopts MD to simulate the single-axial tensile process of nano single-crystal copper. Miyazaki and Shiozaki’s [15] stress calculation equation is applied to calculate the equivalent stress–strain curve during nano thin-film tension simulation tests, and then an equivalent stress–strain relationship equation is regressed, where this article adopts $2.5 \times r_0$ as the value of the outer affecting area of the stress calculation zone. Furthermore, this article uses MD to calculate the atom displacement of the workpiece, of which the result is then combined with the shape function concept in FEM, so as to calculate the equivalent strain of the atomic-scale nodal atoms and elements. Through an equivalent stress–strain relationship equation, the equivalent stress occurring under equivalent strain can be calculated. As to the construction of the stress–strain distribution in terms of single-copper 2D nano-scale orthogonal cutting, it is useful to observe the stress and strain values in terms of the nano cutting of copper materials.