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Multiscale simulation of nanometric cutting of single crystal copper and its experimental validation

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ABSTRACT

In this paper a multiscale simulation study was carried out in order to gain in-depth understanding of machining mechanism of nanometric cutting of single crystal copper. This study was focused on the effects of crystal orientation and cutting direction on the attainable machined surface quality. The machining mechanics was analyzed through cutting forces, chip formation morphology, generation and evolution of defects and residual stresses on the machined surface. The simulation results showed that the crystal orientation of the copper material and the cutting direction significantly influenced the deformation mechanism of the workpiece materials during the machining process. Relatively lower cutting forces were experienced while selecting crystal orientation family {1 1 1}. Dislocation movements were found to concentrate in front of the cutting chip while cutting on the (1 1 1) surface along the $[\bar{1}10]$ cutting direction thus, resulting in much smaller damaged layer on the machined surface, compared to other orientations. This crystal orientation and cutting direction therefore recommended for nanometric cutting of single crystal copper in practical applications. A nano-scratching experiment was performed to validate the above findings.

1. Introduction

Single crystal copper has found its wide applications for the fabrication of high accurate instruments and civil communication equipments because of its explicit properties, such as signal transportation and fatigue resistance [1–3]. Nanometric cutting, in which depth of cut is less than 100 nm, is a perfect choice to fabricate microstructures required for such intrinsic products. Nanometric cutting offers nanometer level surface roughness and submicron form accuracy which can meet the demand on high accuracy for these products. In nanometric machining operation, the ratio of cutting edge radius to the depth of cut is larger which is indeed the distinguishing feature compared to conventional machining [4]. On the other hand, some phenomena in nanometric cutting are difficult to observe by experimental means due to the complexity and miniaturization of the cutting process. However, computational simulation method provides an alternative way to accomplish the "on-line" observation of the machining process.

Since the late 1980s Molecular Dynamics (MD) simulation method has been used to study nanometric cutting processes. Ikawa et al. [5] proposed that the sharpness of the diamond tool had a strong influence on the minimum thickness of cut. Maekawa and Itoh [6] investigated the phenomena of tool wear of a diamond-like tool in micro-machining of single crystal copper. Kim and Moon [7] studied the phenomenon of microcutting with sub-nanometer chip thickness. Kim et al. [8] conducted a three-dimensional MD simulation for AFM-based nano-lithography process which showed that different crystal orientations and ploughing directions had significant influences on the nano-deformation patterns. Liang et al. [9] conducted an integrated MD simulation of scratching and shearing experiments on a single crystal copper specimen. They suggested that the yielding strength of a small-size nanostructure was very sensitive to the imperfection and defect of the copper surface. Zhang et al. [10] simulated the groove fabrication process at atomistic scale using MD method. Results showed that the groove geometry had a huge impact on the groove machining process. In addition, MD method has been extensively applied for the simulation of nanometric cutting, nanoscratching and chemical mechanical polishing processes for other materials, such as silicon, aluminum and multi-layered films [11–14]. However, due to the limitations of computational power, the dimensions of a MD simulation model were usually in the range of few nanometers. Simulation of the full scale of nanometric cutting is still a challenging task.

In recent years, multiscale simulation approach has been developed in the computational materials area. The philosophy of this approach is to retain full atomistic details in the regions of interest

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but uses continuum assumption in the other regions so as to reduce the computational demand. Multiscale method has been used to correlate the mechanical properties of materials with their microstructures [15,16] very little work has been carried out to apply this approach in the study of nanometric cutting. Furthermore, nanometric cutting is basically a multiscale deformation process. The generation, evolution and pile-up of the nanometer level dislocations and breakage of the atomic bonds in the cutting region determine the mechanism of nanometric cutting process. It is essential to explore the atomistic mechanism in this region using MD method. The residual stress in the machined surface and subsurface is a crucial factor for the service performance of the final products. Continuum methods, such as finite element method, can be used to analyze the micro-scale deformation features which are related to the generation of the residual stress. With continuum method the computational time can be saved significantly. In this paper, a multiscale simulation method, Quasicontinuum (QC) [17] was used to study the effect of crystal orientation and the cutting direction on the deformation mechanism in nanometric cutting of single crystal copper.

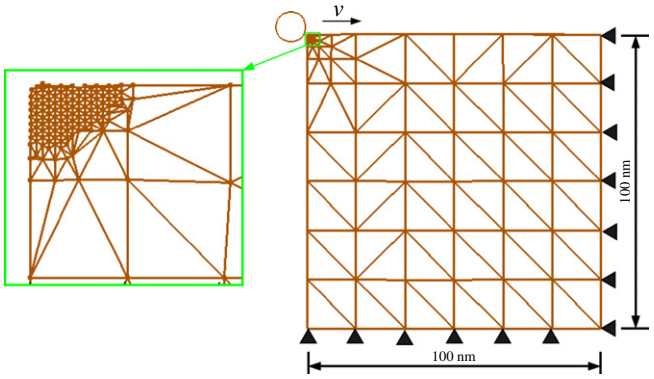

Fig. 1. Multiscale model of nanometric cutting.

Table 1
Computational parameters used in simulations.

Parameters	2-D multiscale cutting model
Workpiece material	Copper, EAM potential
Workpiece dimensions	0.1 × 0.1 μm
Tool edge radius	5 nm
Depth of cut	3 nm
Cutting speed	20 m/s
Workpiece orientation	(0 0 1)[$\bar{1}$ 1 0] (0 0 1)[1 0 0] (1 1 0)[0 0 1] (1 1 0)[$\bar{1}$ 1 0] (1 1 1)[$\bar{1}$ 1 0] (1 1 1)[$\bar{2}$ 1 1]

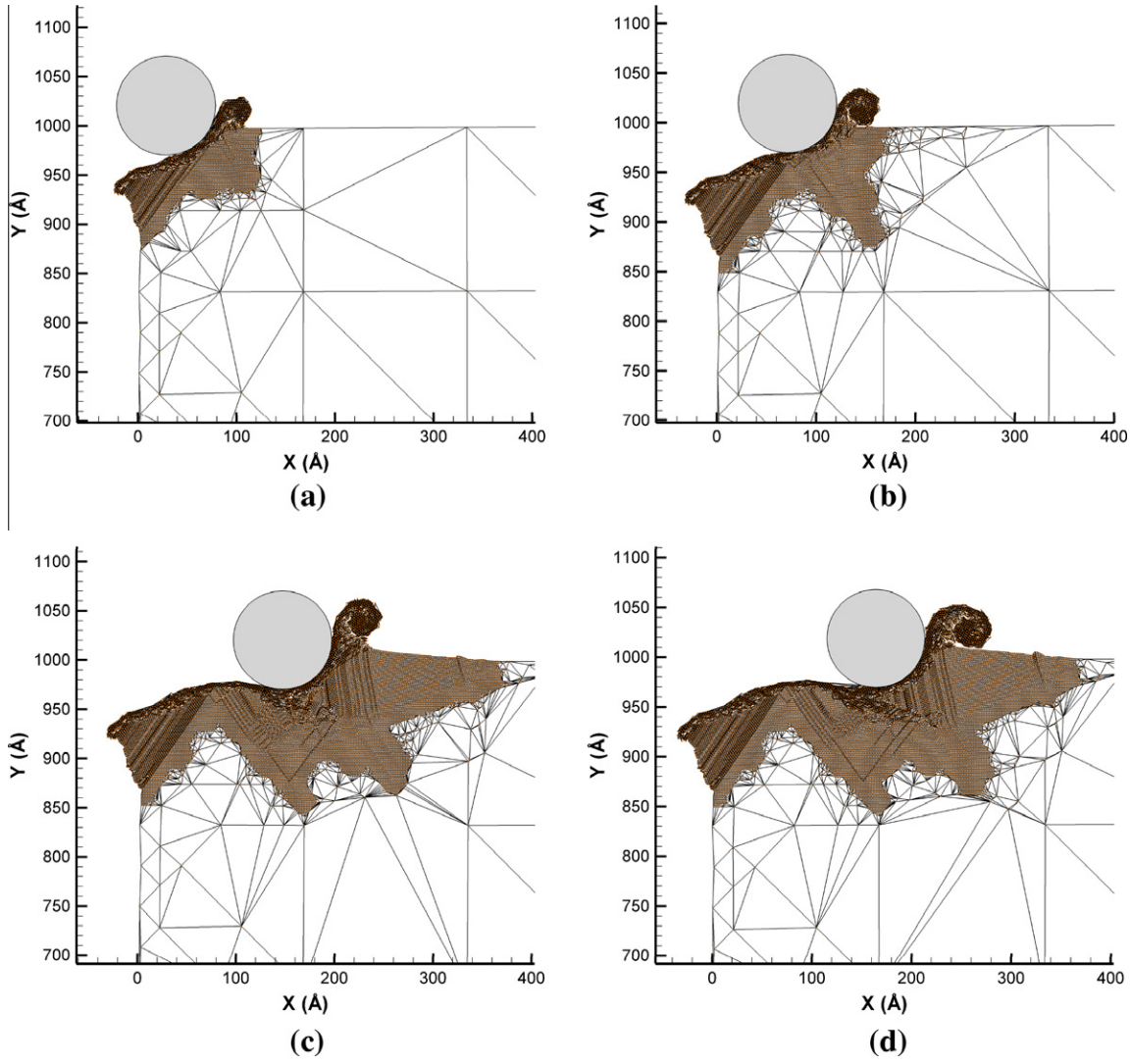

Fig. 2. Snapshots of the multiscale simulation at the cutting distances of 8 nm (a), 12 nm (b), 18 nm (c) and 21 nm (d) in (0 0 1)[$\bar{1}$ 1 0] orientation setup.