Effects of microstructures on the material removal mechanisms in nanomachining of polycrystalline materials

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Abstract

Based on the new three-dimensional polycrystal models proposed by the authors [1-3], atomistic simulations of machining polycrystalline copper by diamond cutting tool have been carried out to investigate the material removal mechanism at nanoscale. Microstructures, including grain cell, grain boundary, triple junction were indentified and the effect of microstructures on workpiece internal stress distribution, machined surface generation, defect structures nucleation and propagation and chip formation have been obtained by large-scale molecular dynamics simulation method. The internal stress at grain boundary and primary deformation zone is much higher than that at grain cell and results in a stress gradient. In particular, the stress field addresses the question whether internal stress responsible for defect structures propagation directions during nanomachining. Our results indicated that for polycrystalline materials the deformation is highly localized. For the large grains in the deformation zone, the material removal mechanism is dislocation-mediated, while for the small grains, grain interface sliding and diffusion tends to be dominated. The atomic analysis shows that the residual defect structures impose a major change on the workpiece physical properties and machined surface quality.

1 Introduction

Most of engineering materials are made of more than one grain or phase, and the neighbouring crystallites across a grain or interface boundary often differ in crystal orientation, structure and property. In nanomachining process, the magnitude of workpiece average grain size is almost in the same order with cutting depth and cutting feed. Nanomachining of polycrystalline materials with realistic microstructures, in which the major microstructures are grain cells (GC), grain boundaries (GB), triple junctions (TJ), is of great importance to practical applications.

Nevertheless, little work has been done for regarding this issue in literature because of the complexities in constructing the precise polycrystalline model and the expensive computation clusters required. The effect of microstructures on machining performance will be examined, and the machining performance is evaluated by chip formation, cutting force, defect structures and internal stresses.

2 Methods

Figure 1(a) shows the equilibrated MD simulation model for nanomachining. For more information about building polycrystalline simulation model, interested reader is referred to Ref. [1-3] for details. In order to show the information of the microstructures of each grain in detail, we choose one grain of the workpiece as shown in Figure 1(b). The atoms with different microstructure entities are colored differently.

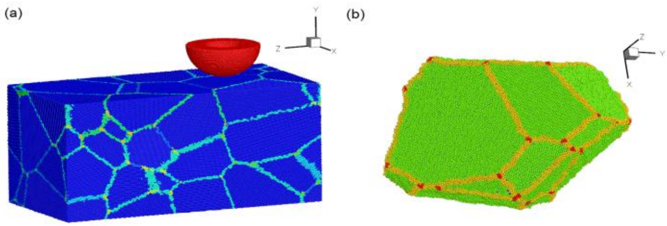

Figure 1: (a) An equilibrated atomic configuration of polycrystalline copper machined with a hemispherical diamond tool; (b) one grain of the nanocrystalline Cu workpiece. The workpiece mean grain size is 20.09 nm and contains about 18 million atoms. Atoms are colored according to their microstructure nature.

3 Results

Figure 2(a) shows the nanocutting topologies of polycrystalline copper. Nano-groove was cut by removing several layers atoms on the top surface of workpiece. Burrs could be clearly observed at the groove edges due to the material deformation and pile-up. Defect structures, are generated and propagated into the workpiece grains interior. Figure 2(b) shows the variation of cutting force in nanocutting process. It can be seen that the cutting force increase rapidly with the progress of machining, and then the growth slows down and enters into a relative steady stage. The conditions of nanocutting with a diamond tool change when the cutting is carried out across grains with various crystallographic orientations, the variations in crystal grain density, hardness and grain interface micro-structures.

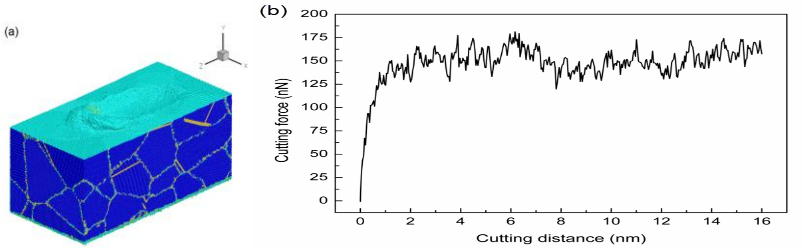

Figure 2: (a) Nanomachining topologies, the diamond cutting tool was not shown for clarity, yellow stands for stacking faults and partical dislocations; (b) cutting force.

Figure 3 shows the defect structure topologies in the sub-layers of workpiece in nanocutting process. The dislocation nucleation event can be viewed as the activation of a dislocation source that lies within or nearby the grain boundary, and grain boundary serves as the dislocation source for dislocation nucleation. Meanwhile, we can find that the line defects activity is blocked or absorbed by the grain boundary due to the constraint imposed by the neighbored grains.

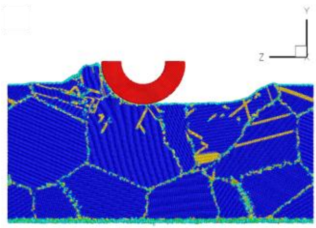

Figure 3: Cross-section view of defect structures inside of polycrystalline Cu workpiece at the cutting distance 20 nm.

Figure 4 shows the internal stress distribution in polycrystalline copper with the progress of nanomachining. The atoms with large internal stress are mainly located in grain boundary and shear zone. The magnitude of the stress in grain boundary ranges from a few to ten times higher than in the grain interior. Atoms with high internal stress are mainly concentrated in grain boundaries. The magnitude of internal stress in the grain interface regions could easily reach the yield stress of the perfect crystal, which makes it easy to initiate atomic motion at the interface regions.

Combined with the external applied stress during nanomachining, the high internal stress will result in defects structures.

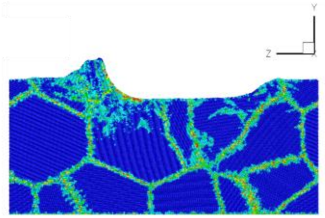

Figure 4: Internal stress distribution of polycrystalline Cu workpiece during nanocutting process.

4 Conclusion

Atomistic simulation of nanomachining polycrystalline materials with a diamond cutting tool was carried out to investigate the material removal mechanism. The new simulation model used for distiguishing microstructure entities enable us to investigate the material removal, chip formation, defect structure nucleation and propagation and calculate the internal stress distribution during nanomachining process.

Acknowledgment

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References:

[1] Y.B. Guo, T. Xu and M. Li. *Philos. Mag.* **92**, 3064 (2012)

[2] M. Li and T. Xu. *Prog. Mater. Sci.* **56**, 864 (2011).

[3] T. Xu and M. Li. *Philos. Mag.* **90**, 2191 (2010).

[4] Y.B. Guo and Y.C. Liang. *Trans. Nonferrous Met. Soc. China*. **22**, 2762 (2012)