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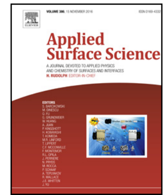

Role of crystal orientation on chemical mechanical polishing of single crystal copper

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ABSTRACT

The material removal mechanism of single crystal copper in chemical mechanical polishing (CMP) has not been intensively investigated. And the role of crystal orientation in CMP of single crystal cooper is not quite clear yet. Quasi-continuum method was adopted in this paper to simulate the process of nano-particles grinding on single crystal copper in CMP process. Three different crystal orientations, i.e. x[100]y[001], x[001]y[110] and x[−211]y[111], were chosen for analysis. The atom displacement diagrams, stress distribution diagrams and load-displacement curves were obtained. After analyzing the deformation mechanism, residual stress of the work piece material and cutting force, results showed that, the crystal orientation of work piece has great influence on the deformation characteristics and surface quality of work piece during polishing. In the A(001)[100] orientation, the residual stress distribution after polishing is deeper, and the stress is larger than that in the B(110)[001] and C(111)[−211] orientations. And the average tangential cutting force in the A(001)[100] orientation is much larger than those in the other two crystal orientation. This research is helpful to revealing the material removal mechanism of CMP process.

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1. Introduction

CMP technology can achieve global and local planarization effectively and meet the demand of high accuracy and ultra-smooth planarization, which has become an indispensable technology in integrated circuit manufacturing [1,2]. Although CMP has been widely used, the material removal mechanism, surface chemistry characteristics, galvanic corrosion problem and chemical-mechanical interactions in CMP are not well known yet [3,4]. Small changes of the variables in the polishing process e.g. silicon, slurry and wafer pad will directly affect the polishing system, and then affect the silicon wafer surface material removal rate and quality change.

Since the changes in CMP process occur only within a few atomic layers from the surface, the problem cannot be solved with the continuum theory. Instead, molecular dynamics (MD) simulation is an appropriate method to study the material remove mechanism in CMP process [5–7]. MD method is generally proved to be a powerful tool in describing microscopic world. Han et al. [8,9] used MD simulation method to study the CMP process of silicon wafer. It was found that huge hydrostatic pressure induced in a local area could lead to the phase transformation of silicon atoms from the classical diamond structure to the metal structure, by which the material was removed in a ductile mode. Si et al. [10] also used MD method to simulate CMP process to study the atomic-scale removal mechanism of single crystalline silicon and particular attention was paid to the effect of scratching depth. However, the system size MD method can simulate is very limited, even high-performance computers can't simulate the real physical system. But quasi-continuum (QC) method can potentially solve this problem. The basic idea of QC method is to combine MD simulation, for critical regions we are interested in, with finite element (FE) method, for continuum description. Currently, QC method has been widely used in basic phenomena of crystal deformation studies, including fracture [11], grain boundary structure and deformation [12], nano-indentation [13] and three-dimensional dislocation interactions [14].

In this paper, QC method was adopted to investigate the role of crystal orientation on CMP of single crystal cooper. In the simulation, the workpiece was set to three different crystal orientations in order to investigate the effect of the crystallographic factors in the CMP process. The characteristics of the plastic deformation, dislocation generation with slip direction, chip formation, and cutting

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force were then studied, attempting to reveal the material removal mechanism of CMP process.

2. Experimental

2.1. Quasi-continuum method

QC method, one of the multi-scale simulation methods, was originally developed by Tadmor [15]. It integrates continuum and atoms, which uses atomic-scale solution in dislocation core regions while uses rough description characterized by "representative atoms" in the regions far away from core regions. It calculates the energy and force of system in the state of reduced degree of freedom, and achieves the coupling of atoms and continuum.

Fig. 1 demonstrates the basic principle of QC method. The black filled circles in Fig. 1(a) are the representative atoms and Fig. 1(b) is the finite element mesh composed of corresponding representative atoms. As shown in Fig. 1(b), atoms B, C and D are finite element nodes and atom A is non-representative atom. The displacements of non-representative atoms are derived from the linear interpolation for representative atoms. This purpose can be achieved by using the interpolation equations of finite element method in QC method. In regions where fully detailed atom description is required, we can choose all atoms as representative atoms and reduce the density of representative atoms in regions with smaller deformation gradient. As Fig. 1 shows, we may choose all atoms in the dislocation core region as representative atoms, and reduce the density of representation atoms in regions away from the dislocation core region.

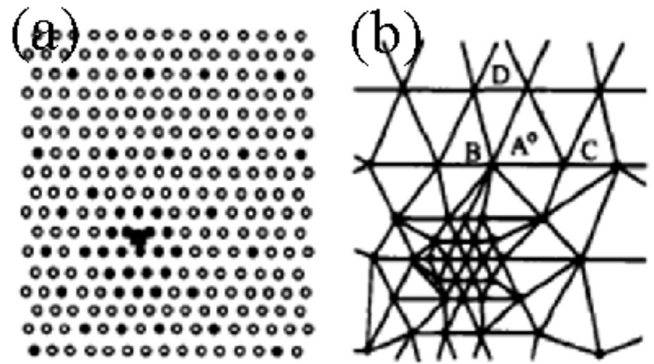

Fig. 1. Schematic representation of rep-atoms.

Ideally, in order to calculate the total energy, all the atoms in the domain need to be visited by

$$E_{tot} = \sum_{i=1}^{N} E_i(x_1, x_2, \cdots, x_N) \tag{1}$$

where E_i is the energy contribution from site x_i.

The precise form of E_i depends on the potential function used. In the regions where the displacement field is smooth, keeping track of each individual atom is unnecessary. After selecting some representative atoms, the displacement of the remaining atoms can be approximated via linear interpolation.

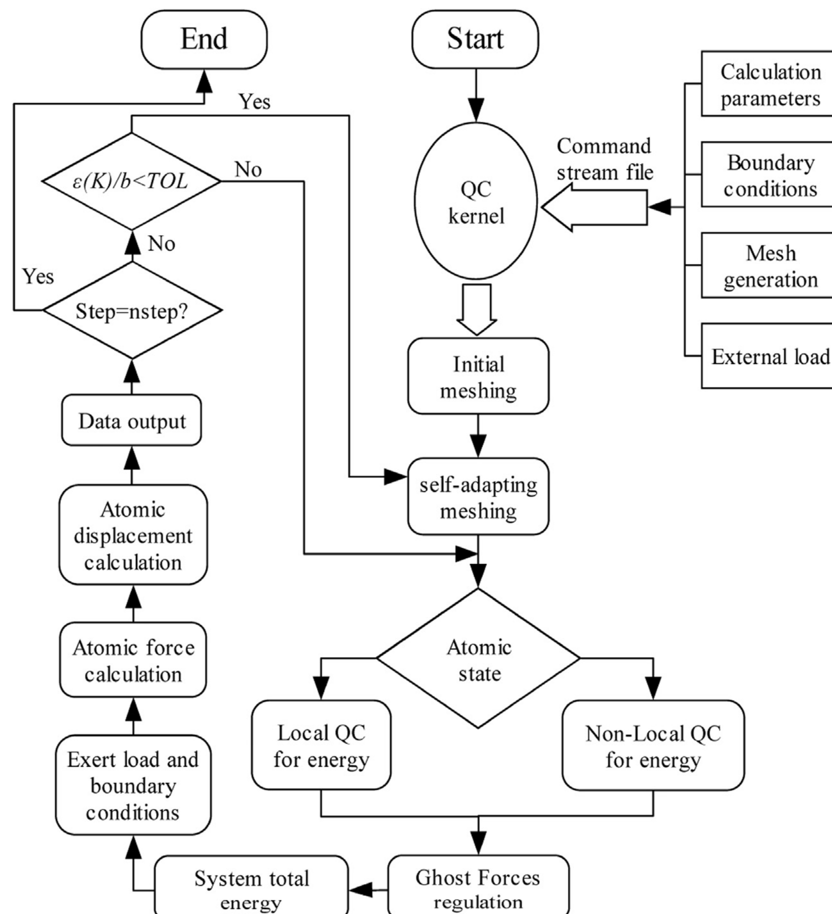

Fig. 2. Flow chart of QC simulation.

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