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Study of material removal processes of the crystal silicon substrate covered by an oxide film under a silica cluster impact: Molecular dynamics simulation

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ABSTRACT

Molecular dynamics simulation was applied in analyzing the material removal mechanism of the crystalline silicon substrate covered by an oxide film under the impact of a silica cluster. With the increasing of the thickness of the oxide film, the optimal film for the maximum of the number of removed atoms from the impact surface would be observed, which is due to the combinational effects of adhesions among the cluster, the oxide film and the substrate, the stability of the oxide film, and the penetration of the atoms of the substrate. Moreover, the optimal oxide film, whose thickness is about 2.5–3.0 Å, is a continuous monolayer molecular structure. Furthermore, the results also showed that the contact–penetration–adhesion (CPA) material removal process, which is different from the traditional indentation-sliding process, would occur during the chemical mechanical polishing process owing to the penetration of atoms of the silicon substrate into the oxide film. These findings are instructive in understanding the material removal mechanism at atom scale during the chemical mechanical polishing process.

1. Introduction

Chemical mechanical polishing (CMP) is widely used in the planarization of semiconductor wafers [1,2]. The diameter of the wafer and the feature size of integrated circuits have been developing towards 450 mm and 14 nm, respectively. With the increasing of wafer sizes and the decreasing of feature sizes, it is becoming more and more important for us to understand the material removal mechanism during CMP in order to improve the polishing process [1,2].

Salient features of a CMP process are shown in Fig. 1. The wafer, which is held firmly on a rotating platen, will be pressed face down against a rotating polishing pad. Meanwhile, the slurry consisting of chemical additives and abrasive particles will be introduced at the interface between the wafer and the polishing pad [3]. During machine process, the wafer reacts with the chemical components of the slurry to form a relatively soft, thin film on the wafer surface. And the thin film is subsequently mechanically removed by the abrasive particles of the slurry. With the combination of chemical action and mechanical action, the material removal and planarization of the wafer surface are realized [4,5]. So, the CMP processes are described as a sequential process of the formation and removal of a thin film of reduced hardness [1,6]. Therefore, the material removal processes of CMP will be significantly affected by the properties of the thin film formed (e.g. thickness, yield strength), and the interactions among the thin film, the wafer and the abrasive particle [7].

Experiments have proven that a metal or silicon wafer during CMP undergoes with the passivation to form a thin film of the oxide or suboxides [6,8,9], whose thickness is very small in the order of several nanometers [8,10,11], even close to the size of several layers of atoms [12]. And the mathematical expressions between the thickness of the passivation film and the material removal rate (MRR) during CMP were established on the basis of the indentation-sliding material removal model [13,14]. However, the mathematical expressions can not explain the experiment phenomenon, which is that the MRR will firstly increase and then decrease with the increasing of thickness of the film during CMP process [4,15].

One of the main reasons for the difference between the mathematical expressions and the experiment phenomenon is that the mathematical expressions usually consider the effect of the passivation film as a single parameter – the thickness of the passivation film, and omit other properties of the passive film, for example, the adhesion strength between the passivation film and the wafer substrate. The reason is that it is very difficult to study the effect of the properties of the passive film on MRR by experimental means

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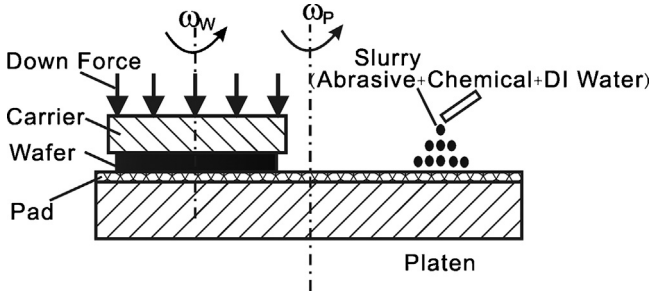

Fig. 1. Schematic of the chemical mechanical polishing (CMP). DI water means the de-ionized water.

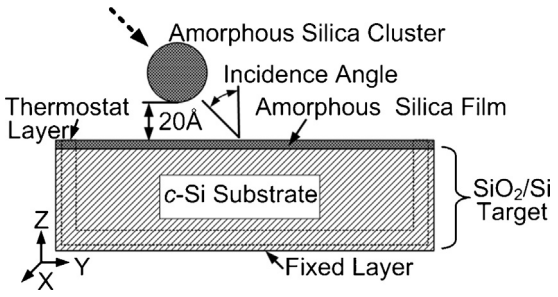

Fig. 2. The schematic diagram of an amorphous silica cluster impact on the crystalline silicon substrate covered by a thin oxidation film for the molecular dynamics simulation.

because the CMP process is transient, dynamic and removes the material of the machined surfaces at nanometer scale. As an alternative, the effect of the passive film could be studied by molecular dynamics (MD) simulation. A few MD simulations have been conducted to investigate the physical essence of the CMP process on the basis of the abrasive wear model [12] and abrasive impact model [16], respectively.

On the basis of the abrasive wear model, Ye et al. [17,18] studied the process of the material removal, and the interplay between mechanistic material abrasion and chemical dissolution during CMP by MD simulations of nanoscale cutting of a copper surface. Agrawal et al. [19] showed that continued transverse motion of the abrasives would lead to tensile pulling, necking, and ultimate separation of the asperity material at silicon wafer by MD simulations. Si et al. [20,21] studied the sliding and rolling effects of the abrasives on material removal of a silicon surface in the nanoscratching process by MD simulations. On the basis of the abrasive impact model, Chagarov et al. [22] studied the mechanical deformation of amorphous silicon dioxide slab under the dry impact of the silica cluster through MD simulations. Han et al. [23,24] studied the surface planarization of the rough silicon surface under the dry impact of multi-nanoparticles through MD simulations. Chen et al. studied the surface damage [25,26] and the material removal processes [27] of the silicon surface under the dry and wet impact of the solid or porous silica cluster by MD simulations.

Most of the simulations reported were performed about the cutting or impact progress of the clusters on the homogeneous and pure substrate. However, no specific result has been reported so far about the effect of the passive film above the pure substrate on the material removal during CMP.

In this paper, to study the material removal mechanism during CMP, we carried out MD simulations of the amorphous silica cluster impacting on the crystalline silicon substrate covered by a thin oxidation film. And the simulation results, which showed that the MRR would firstly increase and then decrease with the increasing of the thickness of the oxidation film, were analyzed on basis of the plough effect and the adhesion effect between the cluster and the impacted surface, and the properties of the oxide film.

2. Simulation model

Fig. 2 illustrates the impact process of the silica cluster toward a SiO_2/Si target, which is composed of the crystalline silicon substrate covered by a thin oxidation film. As described in more detail in our previous work [25–27], Stillinger–Weber-like potential [28] models the interatomic interactions among the cluster, the silica film and the crystal silicon substrate. The Si(0 0 1) substrate contains about 143,360 silicon atoms within a space of 152.04 Å × 217.2 Å × 86.88 Å (i.e. 28 × 40 × 16 unit cells). Then the silicon substrate was covered by an amorphous silica film with a different thickness of 0 Å, 1.5 Å, 2 Å, 2.5 Å, 3 Å, 4.5 Å, 6 Å, 9 Å. The outermost layers of the SiO_2/Si target with the exception of the top surface were fixed in space and have a thickness of 5 Å. In addition, a thermostat layer with a thickness of 10 Å was used to simulate the heat conduction in a reasonable way.

As shown in Fig. 3, the crystalline silicon substrate covered by an amorphous silica film was created in a similar way as in Refs. [29,30]. Firstly, an amorphous silica bulk was created from a beta-cristobalite by firstly melting it and then annealing it. Secondly, the bulk material was sliced to create slabs of amorphous silica with the different thickness. And a few atoms were removed from the slab to enforcing a ratio of two oxygen atoms per one silicon atoms. Thirdly, the layered SiO_2/Si(0 0 1) structures were produced by combining the above amorphous silica slab and a Si(0 0 1) bulk structure and then were relaxed at the ambient temperature. Finally, the relaxed layered structures were replicated and then were used for the impacted SiO_2/Si(0 0 1) target. It deserves noting that the above thickness of the silica film is the nominal thickness owing to the requirement of the preparation of the silica film. Actually, the final true thickness of the silica film is larger than the nominal thickness. For example, the true thickness of the silica film will be close to 3.0 Å under the nominal thickness of 2.5 Å.

The amorphous silica cluster with a diameter of about 54 Å was prepared by quenching melted beta-cristobalite. At the very beginning of the impact, the cluster was located 20 Å above the impacted

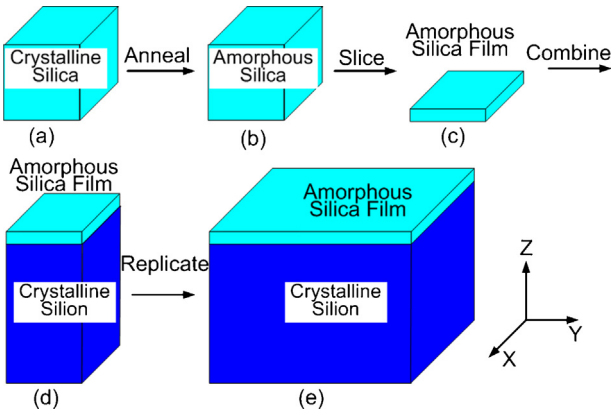

Fig. 3. Building the crystalline silicon substrate covered by an amorphous silica film. (a) A cristobalite unit cell was replicated, filling a cube of 21.72 Å × 21.72 Å × 21.72 Å. (b) To obtain an amorphous bulk, the crystalline silica was annealed, increasing the temperature to 7000 K and then lowering it back to 4500, 3500, 1500, finally to 300 K. (c) The cube of bulk material was sliced and created amorphous silica film with different thickness of 1.5, 2, 2.5, 3, 4.5, 6, 9 Å. (d) The layered SiO_2/Si(0 0 1) structures were produced by combining the above amorphous silica film and a Si(0 0 1) bulk structure. And the dimension of the Si(0 0 1) structure is 21.72 Å × 21.72 Å × 86.88 Å. The combined SiO_2/Si(0 0 1) structure was subsequently relaxed firstly at 0 K and then at the ambient temperature. (e) The combine structure relaxed was replicated by 7 × 10 times in the X- and Y-directions, filling a 152.04 Å × 217.2 Å × 86.88 Å box and generating the SiO_2/Si(0 0 1) target for the simulation system.