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SPUTTERING OF Si(001) AND SiC(001) BY GRAZING ION BOMBARDMENT

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Abstract. The peculiarities of sputtering processes at 0.5-5 keV Ne grazing ion bombardment of Si(001) and SiC(001) surfaces and their possible application for the surface modification have been studied by computer simulation. Sputtering yields in the primary knock-on recoil atoms regime versus the initial energy of incident ions (E_0 = 0.5-5 keV) and angle of incidence (ψ = 0-30°) counted from a target surface have been calculated. Comparative studies of layer-by-layer sputtering for Si(001) and SiC(001) surfaces versus the initial energy of incident ions as well as an effective sputtering and sputtering threshold are discussed.

1. INTRODUCTION

The sputtering process has been the subject of both scientific investigations for a long time and recent rapid developing micro- and nanotechnologies. Processes such as plasma etching and sputter deposition that involve ion bombardment at relatively low ($\sim$ 100 eV) ion energies are widely used in semiconductor processing (Labanda et al. 1997). However, using glancing-angle ion bombardment for surface modification rather than conventional near-normal incidence ions allows expanding the energy range up to $\sim$ 10 keV and has the advantages of reducing damage (such as crater formation) and preferentially removing surface asperities (Dzhurakhalov, 2004) leading to flat surfaces.

Si and SiC crystals have a great importance because of their use in semiconductor technologies. Especially, silicon carbide exhibits a large band gap, a higher breakdown field, a higher thermal conductivity, and a higher saturation velocity, compared to widely used silicon. Besides, SiC is a promising shielding material in nuclear fusion systems such as limiters in Tokamak devices, where the surface erosion is also important (Roth et al. 1976, Bischoff et al. 2001).

In (Kim et al. 2003) atomically clean and flat Si(100) surfaces suitable for nanoscale device fabrication were prepared by wet-chemical etching followed by 0.3–1.5 keV Ar ion sputtering. It was found that wet-chemical etching alone cannot produce a clean

and flat Si(100) surface which can be achieved by subsequent 300 eV Ar ion sputtering at room temperature followed by a 700 °C annealing.

Sputtering yields of crystalline silicon carbide and silicon have been experimentally determined and results have been compared with Monte Carlo simulations for Ne^+, Ar^+ and Xe^+ ion bombardment in the energy range of 0.5-5 keV under 60° sputtering with respect to the surface normal (Ecke et al. 2002). The simulation results depend strongly on the input parameters which are not well known especially for SiC. The TRIM simulation fits the experimental results very well.

The evolution of surface morphology during ion beam erosion of Si(111) at 500 eV Ar^+ ion bombardment (60° from normal, 0.75 mA/cm2 collimated beam current) was studied over a temperature range of 500-730 °C (Brown et al. 2004). Keeping ion flux, incident angle, and energy fixed, it was found that one-dimensional sputter ripples with wavevector oriented perpendicular to the projected ion beam direction form during sputtering at the lower end of the temperature range. For temperatures above approximately 690 °C, growth modes both parallel and perpendicular to the projected ion beam direction contribute to the surface morphological evolution.

Thus, recently sputtering and surface modifications of Si and SiC single crystals are widely studied although there are not sufficient data in the case of grazing incidence. In the present paper, grazing ion sputtering processes of Si(001) and SiC(001) surfaces at 0.5-5 keV Ne^+ bombardment have been studied by computer simulation.

2. COMPUTER SIMULATION TECHNIQUES

The theoretical investigation of atomic collision processes in crystals caused by ion irradiation is more and more done using computer simulation because real physical conditions (e.g. complicated interatomic interaction potential, surfaces, interfaces, defects) can be taken into account much easier than it is possible by using analytical methods (see e.g. Gtirtner et al. 1995).

The simulation used in our calculations to construct the trajectories of the ions or projectile scattered by target atoms is based on the binary collision approximation (see e.g. Parilis et al. 1993) with two main assumptions: (1) only binary collisions of ions with target atoms or between two target atoms are considered; and (2) the path which a projectile goes between collisions is represented by straight-line segments. For the description of the particle interactions the repulsive Ziegler-Biersack-Littmark potential (O'Connor et al. 1986) was used. The inelastic energy losses were regarded as local depending on the impact parameter and included into the scattering kinematics.

Sputtering has been simulated in the primary knock-on regime. Only the primary knock-on recoil atoms ejected from first, second and third layers have been considered. The presence of planar potential energy barrier on the surface was taken into account. The number of incident ions is $4x10^4$. Each new particle is incident on a reset, pure surface. The incident ions and the recoil atoms were followed throughout their slowing-down process until their energy falls below a predetermined energy: 25 eV was used for the incident ions, and the surface binding energy was used for the knock-on atoms. The calculations were performed on the crystals comprising up to 120 atomic layers. The initial energy of incident ions was varied from 0.5 to 5 keV, an angle of incidence ψ counted from target the surface was 0-30° and an azimuth angle of incidence ξ realized by rotating the target around its normal and counted from the $< 100 >$ direction was 0-180°.

3. RESULTS AND DISCUSSION

In Fig. 1a,b the angular dependences of the sputtering yield for Si(001) and SiC(001) surfaces are compared at three values of incident Ne^+ ion energy. Note, the angle of incidence is counted from the surface. It is seen that there is a threshold angle of sputtering in all dependences. At angles of incidence less than the threshold angle the incident ions can not penetrate into the crystal and can not eject target atoms. The threshold angle shifts to the lower values of angle of incidence with increasing the energy of incident ions. The same effect is seen for the main peak of the sputtering yield which increases drastically at first at not too low initial energies and afterwards decreases slowly with increasing angle of incidence. This decreasing is explained by penetration of incident ions to deeper layers at large angles. At low initial energies there is a plateau (shorter for Si and wider for SiC) near the threshold angle because of insufficient ion energy for both a long moving the ions within surface semichannels and their penetration to deeper layers. It is seen that the threshold angle is a bit smaller in the case of Si than for SiC. Besides, in general the sputtering yield is large in the case of SiC. These dependences allow choosing an angle of incidence for an effective sputtering at given initial energy.

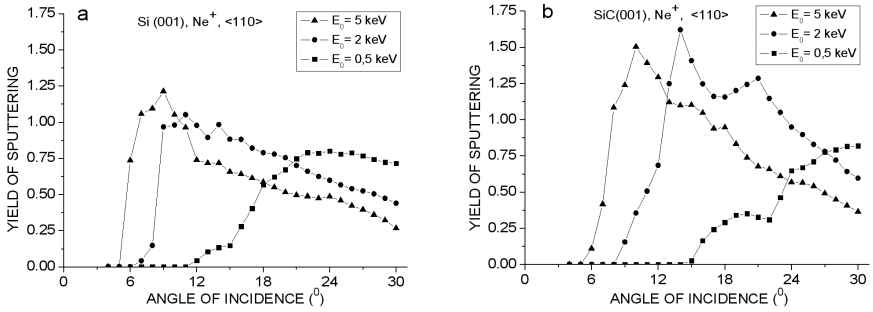

Figure 1: Sputtering yield of Si(001) (a) and SiC(001) (b) versus angle of incidence at Ne^+ ion bombardment.

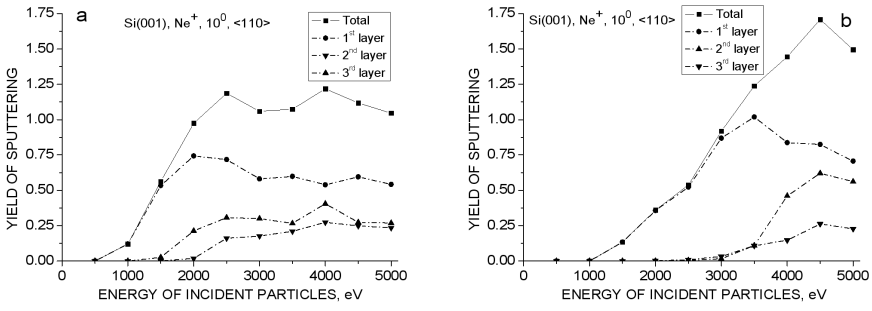

Figure 2: Sputtering yield of Si(001) (a) and SiC(001) (b) versus energy of incident Ne^+ ions at ψ=10°.

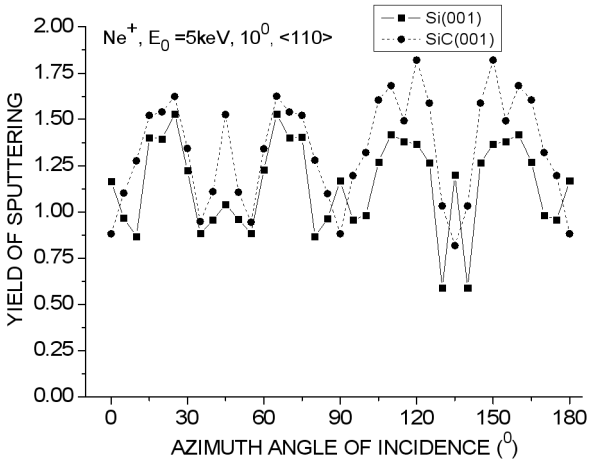

Figure 3: Sputtering yield of Si(001) and SiC(001) versus azimuth angle of incidence at E_0 =5 keV, ψ=10°.

In Fig. 2a,b the sputtering yields of Si(001) and SiC(001) surfaces subdivided into sputtering by the first three surface layers versus the energy of incident Ne^+ ions are shown at $\psi = 10°$. The threshold energy of sputtering is about 1 keV for these cases. There is more drastic increase of sputtering yield in the beginning of dependences for Si than for SiC. It is seen that the main contribution to the total sputtering comes from the sputtering of the first layer. Besides, in the energy range of 1-1.5 keV for Si and 1-3 keV for SiC, sputtering occurs only from the first layer. Further increasing the ion energy results in increasing the contribution from second and third layers. The contribution to sputtering from the third layer is larger than the one from the second layer as the atomic rows in the second layer lies directly under the one of the first layer in the $< 110 >$ direction. Two local maxima at 2.5 and 4 keV are observed in the total sputtering yield dependence in the case of Si. Sputtering from the first layer gives a basic contribution to the first maximum while the second maximum is formed by atoms ejected from the second and third layers. In the case of SiC the maximum of total dependence is formed by atoms ejected from the second layer. These results show that by choosing an angle and an energy of incidence one can produce layer-by-layer sputtering of Si(001) and SiC(001) surfaces.

In Fig. 3 the azimuthal angular dependences of the sputtering yield are compared for Si(001) and SiC(001) surfaces at 5 keV Ne^+ ion bombardment, ψ=10°. Main maxima and minima of dependences are observed in low crystallographic directions and near them. They are caused by the existence of original semichannels and channels in these directions. Thus, there is a good correlation between the sputtering yield dependences and crystallographic structures of studied crystals. From the comparison of the two curves it is seen that at some values of azimuth angle, instead of the peaks of sputtering yield of Si(001) the minima of sputtering yield of SiC(001) are observed. This difference is caused by differences of binding energies, lattice parameters and, of

course, compositions of these single crystals. In most range of the azimuth angle of incidence the sputtering yield for SiC is larger than the one for Si.

4. CONCLUSION

Sputtering yields of Si(001) and SiC(001) surfaces versus the initial energy of incident ions (E_0 = 0.5-5 keV), angle of incidence (ψ = 0-30°) and azimuth angle of incidence (ξ = 0-180°) have been calculated at Ne ion bombardment. It was shown that effective and layer-by-layer sputtering are possible near threshold angle and energy sputtering.

Parameters of single crystals (lattice parameter, binding energy and mass of atoms) influence significantly the angular and energy dependences of sputtering yield. In general, the sputtering yield of the SiC(001) surface is larger than the one of the Si(001) surface.

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