SIMULATION OF BACK AND TRANSMISSION SPUTTERING OF ATOMS UNDER THE ION BOMBARDMENT OF SINGLE-CRYSTAL AND QUASIAMORPHOUS TWO-COMPONENT TARGETS

V. N. Samoilov, V. A. El'tekov, B. Fritzsch, and N. G. Anan'eva

Vestnik Moskovskogo Universiteta. Fizika, Vol. 42, No. 6, pp. 65-69, 1987

UDC 537.534.7:537.534.8

A dynamic model of a block of atoms is used to compare the sputtering parameters of two-component single-crystal and amorphous targets. The simulation is performed for the case of ion bombardment of the (0001) plane of VSi_2 single crystal and a corresponding quasiamorphous target with Ne^+ ions with energies of 10 keV, incident normally.

INTRODUCTION

Ion bombardment of many materials (including two-component media) results in the amorphization of the surface which in turn leads to a change in the propagation of collision cascades and to a change in the parameters of the sputtered particles. The extensive utilization of the sputtering process and the development of methods for the analysis of the structure and composition of surfaces, using ion beams, have been responsible for the growing interest in the interaction between ions and amorphous targets as compared with the corresponding interaction with single-crystal targets of the same composition. Such studies should result in a better understanding of the interaction between ions and solids as a function of the structure of the target. An analytic study of the propagation of collision cascades has already been carried out in the literature in the case of amorphous targets of binary composition. However, the analytical methods encounter serious difficulties in the case of single-crystal targets not only in the case of the two-component media but even for single-component single-crystal targets. Computer simulation has therefore assumed particular importance.

There is now an extensive literature on computer simulation of sputtering from both single-crystal and amorphous solids. The simulation of sputtering under ion bombardment has been based, so far, on the Monte Carlo method and the binary interaction approximation. The binary and dynamic models are quite widely used to calculate sputtering by single crystals. However, there are no published comparisons between the calculated parameters of the propagation of collision cascades and sputtering under ion bombardment of amorphous and single crystal targets (including two-component media), using the same model. An attempt to perform this type of comparison on the basis of the dynamic model of a block of atoms is reported below. We have calculated the sputtering coefficients and the energy spectra of back and transmission sputtered atoms for amorphous and single-crystal targets.

Model. In our previous publications we used the metastable dynamic model of a block of atoms to investigate the back and transmission sputtering from single-component (Co, Ni) (see, for example, [1]) and two-component (VSi_2) [2] single-crystal targets. The same model will be used here. The crystallite consisted of 397 atoms, arranged in five layers of an ideal lattice of a VSi_2 crystal (C40 structure). The layers were parallel to the (0001) plane. Blocks of atoms of this size are widely used in calculations of sputtering from single crystals, based on the dynamic model. The crystallite that we considered was in the form of a cylinder, ~9 Å long and having radius of ~12 Å. The cylinder was surrounded by the interaction region in the form of a rectangular parallelipiped whose faces were at a distance of 4 Å from the block of atoms. The 10-keV $Ne^+ (m_{Ne^+} < m_{Si} < m_V)$ ions were incident normally on the (0001) plane. The ion-atom and atom-atom interactions were described by a potential consisting of two parts, namely, an inverse square potential and the Born-Mayer potential. The constants of this potential were chosen as in [2]. The integration of the equations of motion of the many-body problem was carried out by the "mean force" method. The integration process was terminated when the energy of each of the atoms in the interaction region became less than 4.64 eV. Thermal displacements of atoms in the crystal were not taken into account when sputtering from the VSi_2 single crystal was simulated. The back-sputtering coefficients $S_{t,V}$ and $S_{t,Si}$ and the transmission-sputtering coefficients $S_{t,V}$ and $S_{t,Si}$, and also the energy spectra of the sputtered atoms of the components, were calculated with allowance for the spherical potential barrier on the surface (only particles sputtered through the upper and lower boundaries of the interaction region were taken into account). The difference between the binding energies of the V and Si atoms on the surface was not taken into account. The binding energy was assumed to be 4.64 eV. The liquid model of the amorphous medium was adopted. An attempt to create the liquid block model by using random displacements of all the atoms in a crystallite, uniformly distributed along each coordinate and having the maximum deflection from a site amounting to one-half of the distance to the nearest neighbor, was unsuccessful because it created an internal source of energy in the block because of the strong repulsion between the individual atoms that were too close to one another. The liquid model was therefore developed by anomalously increasing the "thermal" displacements of atoms from the lattice sites in the Debye-Waller model, which corresponded to the melting point. In the calculations reported here, the amplitudes of the displacements of the V and Si atoms from the corresponding lattice sites were assumed to be the same and given by $x_{max} = 0.337$ Å. The displacements of atoms along particular coordinate axes were assumed to be independent of displacements along other axes and of the displacements of the other atoms of the crystal, and were distributed uniformly on the interval $(-x_{max}, x_{max})$. Each successive ion entered a new realization of this quasiamorphous medium.

Results and discussion. The table lists the calculated sputtering coefficients for VSi_2 with the ideal lattice and for quasiamorphous VSi_2. The table also lists the sputtering coefficients for Si atoms, reduced to equal concentrations of the component atoms ($^{1/2}S_{t,Si}$ and $^{1/2}S_{t,Si}$). When sputtering from single-crystal cobalt under bombardment by 10-keV normally incident Ar^+ ions was simulated, the introduction of thermal vibrations led to an increase in the back and transmission sputtering coefficients when the (0001) hcp plane of Co was irradiated. A reduction was observed when the (111) fcc plane of Co was irradiated. The results obtained for cobalt are in good agreement with the experimental data reported in [3] for different transparencies of the single-crystal planes of copper (it was found that, as the target temperature was raised, the sputtering coefficient of the more transparent (011) plane of Cu increased and

Sputtering Coefficients for V and Si Atoms in the Case of Back and Transmission Sputtering (atoms/ion)

	$S_{\uparrow V}$	$S_{\downarrow V}$	$S_{\uparrow Si}$	$S_{\downarrow Si}$	$^{1/2}S_{\uparrow Si}$	$^{1/2}S_{\downarrow Si}$
Perfect lattice	0,31	0,38	0,66	0,83	0,33	0,42
Quasiamorphous target	0,20	0,41	0,56	0,74	0,28	0,37

the sputtering coefficient of the less transparent (111) plane of Cu decreased). Comparison of these data shows that there is an analogy between the bombardment of the (0001) plane of VSi_2 with Ne^+ ions and the bombardment of the (111) hcp plane of Co with Ar^+ ions. Despite the fact that, as we pass from the ideal crystal to the quasiamorphous medium, the probability of collision between the Ne^+ ions and the target atoms increases, which is accompanied by a reduction in the transmission of the ions by the five layers of the crystal and an increase in the energy input into the crystallite, the table shows that $S_{\uparrow V}$, $S_{\uparrow Si}$ and $S_{\downarrow Si}$ increase and $S_{\downarrow V}$ decreases slightly. This reduction is due to the fact that the number of component atoms crossing the upper and lower boundaries of the interaction region with energies $E > 4.64$ eV is reduced (t may increase for $E < 4.64$ eV). The ratio $^{1/2}S_{\uparrow Si}/S_{\uparrow V}$ is greater than unity (~1.06) in the case of the ideal lattice, indicating that the light component is preferentially sputtered. When we pass to the quasiamorphous medium, this ratio is found to be significantly greater (up to ~1.40), so that the preferential sputtering of the lighter atoms is enhanced. The preferential back-sputtering of the atoms of the light component is in agreement with a large number of experiments on sputtering by polycrystalline materials, and also computer simulations of sputtering from amorphous two-component targets (see, for example, [4]). The ratio $S_{\downarrow V}/^{1/2}S_{\downarrow Si}$ is less than unity (~0.92) in the case of the ideal lattice, which corresponds to the preferential transmission-sputtering of the lighter atoms. When we pass to the quasiamorphous medium, the ratio $S_{\downarrow V}/^{1/2}S_{\downarrow Si}$ becomes greater than unity (~1.11). This means that, in the case of the quasiamorphous medium, the heavy atoms are preferentially transmission-sputtered (this was also observed experimentally for polycrystalline targets and was observed in computer simulations of the sputtering by an amorphous traget [5]).

The energy spectra of transmission-sputtered V and Si atoms, $N(E)_{\downarrow V}$ and $^{1/2}N(E)_{\downarrow Si}$, are shown in Fig. 1 in the case of the ideal lattice. Most of the particles in both spectra have energies between 1 and 70 eV. The maximum of the spectrum of transmitted Si atoms is shifted toward lower energies (by ~3 eV) relative to the maximum of the spectrum of V atoms, although the Ne^+ ion transfers more energy to the Si atom on collision than to the V atom (this is due to the fact that the difference between the masses of the ion and the V atom is greater than the difference between the ion and the Si atom). The relative shift of the spectrum of transmission-sputtered Si atoms toward lower energies is due to the large mass difference between the component atoms ($m_V/m_{Si} \simeq 1{,}814$). This means that the lighter Si atoms moving into the crystal have a greater probability of being reflected by the lower-lying heavier V atoms. Hence, silicon atoms passing through the five crystal layers lose a substantial fraction of their energy, transferring it to the vanadium atoms. The heavier V atoms do not come to rest as they penetrate the crystal and collide with the lighter Si atoms, but transfer their momentum to other V atoms when they collide with them. This also leads to the above preferential back-sputtering of Si atoms and the preferential tansmission-sputtering of V atoms. The high-energy

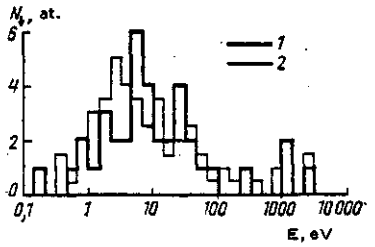

Fig. 1

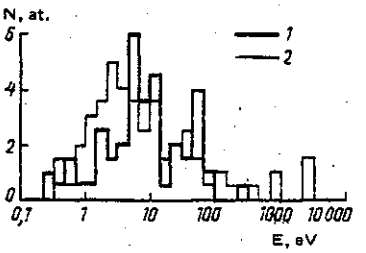

Fig. 2

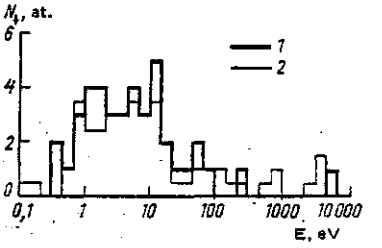

Fig. 3

Fig. 1. Energy spectra of V and Si atoms, $N(E)_{\downarrow V}$ (1) and $^{1/2}N(E)_{\downarrow Si}$ (2) produced by transmission sputtering when Ne^+ ions with energies of 10 keV are incident normally on the (0001) face of a VSi_2 single crystal. The spectrum of the Si atoms is normalized to an equal concentration of the component atoms.

Fig. 2. Energy spectra of back sputtered Si atoms (1) $(^{1/2}N(E)_{\uparrow Si})$ and transmission sputtered Si atoms (2). $(^{1/2}N(E)_{\downarrow Si})$ (single crystal target).

Fig. 3. Energy spectra of V and Si atoms, $N(E)_{\downarrow V}$ (1) and $^{1/2}N(E)_{\downarrow Si}$ (2), produced by transmission sputtering from an amorphous target.

V and Si atoms (with E > 1 keV) in the spectra of transmission-sputtered atoms were probably ejected from the lower layers of the crystallite by ions penetrating the crystal along a channel.

When the ideal VSi_2 lattice is bombarded with ions, the maximum of the spectrum of back-sputtered Si atoms is shifted toward higher energies relative to the spectrum of transmission-sputtered Si atoms (Fig. 2). This shift is due to the high probability that the lighter Si atoms will be reflected by the lower-lying V atoms. The energy of the large fraction of back-sputtered Si atoms is then greater than the energy of the predominant number of transmission-sputtered Si atoms whose ejection is due to the development of the collision cascade. At the same time, the spectrum of transmission-sputtered Si atoms contains atoms with energies in excess of 500 eV (as suggested above, they are knocked out by Ne^+ ions from the lower layers of the crystallite). Si atoms with energies in excess of 500 eV are absent from the back-sputtered spectrum because of the high energy losses accompanying the reversal of the momentum of the atoms (when the Si atom collides head-on with a V atom, it loses approximately 92% of its energy).

When we pass to the quasiamorphous medium, the maximum height and the width of the spectra of transmission-sputtered V and Si atoms (Fig. 3) are reduced, which is in agreement with the changes in the spectra of atoms sputtered under ion bombardment in the case of a single-component single-crystal medium [the (111) planes of single-crystal cobalt] if thermal vibrations of the lattice atoms are taken into account. The spectra of transmission-sputtered V and Si atoms in the case of the quasiamorphous medium are found to be closer to the case of ion bombardment of the ideal lattice (see Figs. 3 and 1). As we pass to the quasiamorphous medium, we encounter V and Si atoms with higher energies than in the case of the ideal lattice. This is due to the fact that the transition to the quasiamorphous model is accompanied by an increase in the probability of collision of an ion penetrating the crystal with the V and Si atoms displaced from the lattice sites. The transition to the quasiamorphous medium is also found to lead to an increase in the mean energy and the total energy transported by the atoms of the two components, both for back and transmission sputtering.

This is explained by the higher probability of a strong collision between an ion and a lattice atom, and the subsequent redistribution of energy in collision cascades between the components in different directions.

CONCLUSIONS

We have tried to apply the dynamic model of a block of atoms to the analysis of sputtering by amorphous targets. The same model was used to calculate sputtering by quasiamorphous and single-crystal targets, and we were able to exhibit the properties of the interaction between ions and solids for different degrees of order in the disposition of their atoms. We were also able to determine the trends in the back and transmission sputtered atoms when thermal vibrations of the crystal atoms were introduced into the model. The properties of the sputtering coefficients and energy spectra of atoms undergoing both back and transmission sputtering under bombardment of two-component quasiamorphous targets (when compared with the ideal crystal) are due to not only the change in the structure but also the two-component nature of the target, including the large mass difference between the components forming the compound.

The authors are grateful to V. E. Yurasova for suggesting the calculation of sputtering by an amorphous two-component target and for discussions of some of the result, and to P. Vaisbrodt, V. S. Chernysh, S. P. Linnik, and Yu. N. Ivashchenko for discussions on the sputtering of two-component media.

REFERENCES

1. V. A. El'tekov, V.N. Samoilov, V. E. Yurasova, and N. A. Motaweh, Nucl. Instrum. Methods B, vol. 13, no. 1-3, pp. 443-448, 1986.
2. P. Vaisbrodt, V. N. Samoilov, and V. A. El'tekov, "Surface diagnostics with ion beams," in: Proc. All-Union Seminar [in Russian], pp. 193-194, Uzhgorod, 1985.
3. I. N. Evdokimov, V. A. Molchanov, D. D. Odintsov, and V. M. Chicherov, Dokl. Akad. Nauk SSSR, vol. 177, no. 3, pp. 550-553, 1967.
4. T. S. Pugacheva, O. V. Gusev, and T. L. Roslyakova, "Interaction of atomic particles with solids," in: Proc. Sixth All-Union Conf. [in Russian], part 1, pp. 3-5, 1981.
5. O. F. Goktepe et al., Nucl. Instrument. Methods, vol. 13B, pp. 434-438, 1986.

23 June 1986

Chair of General Physics for the Physics Department and Chair of Mathematics