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Sputtering Angular Distributions of Individual Elements for Low-Energy Ar Ion Irradiation of PtCu Alloy

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The dynamic Monte Carlo program including a bombardment-induced Gibbsian segregation process was used to calculate angular distributions of individual elements from sputtered $Cu_{0.5}Pt_{0.5}$ alloy in the Ar ion energy range between 0.2 and 1.5keV. Calculated results show that for each investigated incident energy, the angular distribution of the Pt element is more forward-pointed than that of the Cu one; the reason may be that different percentage of sputtered atoms (37~45% of Pt and 12~19% of Cu) come from beneath the topmost layer.

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It is now recognized that under ion bombardment at high dose, an altered layer with the order of the sputtering depth[1,2] exists at the alloy surface due to the preferential sputtering or bombardment-induced Gibbsian segregation (BIGS). The effect of the altered layer at the surface on sputtering angular distributions of alloys has created considerable excitement in sputtering investigations in recent years. The existence of concentration gradients at the CuPt surface was found by Andersen *et al.*[3] under Ar ion bombardment with energies greater than 20 keV by means of measurements of angular distributions of composition, which demonstrated that Pt is preferentially ejected in the near-normal direction. Below 20 keV, their measurement results did not confirm the presence of segregation layers of Cu on the sputtered CuPt alloy. Lately, using different energy Auger line combinations, Li *et al.*[4] have observed bombardment-induced segregation of Cu in the CuPt alloy at Ar ion energies from 0.2 to 2 keV. Li's experiments may imply the preferred ejection of Pt in the normal direction at very low energies. For element targets, it is well established in many papers that as the projectile energy increases from that close to sputtering threshold to keV, the angular distribution will change from under-cosine into cosine-like, or even into over-cosine shapes. However, for alloy targets, very little information has been published concerning the shape change of angular distributions of individual elements in the above projectile energy range by now.

In this work, we try to calculate the angular distributions of individual elements from sputtered $Cu_{0.5}Pt_{0.5}$ alloy in the Ar ion energy range between 0.2 and 1.5 keV at normal incidence with the help of the modified dynamic TCIS (transport and atomic collision cascade of energetic ions in solids) Monte Carlo program including the BIGS process[5], in order to further study the effect of concentration gradients in the order of the sputtering depth on sputtering angular distributions of alloys.

The TCIS program series[5,6] can be used to calculate not only surface composition profiles with depth[5] but also angular distributions[7] for sputtered targets. The modified dynamic TCIS program is employed in the present study to simulate collision cascade, BIGS and BED (bombardment-enhanced diffusion) processes at all. In the program, BIGS is assumed to occur at the surface between the first and second layers, so the sharp variation of the composition is between these layers.

In this simulation, we note that Brongersma *et al.*[8] have found that the topmost surface composition assessed with ISS (ion scattering spectroscopy) is the same as the bulk in the $Cu_{0.20}Pt_{0.80}$ alloy sputtered by 1keV Ne ions when the target temperature is below 100 °C. We also note Sigmund's idea[9] that if the true preferential sputtering has been ignored, at high dose, i.e. assume that the composition of the sputtered flux is equal to the bulk composition, the composition of segregating atoms at the topmost surface is equal to that at the bulk while the sputtering depth is less than the segregation layer. Above notices can be adopted to examine simulated surface composition profiles, which significantly influence sputtering angular distributions of alloys.

Our calculations show that at high enough doses of incident Ar ions, the steady composition gradients appear at the sputtered $Cu_{0.5}Pt_{0.5}$ surface in the energy range from 0.2 to 1.5 keV. In these steady surface composition profiles, the Cu composition enriches in the first layer (50 at.%), depletes in the second layer and increases slowly to the bulk composition. Corresponding to the Cu composition, the Pt composition in the second layer is much denser than that in the first layer. The calculated composition data of Cu and Pt are both shown in Table 1. It should be mentioned here that for all incident energy-ion-target combinations, each layer thickness is chosen to be about 2.5 Å (mean atomic spacings[2]). It is found in our calculations that for all above systems, the mean depths of origin of sputtered atoms for Cu and Pt are either below or close to 2.5 Å, i.e., segregation layer thicknesses of Cu. As explained before, not only the calculated composition data and the tendency of the composition variation with depth may be realistic, but also the chosen segregation layer thicknesses of Cu consent to Sigmund's conclusion[9] about the relation among the sputtering depth, the segregation layer and the surface concentration.

Table 1 Steady-state compositions at the sputtered $Cu_{0.5}Pt_{0.5}$ surface as a function of Ar ion energies.

Ar ion	Steady-state compositions (at.%)			
energy	Cu element		Pt element	
(keV)	first layer	second layer	first layer	secondlayer
0.2	50	38	50	62
0.7	50	34	50	66
1.1	50	29	50	71
1.5	50	25	50	75

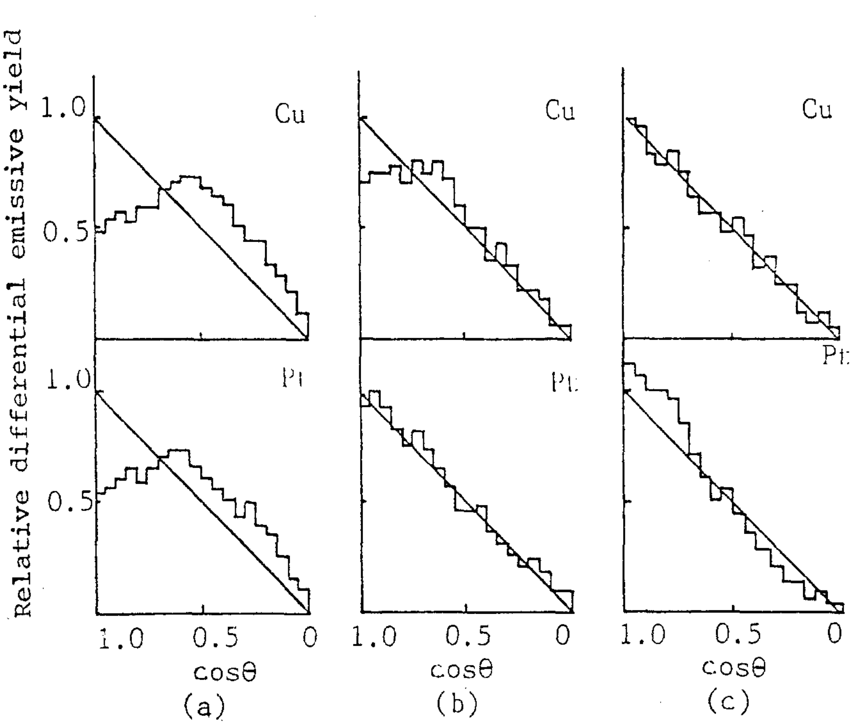

Fig. 1 Stable angular distributions of Cu and Pt from the sputtered $Cu_{0.5}Pt_{0.5}$ alloy under Ar ion bombardment with 0.2 (a), 0.7 (b) and 1.1keV (c). θ is the polar emission angle.

In Fig. 1, the shape transformation of the Pt angular distribution is always ahead of that of the Cu angular distribution as the energy of Ar ion bombardment of the $Cu_{0.5}Pt_{0.5}$ alloy increases. Double under-cosine distributions emerge at quite low incident energies, but the Pt distribution is more outward-peaked than the Cu distribution (Fig. 1a). The Pt distribution shows the cosine-like shape when the Cu distribution still keeps the under-cosine shape (Fig. 1b). The Pt distribution has already showed the over-cosine shape before the Cu distribution changes into the cosine-like shape (Fig. 1c). As a general rule, most sputtered atoms are kicked out of the target from the outer 2~3 atomic layers; and the surface composition spike normally has a width of exactly one atomic layer[2], i.e., it exists at the topmost layer. Sigmund *et al.* have pointed out[1] that the existence of the concentration gradient at the surface causes the difference in the angular distributions because of the surface layer reducing that fraction of the atoms originating deeper in the target which exit at oblique angles. This means that compared with those from the topmost layer, the sputtered atoms from beneath the topmost layer have more possibilities to exit at near-normal direction than at oblique angles. For each investigated system, table 1 shows a large composition difference between the first and second layers at the sputtered $Cu_{0.5}Pt_{0.5}$ surface; furthermore, the concentration of Pt is equal to that of Cu in the first layer whereas the concentration of Pt is much greater than that of Cu in the second layer. Correlated with the surface composition profile of $Cu_{0.5}Pt_{0.5}$, our calculated results also show that 37~45% of the sputtered Pt atoms but 12~19% of the sputtered Cu atoms come from beneath the topmost layer. Therefore, the large difference in the ejective probabilities of Pt and Cu atoms from beneath the topmost layer explains why the angular distribution of Pt is always more forward-pointed than that of Cu. Obviously, it is easily seen in fig.1 that Pt is preferentially ejected in the normal direction at quite low energies.

Andersen *et al.* have paid attention[3] to the significant influence of the surface contamination on the experimental $Cu_{0.5}Pt_{0.5}$ angular distributions due to a combination of low sputtering yields and available beam current under Ar ion bombardment below 10keV. Indeed, such an impurity layer on the $Cu_{0.5}Pt_{0.5}$ surface may strongly perturb the detection of the Cu segregation layer by the measurement of sputtering angular distributions. If the surface contamination could be dispelled during the Ar ion bombardment, the experimental angular distributions of Cu and Pt from the sputtered $Cu_{0.5}Pt_{0.5}$ surface might be similar to those calculated by us for the above combinations.

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