Atomic transport in thermal spike induced ion mixing

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1. Introduction

Ion beam mixing is now recognized as a useful technique to produce some metastable compositions and structures not existing in the equilibrium state. In this study, we present an experimental result for the isotropic atomic transport in Pd/Co bilayer due to thermal spike induced ion mixing, and develope a model to predict the absolute ratio of atomic fluxes of constituents in bilayer systems, which is based on the Vineyard's thermal spike model and the impurity diffusion in solid by a vacancy mechanism.

2. Experimental procedure

Pd(300 Å, top layer)/Au(10 Å,marker)/Co(1000 Å, bottom layer) samples were deposited on single crystal Si substrates by sequential electron beam evaporation. Ion beam mixing was carried out with 80 keV Ar^+ ions at 90 K in order to avoid radiation enhanced diffusion(RED). The ion dose ranged between $1x10^{15}$ and $2x10^{16}$ Ar^+/cm^2 at a typical flux of 1.5 $\mu A/cm^2$.

Fig.1 shows the RBS spectra of Pd and Au layer for the as-deposited and $1.2x10^{16}$ Ar^+/cm^2 irradiated samples. After ion bombardment at 90 K, the broadening of the marker signal and the shift of the low-energy edge of Pd signal are enhanced progressively with increasing ion dose, which demonstrate the atomic transport has occured by ion irradiation. But the marker position remains almost stationary. Thus this result indicates that the atomic mixing of Pd and that of Co across the marker layer is nearly same amount, or the isotrpic atomic transport in Pd/Co system.

The atomic transport fluxes across the marker layer were determined by fitting the computer simulated curves to the experimentally observed RBS spectra.

3. Result and discussion

In order to interpret our experimental results and develope a model to predict the value of J_A/J_B, we introduce the Vineyard's thermal spike model and impurity diffusion in metals.

$$J = C_2 \left[\frac{F_d}{Q} \right]^n \frac{\phi}{\rho^{2/3}} \frac{\partial}{\partial x} f(x)$$

where Q is the effective activation energy for the thermal spike, F_d is the energy deposited per unit ion path length at the interface, and n is the power factor. The value of n is 2 for the cylindrical thermal spike, and 5/3 for the spherical thermal spike. C_2 is a constant, and f(x) is the stoichiometric fration of atom at a depth x.

$$Q_{A(B)}^* = 0.38E_{coh}^B + 0.15E_{coh}^A$$

where E_{coh}^A and the E_{coh}^B are the cohesive energies of pure atom A and B, respectively. When we assume the value of F_d and ρ are constant, odtained the ratio of dimensionless atomic fluxes defined by $J_i^* = J_i/\rho_i^{2/3}$ (i = A or B) becomes as,

$$\frac{J_A^*}{J_B^*} = \left[\frac{Q_{B(A)}^*}{Q_{A(B)}^*} \right]^n \left[\frac{\rho_B}{\rho_A} \right]^{2/3}$$

where $Q^*_{A(B)}$ is the activation energy for a impurity atom of A to diffuse into a matrix atom of B and ρ is the average atomic density of target material. From the above eq. one can easily recognize that the ratio of atomic fluxes depends on the value $Q_{A(B)}^*$ and $Q_{B(A)}^*$, and the system having larger difference between $Q_{A(B)}^*$ and $Q_{B(A)}^*$ shows an anisotropic atomic

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transport, while the system which has similar activation energies of constituents for the impurity diffusion reveals an isotropic atomic trnsport.

In our Pd/Co system, using n = 5/3, we found that the value of J_A^*/J_B^* are 1.11. These values are in good agreement with the experimental results of 1.03 ± 0.09. This near isotropic atomic transport in Pd/Co system is an expected result, since the constituents(Pd and Co) have similiar activation energies for the impurity diffusion. In order to clarify the validity of our presented model, we compared Auner's experimental results. In table 1, we tabulated the measured and calculated values.

4. Conclusion

The ratio of atomic transport fluxes of constituents due to the thermal spike is related with the activation energy for the impurity diffussion. A model to describe the ratio of atomic fluxes in thermal spike induced diffusion correctly predicts the trend in experimental observation and agree fairly well quantitatively.

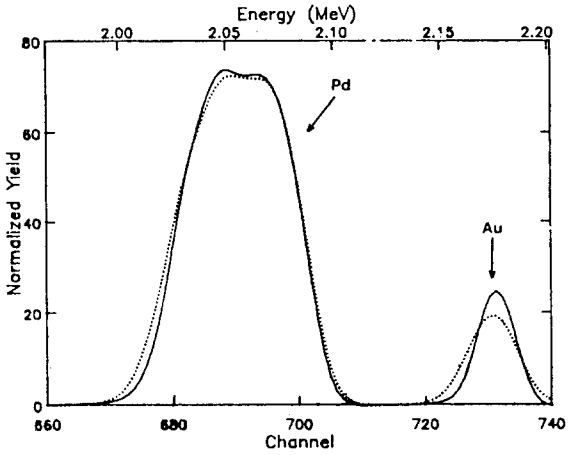

Fig. 1 Rutherford backscattering spectra of the Pd and Au layer for the as-deposited(——) and 1.2×10^{16} Ar^+/cm^2 irradiated(------) Pd/Co system.

Table 1. System geometries, cohesive energies(E_{coh}), atomic densities(ρ), activation energies for impurity diffusion($Q_{A(B)}^*$), the experimental and the calculated values of the ratio of dimensionless fluxes ($(J_A^*/J_B^*)_{exp}$, $(J_A^*/J_B^*)_{cal}$).

System configuration	E_{coh}^A	E_{coh}^B	$Q_{A(B)}^*$	ρ_A	ρ_B	(J_A^*/J_B^*)	
(A/B/substrate)	(eV/atom)			($\times10^{22}/cm^3$)		exp	cal
W/Pd	8.90	3.89	2.81	6.30	6.80	1.18	2.09
Pd/W	3.89	8.90	3.97	6.80	6.30	0.73	0.48
Nb/Cu	7.57	3.49	2.46	5.56	8.45	2.78	2.53
Cu/Nb	3.49	7.57	3.41	8.45	5.56	0.48	0.39
V/Ag	5.31	2.95	1.92	7.22	5.85	1.54	1.43
Ag/V	2.95	5.31	2.46	5.85	7.22	0.50	0.70
Ni/Pd	4.30	3.89	2.12	5.14	6.80	1.18	1.33
Pd/Ni	3.89	4.30	2.22	6.80	5.14	0.96	0.88