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A calculation on the Metal-Film Mixing by Intense Pulse Ion Beam (IPIB)

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Abstract

In this paper, we studied, by numerical calculation, a system, which was composed of metal-film and metal-substrate irradiated by IPIB with beam ion energy 250 keV, current density 10 to 250 A/cm^2. While the IPIB irradiation was going on, an induced effect named mixing occurred. In this case, metal-film and part of metal-substrate melted and mixed. The mixing state was kept as it was in melting phase due to the fast cooling rate. Our works were simulating the heating and cooling process via our STEIPIB program and tried to find proper parameters for a specific film-substrate system, 500 nm titanium film coated on aluminum, to get best mixing results. The parameters calculated for such Ti-Al system were compared with the experimental results and were in good accordance to the experimental results.

Keywords : IPIB, mixing, coatings, computer simulation

1. Introduction

For surface treatment, intense pulse ion beam (IPIB) is expected to be an effective method because of its high power density. In comparison to laser beams, IPIBs have several advantages. These are: noticeably higher efficiency, larger areas of treatment (~10^2 cm^2), high levels of absorption in various materials, deeper layer of modification and lower fluences (10^{13}~10^{14} ions/pulse) which makes it possible to produce film with moderate impurity levels (<0.1 at.%).

By using the thermo-dynamical effects it induced, we can modify the target material surface directly or deposit protective coatings on metals. And there is an increasing interests in the development of new technology on corrosion and adhesion enhancements-- ion beam mixing for various combinations of thin film and substrates [1,2,3].

But it must be noted that ion mixing to creating transition layer could be provided in different ways. There are many factors affecting the efficiency of each way. They are ion energy, current density, ion dose, the masses of ion and target atom, and irradiation conditions. So the objectives of this paper were: (1) to study beam energy deposition profile in Ti/Al film-metal system; (2) to calculate thermal effects in the surface layer of such system by our STEIPIB codes [4]; and (3) find out a proper parameter for IPIB mixing technique.

2. Simulation Method

In our calculations, we consider ion beams has an energy spectrum with current density varying versus time. The ion energy and beam current density could be described by pulse functions according to the discussion before [5]. Energy deposition profiles are calculated with SRIM code.

We assume that ion deposited energies are completely

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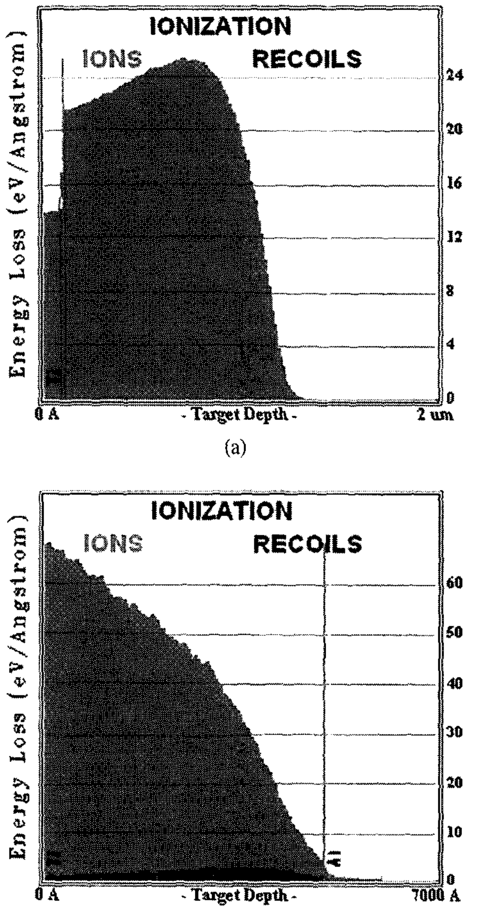

(a)

(b)

Fig. 1. shows the energy deposition profile of 250 keV H^+ and C^+ respectively.

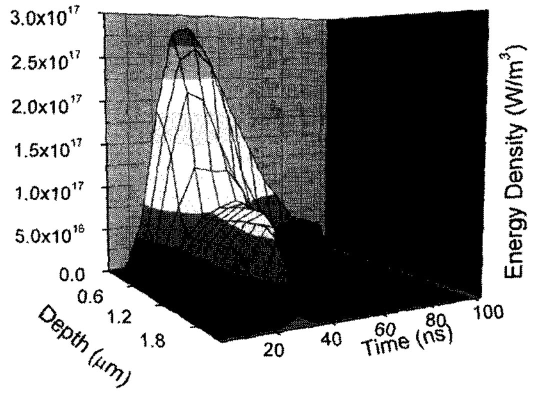

Fig. 2. shows energy deposition profiles of these two ions at different time.

transformed into heat energy, so the energy absorption profiles in the surface layer of Ti/Al film-metal system are considered the same as ion deposited energy curves.

Because the cross-section areas of IPIB are from few cm^2 to 10^2 cm^2, hence the distortions at the beam margin are too little to be considered, so it may be considered as one-dimension problem. With the codes named STEIPIB developed in our lab, we calculate the temperature distribution and phase transformation generated by IPIB. IPIB parameters are: 250 keV beam ion peak energy, 10 A/cm^2 to 250 A/cm^2 beam peak current density (10 A/cm^2, 30 A/cm^2, 50 A/cm^2, 80 A/cm^2, 100 A/cm^2, 120 A/cm^2, 150 A/cm^2, 180 A/cm^2, 200 A/cm^2, and 250 A/cm^2, respectively), 100 ns pulse duration. Compositions of IPIB ions are 70% H^+ and 30% C^+. The results are shown below.

3. Calculation Results and Discussion

With the same beam ion energy spectrum, we change the beam current density to evaluated Ti/Al system's surface phase transformation. Fig. 3 and fig. 4 demonstrate temperature distribution of Ti/Al film-metal system irradiated by IPIB of 100 ns duration time, 250 keV beam ion energy, but 120 A/cm^2 and 50 A/cm^2 current density respectively.

Fig. 5 shows temperature distribution at the time when the thickness of Ti layer gets a maximum value. For IPIB of 250 keV, 80 A/cm^2, 100ns, it happened at

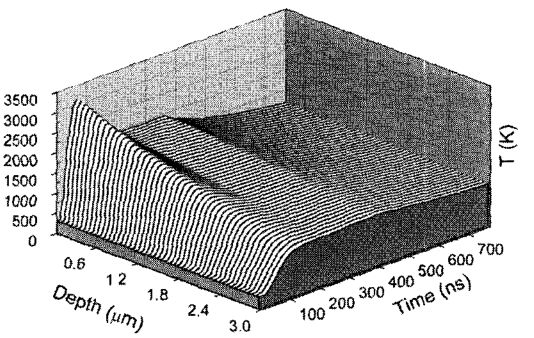

Fig. 3. Temperature near the surface of Ti/Al irradiated by 250 keV, 120 A/cm^2, 102 ns IPIB

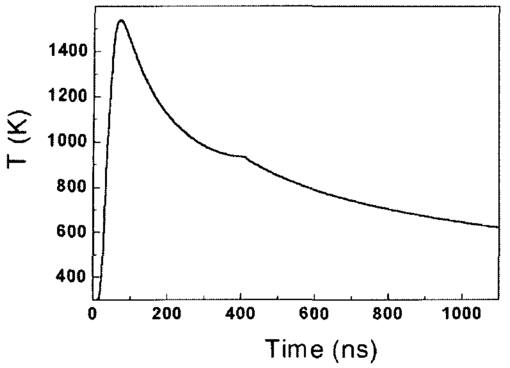

Fig. 4. Temperature at the Ti/Al interface irradiated by 250 keV, 50 A/cm^2, 100 ns IPIB

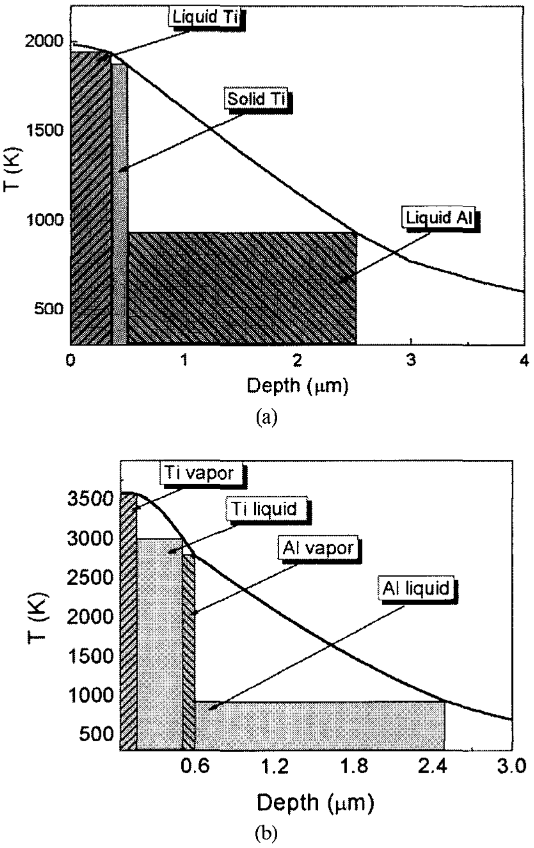

Fig. 5. Temperature distribution at the time when the thickness of Ti layer gets a maximum value: (a) at 89 ns, with beam parameters 250 keV, 80 A/cm^2, 100 ns IPIB; (b) at 57 ns, with beam parameters 250 keV, 150 A/cm^2, 100 ns.

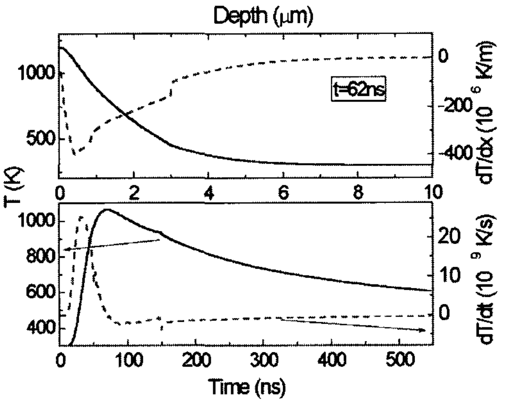

Fig. 6. Temperature, its gradient and its varing rate at the interface of Ti/Al irradiated by 250 keV, 30 A/cm^2, 100 ns IPIB.

89 ns, as (a) shown; while it happened at 57 ns for IPIB of 250 keV, 150 A/cm^2, 100 ns.

These figures demonstrate that for some film-metal structure with bigger difference of melting points, like Ti/Al in this paper, substrate melted more easily than film layer outside. And while the inside layer of film (Titanium film) kept solid, substrate (Aluminum) began melting.

Furthermore, the thickness of melted Al substrate could access to several micrometers, even though Ti film layer did not get to melt (as Fig. 4 shown). According to our calculation, the highest temperature of Ti film, which was 1756 K, hadn't got to melting point of Ti (1941K), but Al substrate had melted as pulse energy rising to its highest value when current density was only 50 A/cm^2 or lower.

Through our calculation, we can read that while current density increasing, there are at least four kinds of phase state of Ti/Al system appeared during IPIB irradiation. These are solid-solid, solid-liquid, liquid-liquid, liquid- vapor (two of them shown in Fig. 5).

For purpose of obtaining transition layer between Ti film and Al substrate, which acts as increasing film adhesion, we have two ways to realize mixing technique. One is fast melting of surface layer and convective mixing. The other is noticeable high gradient of temperature near Ti/Al interface and mixing through the enhancement of thermal diffusion.

At low current density, such as 30 A/cm^2 shown in

Fig. 6, Ti film kept solid state and it could not mixing with Al through convection. But the temperature gradient at interface is quite high, nearly 4.0×10^8 T/m (see Fig. 6). It is big enough to be a driven force for thermal diffusion.

When we get enough current density, convective mixing is a preferable way for us. Because during the irradiation of IPIB, surface layer is heated to melting very fast (as Fig. 6 shown heating rate access to 1010 K/s), mixing together and then cool also very fast (as Fig. 6 shown heating rate access to 109 K/s). Therefore, convection or Raleigh-Taylor instability state during fast heating process can be kept up.

On the other hand, temperature gradient still keeps at a high level when melting process occurs (see Fig. 7). This high gradient, accompany with a little amount of aluminum substrate vaporization, could contribute to Raleigh-Taylor instabilities and let two metals mixing sufficiently. Through the estimation of time needed for the first mode instability to develop in ref. [2], we got 3×10^{-8}s. That just falls in the heating process.

Therefore, for convective mixing, the best state is melting of the whole Ti layer, Al substrate and in addition a little amount of Al substrate vaporizing. According to such principle, we first got a development of thickness of melting layers and vaporizing of film and substrate via different current density (shown in Fig. 7). From Fig. 7, we got the best current density or 250keV, 100ns IPIB locating between 120~150 A/cm^2.

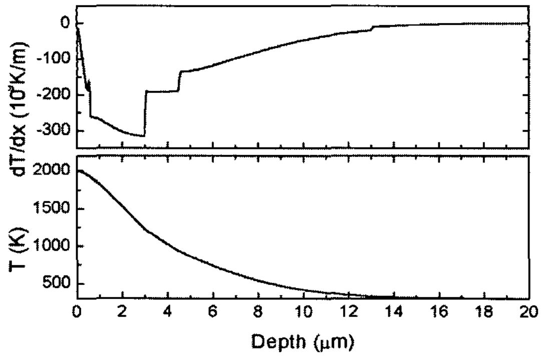

Fig. 7. Temperature and its gradient at time=194 ns (IPIB parameters: 250 keV, 120 A/cm^2, 100 ns).

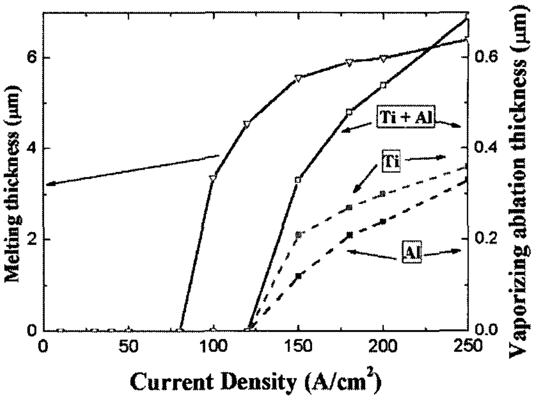

Fig. 8. Melting layer thickness and vaporizing of film and substrate at different current density.

The experiments results done in ref [2] is around 150 A/cm^2. This is in agreement with our calculation. Furthermore, the evaporated layer thickness calculated here is 120 nm. It's also good correspondence to the Auger profile measurement results done in ref. [2].

4. Conclusions

There are two kind of mixing techniques for IPIB: convective mixing and thermal diffusion. Through our calculation, they are all practical. For IPIB of 250 keV, 100ns, the best current density fall in a range between 120~150 A/cm^2.

Acknowledgments

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