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Two-dimensional numerical research on effects of titanium target bombarded by TEMP II accelerator

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Two-dimensional numerical research has been carried out on the ablation effects of titanium target irradiated by intense pulsed ion beam (IPIB) generated by TEMP II accelerator. Temporal and spatial evolution of the ablation process of the target during a pulse time has been simulated. We have come to the conclusion that the melting and evaporating process begin from the surface and the target is ablated layer by layer when the target is irradiated by the IPIB. Meanwhile, we also obtained the result that the average ablation velocity in target central region is about 10 m/s, which is far less than the ejection velocity of the plume plasma formed by irradiation. Different effects have been compared to the different ratio of the ions and different energy density of IPIB while the target is irradiated by pulsed beams.

Keywords: intense pulsed ion beam, two-dimensional numerical model, ablation process, titanium

PACC: 6180J, 0570, 5265

1. Introduction

In the recent twenty years, intense pulsed ion beam (IPIB) techniques have been researched extensively in the material science field.[1−3] This is mainly due to the construction of the equipment of moderate size with high power load that generates the ion beam which has the advantages of high density ($\sim$1 kA/cm^2), short pulse time (10–1000 ns), and high ion energy ($\sim$MeV), etc.

IPIB is generated by a magnetically insulated diode (MID),[4,5] the energy of the ion is determined by voltage applied to the diode. The sort of ions and the composition of beam are determined by anode material of MID. For the TEMP II accelerator, where graphite is used as the anode of MID, the beam consists of H^+ ions and C^+ ions. When the beam impacts on the target, the energy mainly deposits on the surface, and melting and boiling both begin from the surface of the target. A temperature gradient will form due to the deposited energy, and thermal stress will be generated. If the surface absorbs enough energy, evaporation happens and plasma ejects from the surface; meanwhile, because of the reaction of emission of material a shock wave will be generated and propagates inside the target.

The beam generated by IPIB shoots to the focus region of MID, therefore at different distances from the target in the vacuum chamber, the IPIB density will be different. Actually, from the experiments we know that IPIB density has a spatial distribution when IPIB interacts with the target. On the target surface, the central region where IPIB interacts with the target absorbs more energy, and during the irradiation process the ablation of material reaches a maximum value here, and the farther from the centre, the shallower the irradiation depth is, so there are shortcomings in dealing with the problem with one-dimensional models,[6] in which the real process cannot be reflected correctly.

In this paper, by combining the characteristic of TEMP II accelerator, we establish a temperature model with phase transformation in Section 2, and calculate the temporal evolution of titanium target, and give the results of thermal effects and the irradiation process for Ti target irradiated by IPIB in Section 3. Section 4 gives our conclusions.

2. Physical models

2.1. IPIB model

IPIB is mainly determined by ion species, MID voltage, ion beam density and pulse duration. For

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different types of IPIB accelerators, the sort of ions and the component of beam will be different, and the effects caused by accelerator will be different also. H^+ ions have long range, they can impact into the deep layer of the target, but C^+ with the same energy can only shoot into the shallow layer. The energy of ions is determined by the voltage of MID: the higher the voltage is, the higher energy an ion has. The voltage of the diode is zero at first, and then increases to a maximum value, then decreases, and at last disappears during a pulse. The energy of the ions are not a single one: they have distributions. The higher the energy the ions have, the deeper the ions shoot into the target, and the more widely the ions affect it; the number of ions arriving at the target is determined by IPIB density, it is affected by the distance between MID and the target, and at the focus region of MID, the density reaches peak value. High voltage and IPIB density create intense power density. Energy transform from IPIB to target per unit time is more efficient. Therefore, the voltage of MID and IPIB density are the decisive factors for melting depth and evaporating mass of target.

Generally, an average energy of ions is used to discuss the IPIB irradiation problem, but in looking for the instantaneous change of temperature and ablation mass, a model changing as function of time must be used. According to the fitting results of MID voltage and the wave of IPIB density near the focus of MID, considering the axis-symmetric profile of the deposited energy, we take an arbitrary direction as positive direction of y axis on the target surface, and the direction pointing to the inside of the target as positive direction of x axis. The voltage and ion density are given as follows respectively:[7]

$$U(t) = A\exp\left[-\frac{(t-t_{0U})^2}{2\sigma_1^2}\right], \tag{1}$$

$$J(y,t) = B\exp\left[-\frac{(y-y_0)^2}{2\sigma^2}\right]\exp\left[-\frac{(t-t_{0J})^2}{2\sigma_2^2}\right]. \tag{2}$$

Here y_0 represents central position of y where the ion beam bombards the target. A and B represent maximum value of MID voltage and IPIB density respectively. At the position y, power density of absorbed energy is:

$$P(y,t) = U(t-\Delta t)J(y,t), \tag{3}$$

where $\Delta t = t_{0J} - t_{0U}$.

Let $\mathrm{d}N(y,t)$ represent number of ions impacting on the target at position y between time t and $t + \mathrm{d}t$:

$$\mathrm{d}N(y,t) = \frac{J(y,t)\mathrm{d}t}{q}, \tag{4}$$

where q is the charge of a single ion. The energy of an ion impacting on the target between time $t \to t + \mathrm{d}t$ is:

$$E(t) = qU(t-\Delta t). \tag{5}$$

Let $x = 0$ on the surface, then between time $t \to t + \mathrm{d}t$ the energy deposited at (x, y) is

$$\mathrm{d}E_\mathrm{s}(x,y,t) = \frac{\mathrm{d}E(x)}{\mathrm{d}x}\mathrm{d}N(y,t). \tag{6}$$

To time t, total energy deposited at (x, y) is:

$$E_\mathrm{s}(x,y,t) = \int_0^t \frac{\mathrm{d}E(x)}{\mathrm{d}x}\frac{J(y,t)}{q}\mathrm{d}t \tag{7}$$

The deposited energy $\mathrm{d}E(x)/\mathrm{d}x$ was calculated by TRIM code.

2.2. Thermodynamic model with phase transformation

The energy on the target transferred by ions will increase with time during pulse time, it will change the temperature of target, especially in the near surface layer.

Taking the deposited energy varying with time in the target as the thermal source term, thermodynamic model has been constructed to calculate the temporal and spatial evolution profile of the ablation process in the target. The two-dimensional model is given as

$$\rho C(T)\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}(\kappa(T)\frac{\partial T}{\partial x}) + \frac{\partial}{\partial y}(\kappa(T)\frac{\partial T}{\partial y}) + E_{\rm tot}(x,y,t), \quad (8)$$

$$E_{tot}(x,y,t) = E_{\rm s}(x,y,t) - E_{\rm ph}, \quad (9)$$

$$E_{\rm ph} = L_{\rm l}\delta(T(x,y,t) - T_{\rm m}) + L_{\rm v}\delta(T(x,y,t) - T_{\rm v}), \quad (10)$$

where ρ, $C(T)$ and $\kappa(T)$ are mass density, specific heat and thermal conductivity, respectively, $E_{\rm s}(x,y,t)$ denotes the term of deposited energy, $E_{\rm ph}$ is the term which relates to latent heat, $L_{\rm l}$ and $L_{\rm v}$ denote latent heat of fusion and latent heat of evaporation, respectively. Set δ function equal to one if temperature reaches melting or boiling point, and to zero otherwise. The initial condition is $T(x,y,0) = T_0$. Adiabatic conditions have been taken as boundary conditions, longitudinal depth is 50 μm, and surface width is 50 mm. The initial target temperature T_0 is 20°C. Finite differential method has been used.

3. Numerical results and discussion

The irradiation process of Ti target by IPIB has been calculated. The temperature dependent thermophysical parameters of metal titanium used in our calculation are listed in Table 1.[8]

Table 1. Thermophysical properties of titanium.

Solid density/(kg/m^3)	4530	
Liquid density/(kg/m^3)	4110	
Melting temperature/K	1933	
Boiling temperature/K	3575	
Mole weight/(kg/kmol)	47.9	
Thermal conductivity/(W/(mK))	21.1	
Specific heat of solid phase/(J/K · mol)	298–1155K	$2.29+2.45\times10^{-3}T$
	1155–1933K	$4.74+1.89\times10^{-3}T$
Specific heat of liquid phase/(J/K · mol)	8.5	
Latent heat of fusion/(kJ/mol)	18.6	
Latent heat of evaporation/(kJ/mol)	425.9	

The width of the irradiated surface is 50 mm, the thickness of target is 50 μm, σ is 6.25 mm. σ_1 and σ_2 are 17, 19 ns, respectively. Graphite has been used as anode of MID, the beam consists of 30% H^+ and 70% C^+,[4] the pulse duration is 70 ns. The average energy is calculated based on the detected wave, it is 295 keV. The maximum range of H^+ with this energy impacting on titanium target is 1.9 μm, and for C^+, it is only 0.44 μm. H^+ affects the physical properties of deep layer, and C^+ affects the shallow layer.

Figure 1 shows the temperature field along the axis at the centre of target surface irradiated by IPIB during a pulse width of 70 ns under the energy density of 15 J/cm^2, where cases (a), (b), and (c) correspond to time 6 ns, 12 ns, and the end of a pulse respectively. We can see that at time 6 ns neither melting nor evaporating happened, but at time 12 ns, melting happened, the solid and liquid co-exist. After a pulse, temperature almost everywhere on the surface has been changed. It reaches highest value in central area. The nearer to the edge, the lower the temperature; The deeper into the target, the lower the temperature, and the narrower the temperature rising region. This is mainly due to the central area obtaining more energy than elsewhere. During the phase changing process, target will absorb latent heat, so the temperature plateau of solid and liquid, liquid and gas phase transformation appeared. The liquid and gas phase transformation plateau was larger than that of solid and liquid, because the latent heat of evaporation is much larger than the fusion one. We can also see from Fig.1 that at the end of a pulse the temperature of part target was above the boiling point, they evaporated as plasma off the surface.

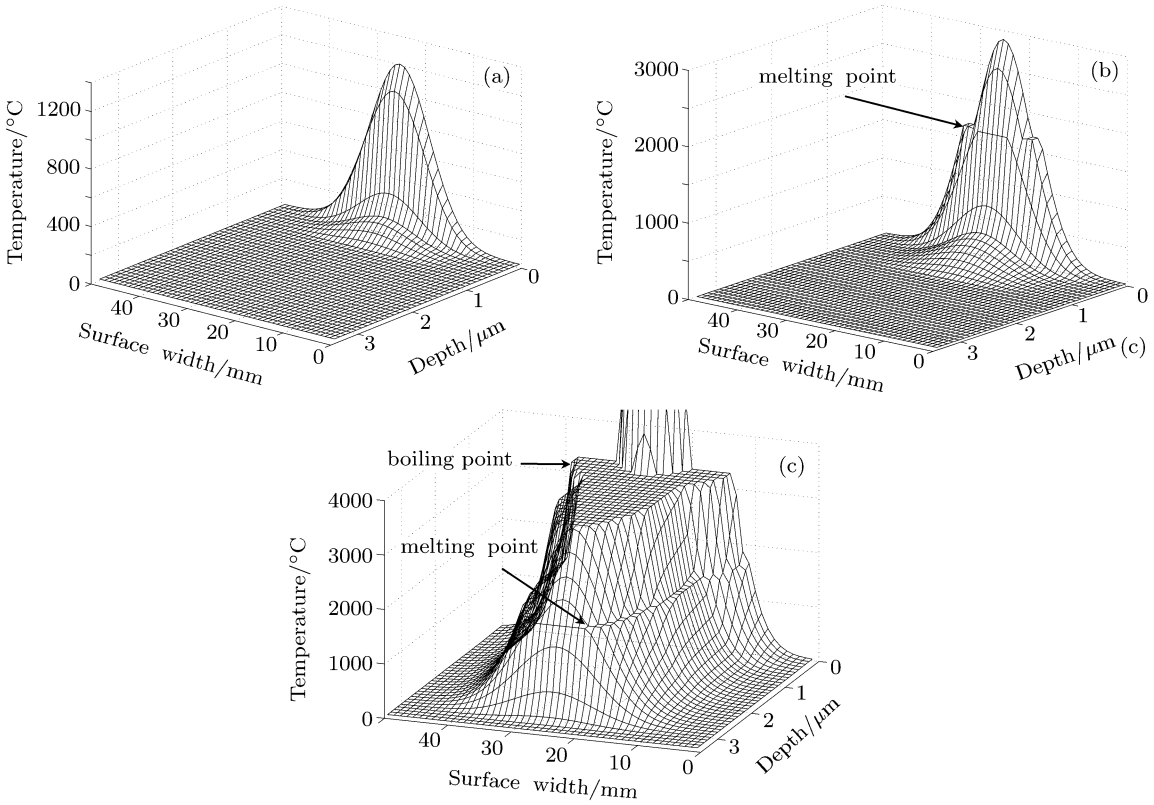


Fig.1. Temperature fields of titanium target irradiated by IPIB with energy density of 15 J/cm^2 at time (a) 6 ns, (b) 12 ns and (c) 70 ns respectively.

The evaporizing temporal evolution profile of irradiated area is shown in Fig.2 by treating the data obtained for purpose of discussing the ablation process.

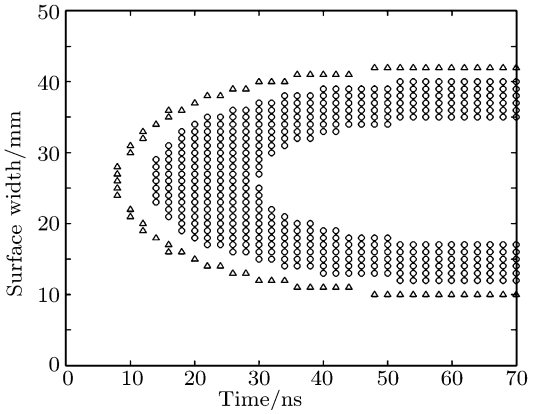


Fig.2. Temporal evolution profile of evaporizing ablation of target surface.

Sign 'Δ' and '$\bigcirc$' denote solid liquid and liquid gas, respectively, in the two phase co-existing state. Ten nano seconds after the beginning of a pulse, the centre of irradiated surface began ablation, it needed about 5 ns for the surface to absorb enough energy for the temperature to rise to the boiling point. The coexisting time of liquid and gas was much longer than that of the solid and liquid, because the latent heat of evaporation is much larger than latent heat of fusion. 30 ns after the beginning of a pulse, central surface began evaporizing, at the end of a pulse, diameter of evaporizing ablation area on the surface reached about 20 mm. The diameter due to melting ablation reached 30 mm. It took a short period of time to finish solid to liquid phase transformation in the central region; comparatively, the changing of liquid to gas phase took a longer time. Figure 3 shows the spatial evolution of evaporizing ablation of the central area.

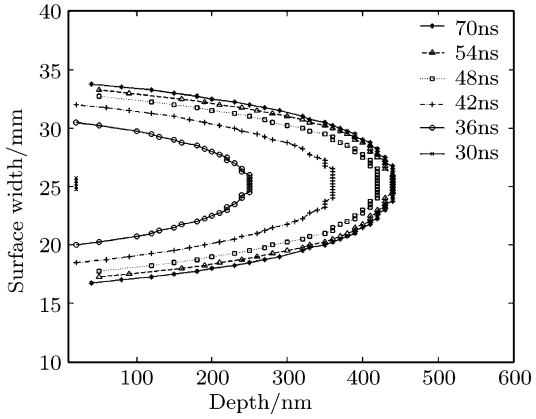


Fig.3. Temporal and spatial evolution profile of titanium target irradiated by IPIB.

It can be seen that target began ablation at time 30 ns

from the beginning of a pulse. By time 36 ns the maximum ablation depth reached 250 nm in target, the diameter of evaporizing ablation area on surface was a little bigger than 10 mm. At time 42 ns, maximum evaporizing ablation depth reached 360 nm, by the end of the pulse, the value was 450 nm, at the same time the evaporizing ablation diameter on the surface was about 20 mm. Figure 4 shows the ablation extent as function of time in the target on central impacting region and at 4 mm and 6 mm distances away from it.

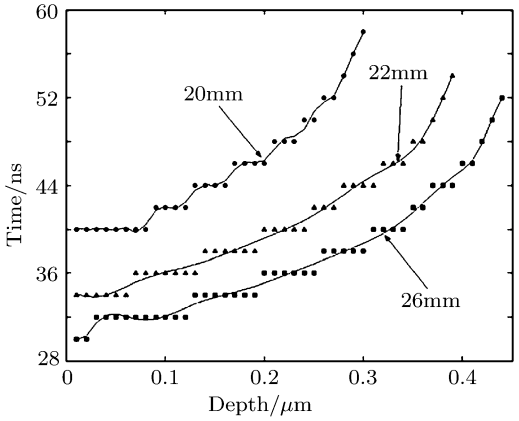


Fig.4. The ablation evolution profile of surface centre and at 4 mm and 6 mm distances away.

We know that evaporation began from 30 ns on central region of target surface, at 4 mm, 6 mm away the time were 4 ns and 10 ns later, respectively. The ablation extent was different in target at different time, as was clearly shown in the figure. In the central region, the ablation velocity as function of time is shown in Fig.5.

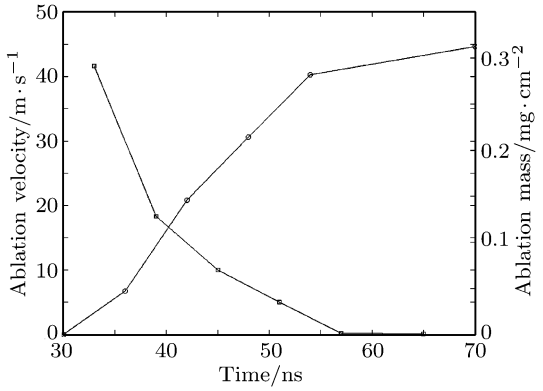


Fig.5. Ablation mass and velocity as function of time at central region.

From the time the ablation began, the ablation velocity decreased. This was the result that ions beam density reached maximum value after half of the pulsed time, and at that time the energy transferred to target per unit time reached maximum value, afterwards it decreased. The average ablation velocity calculated based on the data was about 10 m/s during a pulse. It is far less than the ejection velocity of plasma generated by IPIB irradiation target.[9]

Figure 5 also shows the ablation mass changing as function of time calculated from rotational parabolic ablation volumes by fitting the time dependent ablation curves. We got the result that 0.3 mg/cm^2 target material evaporated after a pulse while the energy density was 15 J/cm^2. At first, mass evaporation rate was larger, then it decreased slowly. The evolution of evaporizing ablation depth changed with energy density of IPIB as shown in Fig.6, which the energy densities were 10, 15 and 30 J/cm^2 respectively. When the energy density was 30 J/cm^2, at 20 ns from beginning of a pulse, evaporation emerged; and the energy density was 15 J/cm^2, at time 30 ns, and 10 J/cm^{2}at 35 ns. The maximum ablation depth increased as the energy density evolved, as shown in Fig.7.

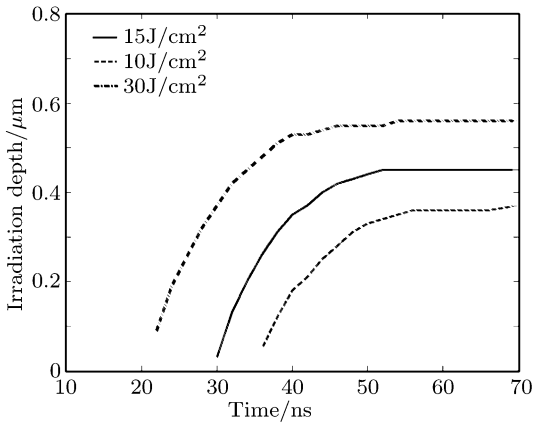


Fig.6. The ablation depth as function of time under the irradiation energy of 10, 15 and 30 J/cm^2 respectively.

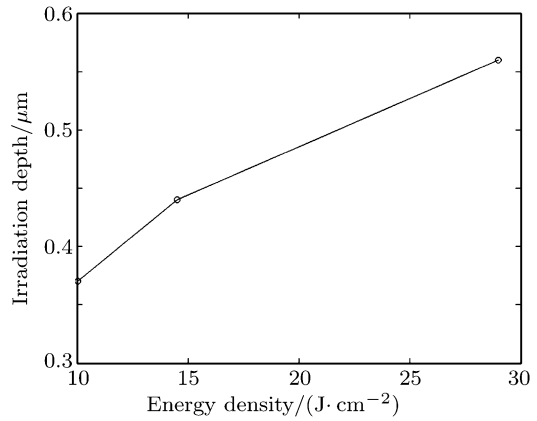


Fig.7. The ablation depth as function of energy density range from 10 to 30 J/cm^2.

The anode of MID can also be coated with polyethelene; in this case, the beam consists of

70% H^+ and 30% C^+, the evaporizing ablation profiles of IPIB impacting on titanium target with energy density of 10, 15 and 30 J/cm^2 after a pulse are shown in Fig.8. The diameters of evaporizing ablation area on surface were smaller than that for the graphite one under the same energy densities, and graphite anode MID generates more emission materials than polyethelene coating one.

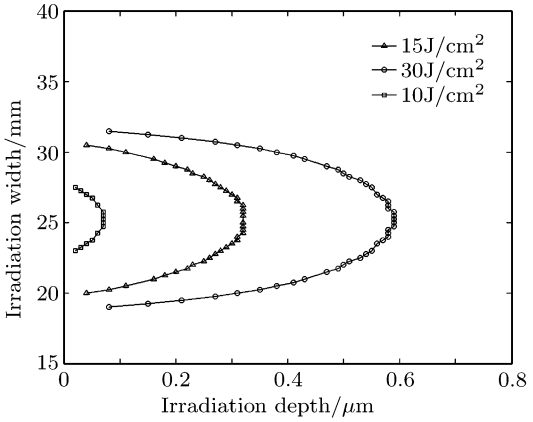


Fig.8. The evaporating ablation profile of titanium target irradiated by IPIB produced by MID with polyethelene coated anode under energy density of 10, 15 and 30 J/cm^2 respectively.

4. Conclusions

By simulating the thermodynamic evolution process of titanium target irradiated by IPIB, we know that after the target evaporation happening, the impacting ions still interact with them, and they will absorb more energy, the interaction between evaporated materials and impacting ions creates the result that the target emitted violently. The average ablation velocity is about 10 m/s, it is far less than the emission velocity of plasma.

The size of emission particles are small, they are about 0.1 nm, during the pulse, the ejection mouth on target increases with time obviously at first, but it increases slowly at last. For the ejection particles, the ablation region turns from a bowl to a well. At the beginning, plasma spreads around, but quickly a large amount of particles will eject almost in perpendicular direction to the target plane, just like oil ejects from a well. This is the phenomenon we have observed during the experiments.

Different kinds of material of MID anode have shown different effects under the same energy density, a graphite anode of MID will generate more emission materials, it is suitable for formation of film and synthesis of nano powder; the polyethelene coated anode can be better used to modify the physical properties of target.

IPIB generated by TEMP II type accelerator transfers more energy to the target surface, so melting and evaporating both begin from the surface. This is different from ETIGO equipment.[10]

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