Ablation Behavior of Titanium Irradiated by High-Intensity Pulsed Ion Beams

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A complementary study on experimental observation and theoretical modeling has been performed to investigate the ablation behavior on titanium irradiated by high-intensity pulsed ion beams (HIPIB) with energy density of 70 J/cm² up to 3 shots. The surface morphology with a typical waviness feature on the irradiated surface was observed by scanning electron microscopy (SEM). The observed surface morphology indicates a severer ablation in the center of irradiated area, leading to a fluctuation of liquid layer spreading radially to the peripheral area, due to the spatial distribution of ion beam energy density along the radial direction. The ablation process was simulated from the modeling of heat transfer in the irradiated samples using an axisymmetric model based on enthalpy formulation. The computational results are in good agreement with the experimental findings in the ablation mass with a trend of severer ablation in the center of irradiated area.

Keywords: High-intensity pulsed ion beam, ablation, modeling, surface morphology, titanium

1. Introduction

The high-intensity pulsed ion beams (HIPIB) efficiently deliver energy onto materials in the ion range (0.1-10 µm) during a short pulse width (t ≤ 1 µs) to rapidly melt and strongly vaporize (or ablate) the near-surface layer of materials (1). The plasma plume formed by HIPIB ablation expands away from the ablated surface and generates strong shock stress in the irradiated materials. These nonequilibrium processes led to a significant change in composition, microstructure and morphology on the irradiated materials, affecting the performance of materials. The understanding of ablation behavior on the surface irradiated by HIPIB is very helpful to explore the interaction mechanism of HIPIB with materials. However, experimental observation during HIPIB irradiation is limited due to the extreme high-density energy in a short pulse width, and thus the observation of surface morphology after irradiation is being considered as a useful means (2-5). Meanwhile, theoretical modeling is desired according to the numerical analysis of heat transfer on surface irradiated by HIPIB, though the process of heat transfer in substrate is mainly simulated by an one-dimensional model (6-9). Moreover, there is lack of a complementary study, despite of an effort having been made in experimental or theoretical studies, respectively.

In this article, both experimental observation and theoretical calculation are investigated for ablation behavior of pure metal Ti samples irradiated by HIPIB. The surface morphology and the ablation mass of irradiated Ti samples have been observed and measured, respectively, and also been modeled using a two-dimensional axisymmetric numerical model based on enthalpy formulation, in order to explore the interaction mechanism of HIPIB with materials.

2. Experimental Study

The HIPIB irradiation was carried out in an ETIG-7 type high-intensity pulsed ion source apparatus (9-10). The apparatus mainly comprises of two parts, i.e. pulse power system and ion diode system. A geometrically focused magnetically insulated ion diode (MIID) was used to generate HIPIB, using a polyethylene sheet coated on an aluminum anode as an ion source. When the high-voltage pulse is applied to the MIID, anode plasma is formed on the surface of polyethylene sheet based on high-voltage flashover and then ion beam accelerated simultaneously and extracted through the output slits of the cathode. The ion beam mainly composed of proton (peak energy: 1 MeV, peak current: 60 kA, and beam pulse width: ~70 ns) was used to irradiate pure Ti (99.9%) in this study. Plate samples with diameter of 50 mm and thicknesses of 5 mm were mechanically polished with silicon carbide paper and were cleaned in acetone followed by air-drying before irradiation. A schematic drawing for the sample irradiated by HIPIB with surface normal to the beam axis is shown in Fig. 1. The surface morphology on the irradiated surfaces was observed using a JSM-5600LV scanning electron microscope (SEM). The weight change of the samples before and after HIPIB irradiation was measured using an electronic microbalance with a mass resolution of 0.1 mg.
3. Numerical Modeling

According to the characteristics of HIPIB irradiation, the heat transfer in the irradiated samples was described by a two-dimensional heat conduction equation as follows:

\[
\rho C(T) \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r k \frac{\partial T}{\partial r} \right) + Q(r, z, t), \quad \text{------- (1)}
\]

where \(\rho\) is density, \(C(T)\) the specific heat, \(k\) the thermal conductivity, \(Q(r, z, t)\) the volumetric source term.

Moreover, in order to accurately describe the process of heat transfer, two reasonable assumptions are made: (i) the plasma plume, possessing the thermal properties of liquid at boiling temperature, remains on the sample surfaces during a pulse without any contribution to the heat transfer; and the plasma expands rapidly away from the surface after termination of a pulse; (ii) all the energy losses including the absorption by plasma plume, the reflection, radiation and convection at the surface are counted by introducing an effective energy absorption coefficient.

Initially, the entire computational region is at the ambient temperature \(T_a\) and the boundary condition at the exterior surface is treated as adiabatic. As a consequence of HIPIB irradiation, the sample underwent rapid melting, vaporizing and ablation from surface toward the interior region, and thus the solid/liquid and/or liquid/vapor interfaces emerged correspondingly where the temperatures at the two interfaces were taken to be \(T_m\) and \(T_v\), respectively.

To avoid the need for explicit tracking of the solid/liquid interface location, the enthalpy formulation was used to model the heat transfer in HIPIB-irradiated samples. The enthalpy form converted from the heat conduction equation was given as follows:

\[
\frac{\partial H}{\partial t} = \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r k \frac{\partial T}{\partial r} \right) + Q(r, z, t), \quad \text{------- (2)}
\]

where \(H\) is the enthalpy per unit volume. The enthalpy-temperature relation for a finite-difference cell was given as:

\[
H = \int_{z_0}^{z} \rho C(T) dT + f_l \rho L_v + f_v \rho L_s, \quad \text{------- (3)}
\]

where \(f_l\) and \(f_v\) are volume fractions of the liquid and vapor phases, respectively.

For modeling of the heat transfer in HIPIB-irradiated samples, the Eqs. (2),(3) are solved numerically using a finite difference scheme with an implicit time integration technique in the fixed grids. The full lengths in radial direction \(r\) and axial direction \(z\) of computational region are \(R\) and \(Z\), respectively, where the computational region is subdivided into numerous small control volume, as shown in Fig. 1.

4. Results and Discussion

A set of SEM images of typical surface morphology on titanium irradiated by HIPIB with 70 J/cm² up to 3 shots are given in Fig. 2. The zones I-III indicate the observed regions on the irradiated surface along the radial direction of 0–3 mm, 14–17 mm and 22–25 mm, respectively, where the ion-beam energy densities are decreased correspondingly from the center to the edge regions. The surface morphology without crater formation presents a slight wavy feature in zone I (with a maximal energy density) under 1 shot [Fig. 2(a)]. A more obvious wavy feature obtained at zone II seems to be caused by fluctuation of liquid layer spreading from central zone to the edge of the irradiated surface [Fig. 2(b)]. Although the polishing marks formed during samples preparation were not entirely removed at zone III due to a further decrease in the energy density, the molten morphology with a spread of waviness is also observed [Fig. 2(c)]. It confirms that lower ion beam intensity led to less melting and ablation of titanium. With 2 and 3 shots, a similar trend of ablation on the irradiated surface is observed at zones I-III [Fig. 2(d),(e)]. However, a smoother surface at zone I and a more acute waviness at zone II are observed with 2 shots [Fig. 2(d),(e)]. The surface at zone III were entirely melted and presented a feature with crater formation [Fig.2(f)]. Moreover, surface morphologies with typical wavy feature was respectively obtained at zone I-III on the irradiated surface with 3 shots [Fig. 2(g),(h)]. In sum, the surface morphology in the micro scale reveals that severer local ablation took place at the center of irradiated area as compared to the peripheral zones due to radial distribution of ion beam intensity, and a fluctuation of liquid layer spreads out from the center.

The modification of resistance to wear and corrosion on the materials irradiated by HIPIB is greatly affected by the ablated surface morphology, which was determined by geometrical shape of liquid/vapor interface during the subsequent resolidification at a high cooling rate typical of \(10^2-10^3\) K/s. Therefore, the ablated

<p>| Table 1. Thermophysical properties of titanium |
|-----------------|-----------------|
| Solid density/(\rho_s), kg/m³ | 4530 |
| Liquid density/(\rho_l), kg/m³ | 4110 |
| Melting temperature/(T_m), K | 1933 |
| Boiling temperature/(T_v), K | 3575 |
| Mole weight/M, kg/(kmol) | 47.9 |
| Thermal conductivity/(k), W/(m·K) | 21.1 |
| Specific heat of solid phase/(C_p), J/(K·mol) | 2.29·10³·T, 298–1155 K |
| | 4.74·1.89·10³·T, 1155–1933 K |
| Specific heat of liquid phase/(C_p), J/(K·mol) | 8.5·1933–3575 K |
| Latent heat of fusion/(L_m), kJ/mol | 18.6 |
| Latent heat of evaporation/(L_v), kJ/mol | 425.9 |</p>
<table>
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Fig. 2. The SEM images of typical surface morphology at the different zones on the titanium irradiated by HIPIB with a maximal energy density of 70 J/cm² up to 3 shots; The observed regions apart from the irradiation center with distance from 0 to 3 mm (zone I), from 14 to 17 mm (zone II) and from 22 to 25 mm (zone III); All the scale bars are of 100 μm.

Surface morphology is represented by the geometrical shape of liquid/vapor interface, which is simulated by the modeling of heat transfer in the irradiated sample. In our calculation, the temperature-dependent thermophysical parameters of titanium are used (3), as listed in Table 1. The other parameters are as follows:

\[ R_1 = 12.5 \text{ mm (spatial FWHM of ion current)} \]

\[ R_2 = 25.0 \text{ mm} \]

\[ Z = 50.0 \mu \text{m} \]

Fig. 3 shows the ablated surface morphology represented by the geometrical shape of liquid/vapor interface with the shots up to 3 at the energy density of 70 J/cm². The trend of ablation on the irradiated surfaces along the radial direction is in accordance with the experimental observation as implied by the calculated surface morphology, i.e. much severer ablation taking place in the central regions due to the spatial distribution of HIPIB energy density. From the ablated volume of calculated surface morphology, the ablation mass for titanium during HIPIB irradiation was derived for the energy density of 70 J/cm² up to 3 shots, as given in Fig. 4. The experimental data are also shown in Fig. 4, obtained from mass loss measurement for irradiated titanium samples under the same conditions. As an effective energy absorption coefficient and the existence of liquid phase were taken into account in our model,
the calculated results agree well with the experimental data, considering the effect of back-deposition of ablated droplets on the measured ablation mass. The effective energy absorption coefficient of 0.75, which was referenced from the pulsed laser irradiation onto metals, has been introduced to count the total energy loss in the calculation, in order to reasonably estimate the deposited energy by HIPIB in the sample. The occurrence of liquid phase indicated more energy dissipation into the substrate other than ablation of materials in our model as compared to the previous one proposed by Davis et al. In that case, the neglect of liquid phase would cause the numerical results overestimated on the ablation mass with respect to the experimental data, because the energy to be stored in the liquid phase (subsequently transferred to the solid phase) thus contributed to overcome the latent heat of ablation. Moreover, SEM observation on the surface morphology in a micro scale also indicates existence of liquid phase and its disturbance under the ablation. Note that disturbance of the liquid layer plays a important role in the formed surface morphology under fast resolidification after termination of the irradiation pulse, even though the process has little influence in ablation mass and macro surface morphology as indicated by the present study without modeling in such a micro scale.

5. Conclusions

HIPIB irradiation into pure Ti with the shots up to 3 at the energy density of 70 J/cm² led to ablated surfaces with a typical waviness feature. Surface morphology in a micro scale observed using SEM indicated a severer ablation in central zones of irradiated surfaces (higher ion beam intensity) as compared to that of the peripheral regions due to the distribution of ion beam energy density along radial direction.

An ablated surface morphology represented by the geometrical shape of liquid/vapor interface was obtained from the modeling of heat transfer in samples irradiated by HIPIB, in which an axisymmetric model with considering a HIPIB energy absorbed coefficient based on enthalpy formulation was used. Severer ablation in the central region of irradiated surfaces was also showed by the calculated surface morphology in a macro scale. Moreover, the good agreement in ablation mass of titanium between experiment and calculation indicated the feasibility of introducing an effective energy absorption coefficient (0.75) in our numerical model to count the total energy loss.

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