Hydrodynamic Effects on Surface Morphology Evolution of Titanium Alloy under Intense Pulsed Ion Beam Irradiation *

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The hydrodynamic effects of molten surface of titanium alloy on the morphology evolution by intense pulsed ion beam (IPIB) irradiation are studied. It is experimentally revealed that under irradiation of IPIB pulses, the surface morphology of titanium alloy in a spatial scale of μm exhibits an obvious smoothening trend. The mechanism of this phenomenon is explained by the mass transfer caused by the surface tension of molten metal. Hydrodynamic simulation with a combination of the finite element method and the level set method reveals that the change in curvature on the molten surface leads to uneven distribution of surface tension. Mass transfer is caused by the relief of surface tension, and meanwhile a flattening trend in the surface morphology evolution is achieved.

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Intense pulsed ion beams (IPIBs) have been extensively studied in material processing in the past two decades[1−3] and have seen applications in surface cleaning, surface hardening, crack healing, etc.[1−3] IPIB irradiation may make a high energy flux (approximately 10^8 W/cm^2) deposited in the near surface region (within a depth of several μm) of the target in a temporal scale of tens of ns to one ms,[4,5] resulting in ultrafast heating and cooling on the surface with shocked stress ignited and propagated in the target.[6,7] Material treatment can be achieved as a result of these processes.

As have been widely observed in previous studies, the surface morphology of a solid target may change significantly in spatial scale of μm. Micro craters may be formed on the surface of the target during IPIB irradiation,[8] and can be flattened during the irradiation of succeeding pulses.[8−10] As the existence of craters and the revolution in surface morphology may impose influence or even deterioration on the service properties of processed materials, much attention has been paid to the formation and evolution mechanism of surface morphology. Studies have been carried out on various materials such as steel,[11] copper,[12] silicon,[12,13] titanium[8−10] and refractory alloys.[14,15] It has been revealed that several factors such as the non-uniformity and impurities of the beam, the crystalline structure and the impurities of the target may contribute to the formation of craters, and when the beam flux succeeds a certain value, craters are inevitable.[8−15] On this account, the mechanism in the evolution of surface morphology is of crucial significance. Some models, such as temperature field and thermal stress analysis have been carried out to understand the mechanism of surface evolution under IPIB irradiation,[7,16,17] and the main limitations in these models are that they were based on theories for solid states and the liquid state formed during IPIB irradiation was not fully taken into consideration, and the mechanism of mass transportation which leads to the changing of surface morphology was not well explained.

In this Letter, the effects of surface tension of the liquid metal formed by IPIB are considered to express the mechanism of mass transportation by IPIB irradiation. Titanium alloy is chosen as an example for verification by experimental and theoretical means both. The samples are TC4 alloy taken from the blades of a turbine engine after service with compositions of 6 wt.% Al, 4 wt.% V, 0.3 wt.% Fe, 0.2 wt.% O, 0.1 wt.% C, 0.05 wt.% N, 0.015 wt.% H and Ti balance. The samples were cleaned with ethyl alcohol without polishing. The irradiation was carried out on a pulsed ion beam accelerator TIA-450.[18,19] The IPIB was generated by a passive magnetically insulated diode (MID) with a graphite anode and accelerating voltage up to 250 kV, pulse width of 80 ns (FWHM). The beam was approximately composed of carbon ions (70%) and protons (30%) and the irradiation was carried out with various beam currents and

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shot numbers. The time interval between pulses is 5 s and the surface of the sample has already cooled down to room temperature before the succeeding pulse arrives.[20] The surface morphology of the samples was examined with a scanning electron microscope (SEM).

As revealed in previous studies, under irradiation of a single IPIB pulse, in a depth of several µs, the surface region of titanium alloy can be in a molten state in a temporal scale of hundreds of ns.[21] To explain the mass transfer on the surface region, the molten alloy and the surrounding gas are described by the Navier–Stokes (N-S) equations for incompressible laminar flow,

$$\rho\frac{\partial \boldsymbol{u}}{\partial t}-\nabla\cdot\mu(\nabla\boldsymbol{u}+(\nabla\boldsymbol{u})^T)+\rho(\boldsymbol{u}\cdot\nabla)\boldsymbol{u}+\nabla p=\boldsymbol{F}, \quad (1)$$

$$\nabla\cdot\boldsymbol{u}=0, \quad (2)$$

where ρ is the density of fluid, $\boldsymbol{u}$ is the flow velocity vector, μ is the dynamic viscosity, p is the pressure, and $\boldsymbol{F}$ is the source term, i.e., the surface tension at the liquid-gas interface.

To describe the liquid-gas interface, the level-set (LS) method[22] was used. To track the liquid-gas interface, a scalar function φ is defined (the LS function) and its value is negative for liquid, zero at the interface and positive for gas. The advection of φ follows

$$\frac{\partial\varphi}{\partial t}+\boldsymbol{u}\cdot\nabla\varphi=0. \quad (3)$$

The change of physical properties across the interface is defined as

$$\rho=\rho_{\rm g}+H(\varphi)(\rho_{\rm l}-\rho_{\rm g}), \quad (4)$$

$$\mu=\mu_{\rm g}+H(\varphi)(\mu_{\rm l}-\mu_{\rm g}), \quad (5)$$

where $H(\varphi)$ is the smoothed Heaviside function and the value is 1 for liquid, zero for gas, and n is a parameter for the transition width

$$H(\varphi)=(1+\tanh(-\varphi/n))/2. \quad (6)$$

Surface tension is induced as the driving force in the N-S equations and takes the following form

$$\boldsymbol{F}_{\rm st}=\gamma\kappa\delta(\varphi)\boldsymbol{n}, \quad (7)$$

where $\boldsymbol{F}_{\rm st}$ is a body force vector field, γ is the surface tension, κ is the interface curvature, $\delta(\varphi)$ is the Dirac function, and $\boldsymbol{n}$ is the unit normal vector to the interface. Here $\delta(\varphi)$ takes the form

$$\delta(\varphi)=\frac{n_2}{\sqrt{\pi}}e^{-n_2^2\cdot\varphi^2}. \quad (8)$$

The normal vector to the surface and the curvature are given in terms of φ

$$\boldsymbol{n}=\frac{\nabla\varphi}{|\nabla\varphi|}, \quad (9)$$

$$\kappa=\nabla\cdot\frac{\nabla\varphi}{|\nabla\varphi|}. \quad (10)$$

In the simulation, the evolution of a protuberance and depression was calculated to show the mass transportation caused by surface tension. The density of air is $1.293\times10^{-7}\,{\rm g/cm^3}$ (air pressure of 0.01 Pa in the vacuum chamber), the density of molten TC4 is $4.5\,{\rm g/cm^3}$, the dynamic viscosity of molten liquid is $2\times10^{-3}\,{\rm Pa{\cdot}s}$, and the surface tension on the interface is 1.4 N/m. The equation is solved with the finite element method (FEM) software Comsol Multiphysics.

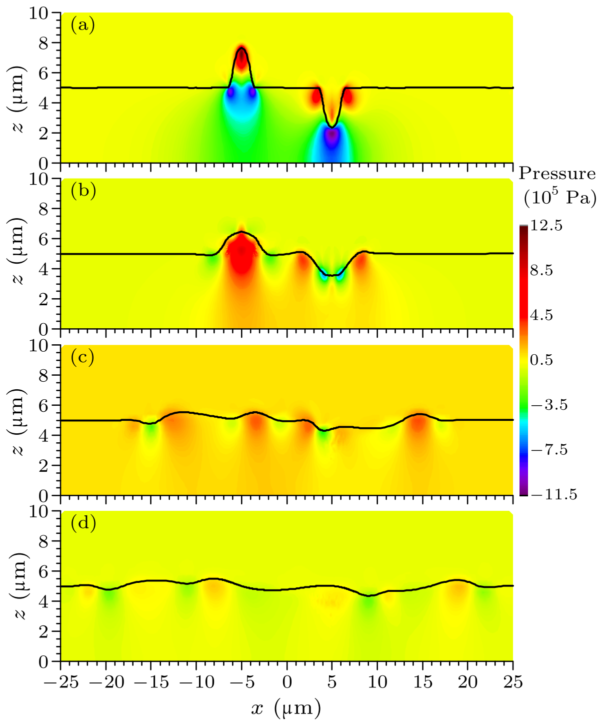

Fig. 1. Interface (the grey line) evolution and pressure distribution (Pa) of liquid protuberance and depression at (a) 0 ns, (b) 100 ns, (c) 500 ns, and (d) 800 ns.

As demonstrated by the results of interface evolution simulation (Fig. 1), mass transportation can be induced by surface tension of the molten surface. At the positions on the surface where relatively larger curvature exists (e.g., at the tips of protuberance and the bottom of depression), stronger surface tension comes correspondingly. The mass is pulled away to a nearby region and thus changes in surface morphology are brought about simultaneously. As a result of mass transportation, surface curvature decrease and surface tension release are achieved, meanwhile the surface energy of the whole system becomes smaller, making the surface system reach a steadier state. Although the real surface morphology is more complicated, the above analysis can describe the general trend in surface morphology evolution. It can also be deduced that surface morphology with smaller dimensions, such as edges, may generate much larger surface tension density at the molten state and is thus easier to be smoothened under IPIB irradiation. When the surface becomes smoother and tension is released, the mass transportation tends to be slower and this can be observed. When the surface becomes smoother after irradiation of initial pulses, the surface morphology may not undergo obvious change under succeeding pulses. The movement of the surface caused by fluctuations at different positions may interfere with each other and this makes the surface forming a smoother waving morphology under a series of pulses irradiation.

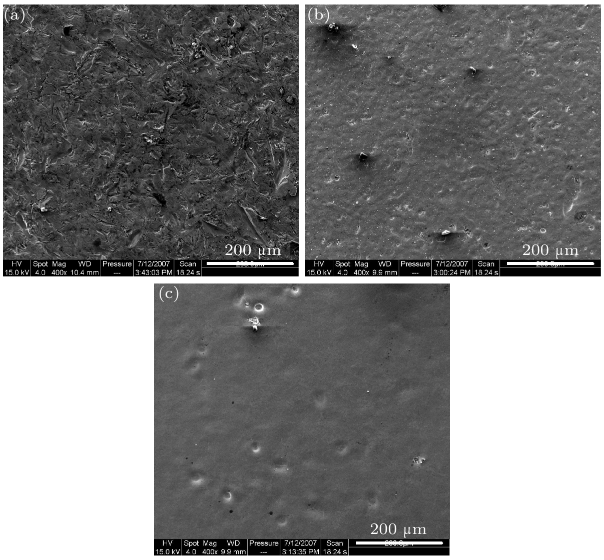

Fig. 2. Surface morphology by IPIB irradiation ($150\,A/cm^2$): (a) original sample, (b) 1 pulse, and (c) 5 pulses.

Figure 2 demonstrates the surface morphology evolution after irradiation of IPIB series with current density of $150\,A/cm^2$. On the original sample, the surface is quite rough as a result of the corrosion by high-temperature gas. After one pulse, the melting on the surface is obvious and the sharp edges and ridged bumps on the original samples are smoothened with cracks and pits shrink to pores with a round shape. After 5 pulses, the surface is further smoothened. Edges of the pits become smoother and pits with smaller size vanish. Only round pits with larger size remain, this can be explained as the surface tension of larger pits are weaker due to their smaller curvature, thus the traction of tension is weaker, making the surface morphology evolution slower at these positions.

Under IPIB with higher energy density ($250\,A/cm^2$), after a single pulse, the surface exhibits larger roughness than irradiated with lower energy density. This can be attributed to the strong disturbance by the evaporated gas plume on the molten metal. After five pulses, the surface is obviously melted with the surface smoothened and a waving morphology formed and there exist deep pores which are formed by the local eruption of ablated gas. After ten pulses, most of the pits vanish and the surface exhibits a waving morphology with smaller roughness. This reveals the two stages of surface morphology evolution under IPIB irradiation with large energy density. The grain boundaries in the original samples may cause local uneven distribution of thermal resistivity and this may lead to local eruption under IPIB irradiation. As a result, under the irradiation of preliminary pulses, local eruption may lead to the formation of micro pits or craters and if the density of local eruption is high, the surface may be roughened with a boiling-like morphology in this stage. As described by previous studies, after IPIB irradiation, the surface region of the target may have a glass state or grain refinement formed.[23,24] The size of erupted region may be decreased, and even when local evaporation occurs, the formed pits or craters may be smoothened very soon due to the high surface tension density for the large surface curvature. In this stage, the effects of local eruption are weaker and the surface tension of the molten surface dominates the change in surface morphology. The surface may finally be in a waving feature as a result of the competition between the surface tension of molten metal and the disturbance imposed by evaporated gas.

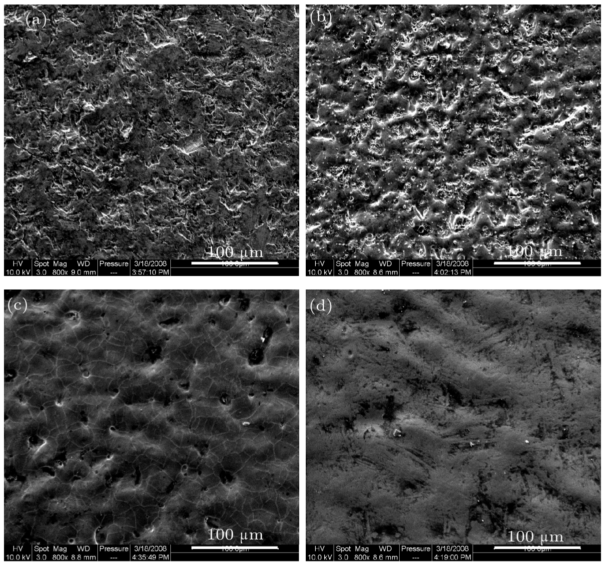

Fig. 3. Surface morphology by IPIB irradiation ($250\,A/cm^2$): (a) original sample, (b) 1 pulse, (c) 5 pulses, and (d) 10 pulses.

It can also be predicted that for metals and alloys with a relatively high evaporating point, strong surface tension and high viscosity, such as copper, steel and nickel based alloys, the surface evolution is largely dominated by the hydro effects of the molten metal and may exhibit a similar trend under IPIB irradiation like TC4 in this work. However, if the energy density of IPIB is high enough to produce a strong gas plume on the surface, the surface tension of the molten metal may fail to confine the surface and surface with large roughness or even a splashing pattern may appear on the surface. For surface treatment in which a smoother surface is usually preferred, this causes a dilemma. Based on the effects of the surface tension, IPIB should be strong enough to keep the surface region under the molten state as long as possible. On the other hand the thermal effects of IPIB cannot be too strong to avoid the violent disturbance by surface ablation. This implies that during the surface treatment with IPIB, the current density should be adjusted as the states of the irradiated target changes.

In conclusion, the hydro effects of molten TC4 alloy under IPIB irradiation on the surface evolution have been studied. The trend in surface morphology evolution in a spatial scale of μm can be explained by the flowing of molten metal formed by the thermal effects of IPIB. Flow field simulation with the LS method reveals that the release of surface tension of the molten surface is the cause of mass transportation and thus is the driving force of the surface morphology evolution in the situation that no obvious ablation or evaporation is induced by IPIB irradiation. Experimental results show that the surface of TC4 can be smoothened under IPIB irradiation, the surface morphology evolution may be influenced by surface tension and the material properties both, and this makes the trend in surface morphology different for IPIB irradiation with low and high energy densities. In the case of strong ablation plume, the hydro effects of the gas phase should not be neglected, and surface morphology is then determined by the hydro processes by both liquid and gas states.

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