Simulation of Crater’s Formation Mechanism on Target GH3536 Surface Irradiated by High Intensity Pulsed Ion Beams

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Abstract: Body Heat Flux Mode characterised by Element Birth and Death method is built to simulate the thermal effect of target GH3536 irradiated by HIPIB with different energy parameters using the FEM (Finite Element Method) software. The thermal data of the metal surface irradiated by HIPIB is obtained. The simulated result has proved that the explosive eruption of the inner surface is the dominant mechanism of the formation of dense craters with large sizes when the ion current energy input is high.

High-intensity pulsed ion beams (HIPIB) irradiation into engineering materials can realize the deposition of high-energy density rapidly on a surface layer of target materials if the pulse duration is less than 1µs and typical ion range is shorter than 10µm, and this can cause a high heating and cooling rate of $10^7$-10$^9$ k/s together with fusion, vaporization and ablation. Meantime, the high changing rate of surface temperature in time and in space also produces thermal stresses and shock waves that induce changes of the surface in phase structure, microstructure, surface hardness, abrasive resistance and corrosion resistance, etc [1~3]. However, irradiated surface may exist particle impacting or craters which are caused by ablation, and this can lead to the imbalance of geometry, structures and chemical compositions of micro surface, and then cause bad effects on the abrasive resistance and corrosion resistance of the surface. At present, theory on particle impacting is used both at home and abroad in explaining craters’ generation, however, studies on formation mechanism of craters are still insufficient [4,5], thus, it is necessary to study the formation mechanism and controlling factors of irradiated surface craters. Body Heat Flux Mode using Finite Element Method with ABAQUS software is built in this paper to simulate the thermal effect of target materials. Heating and cooling thermal effects of target materials under different process conditions are analysed to provide theoretical foundations for the formation mechanism of craters in the material surface irradiated by HIPIB.

Build calculation model

Based on Fourier transient thermal transfer equation, hypotheses of thermal transfer equation for metal surface irradiated by HIPIB are built[5]. Suppose the length (x direction), width (y direction), height (z direction) of the model are l, b, h, respectively, and the ion irradiation direction is along z direction. During thermal transfer process, temperature t is a function of time τ: t(x, y, z, τ). Suppose the ion beam energy is E, melting point of the material is $T_m$, latent heat of fusion is $H_f$, boiling point is $T_v$, latent heat of vaporization is $H_y$, and we introduce a conditional function $f(x)$, then transient thermal transfer equation of HIPIB is built[5].

Set relevant parameters as follows: model size 0.1mm×0.1mm×0.1mm, element number 20×20×40, 20×20 elements uniformly distributed on irradiated surface, 40 elements nonuniformly
distributed along irradiated direction ($z$ direction), deviator ratio 1.15, element thickness of the first layer 0.0526µm, as shown in Fig. 1. Suppose we choose an inside element, set the four surfaces adjacent to the loading surface are under adiabatic condition, the initial temperature of the model is 25°C. The emissivity $\varepsilon$ is a linear increasing curve (0.1–0.9) within burst length, while it is a linear decreasing curve (0.9–0.1) after burst length. Since target material is irradiated in vacuum, no heat transfer coefficient is set in the surface layer.

Since ionic clusters may emerge during the motor process of ions, the energy distribution of target material irradiated by ions is random. Thus, the energy distribution for load should also show random nature. Elements in deep color in Fig. 2 are randomly loaded elements.

**Parameters in simulation**

The experimental foundation of simulation is TLA-450 type ion accelerator of China-Russia joint high energy beams laboratory of Shenyang Ligong University, and the composition of ion beams are C$^+$ and H$^+$. Its typical working parameters are shown in Table 1.

| Ion component       | Pulse voltage/keV | Current intensity/(A/cm$^2$) | Pulse width/ns |
|---------------------|-------------------|-----------------------------|----------------|
| 70%C$^+$+30%H$^+$   | 100-450           | 80-350                      | 50             |
GH3536 high temperature alloy (vacuum response add electroslag) is chosen as experimental materials. Specimens were cut into 20mm×10mm×2.5mm plates, and the relevant parameters are chosen [5]. Irradiated experiment is carried out at the beam parameters of accelerating potential 200KV, pulse duration 50ns, current density 100~120A/cm² and 230~250A/cm².

Results and discussion

Body Heat Flux Mode is built to simulate target material at the beam parameters of pulse duration 50ns, pulse voltage 200keV, and current density 80, 150, 200, 250, 300 A/cm², respectively.

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Fig. 5 shows the temperature distribution curve on the surface along the irradiated direction at the end of one pulse. Apparently, the vaporization layer gets thicker as ion current density increases. The temperature gradient along the irradiated direction is slightly affected by ion current density if the energy of HIPIB is capable of making vaporization happen on the surface, otherwise, it increases with the ion current density. Heating curves of nodes in the 1, 3, 5, 7, 8, 9 layer are measured in the ion beams irradiation at the energy parameter of $400\text{keV}\times350\text{A/cm}^2$, as shown in Fig. 6. The simulation results showed that the temperatures of nodes in the former seven layers rise rapidly and all reach the melting point at about 10ns, and reach the boiling point between 25ns and 30ns. Thus, there is a temperature region of more than ten nanoseconds, as a result, quite a few of atoms sublimated into metallic vapor directly without melting.

Therefore, the simulation results show that, when the energy input is $200\text{keV}\times250\text{A/cm}^2$, the energy of ion current can make the surface of target materials reach or pass the boiling point, thus cause evaporation and ablation in a short period of time and form craters. When the energy parameters achieve $300\text{keV}\times350\text{A/cm}^2$, it changes into multilayer vaporization, and the explosive eruption of gaseous atoms is the main formation mechanism of craters. Therefore, besides the explanation of “raindrop” and “vaporization and ablation” for the formation of craters under a low energy, the explosive eruption of the inner surface is the dominant mechanism of the formation of dense craters with large sizes when the ion current energy input is high.

**Conclusions**

1. In the irradiation process by HIPIB, increasing the ion current density can markedly improve the heating rate of target materials surface layer, but ion current density have little effect on cooling rate.
2. When target materials is irradiated by HIPIB of high power density (pulses voltage is higher than $300\text{keV}$, ion current density is higher than $350\text{A/cm}^2$), the explosive eruption of gaseous atoms is the main formation mechanism of craters.
3. When ion current energy is capable of making the temperature of target materials surface reach or get close to the boiling point, the local vaporization caused by the heterogeneity of ion current can form local craters in the surfaces.

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