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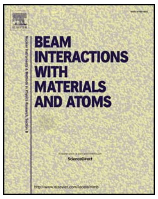

Anisotropy effect of crater formation on single crystal silicon surface under intense pulsed ion beam irradiation

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ABSTRACT

Due to the induced extremely fast thermal and dynamic process, Intense Pulsed Ion Beam (IPIB) is widely applied in material processing, which can bring enhanced material performance and surface craters as well. To investigate the craters' formation mechanism, a specific model was built with Finite Element Methods (FEM) to simulate the thermal field on irradiated single crystal silicon. The direct evidence for the existence of the simulated 6-fold rotational symmetric thermal distribution was provided by electron microscope images obtained on single crystal silicon. The correlation of the experiment and simulation is of great importance to understand the interaction between IPIB and materials.

1. Introduction

The treatment of material surfaces and thin layers with intense pulsed ion beams (IPIB) has been a novel technique developed during the past several decades [1–3]. IPIB are energetic and charged ion beams with high intensity (1–10^4 A/cm^2), short pulse duration (≤ 1 μs) and high instantaneous power density (10^6–10^{10} W/cm^2). Due to the fast energy deposition on material surface, it results in fast temperature rise (up to 10^{10} K/s [4]), melt, vaporization, sublimation, ablation and shock wave pressure effects by the interaction between beams and target materials. Therefore, IPIB have been proved promising in material surface enhancement [5], polishing [6], mixture [7], film deposition [8] and nanopowder synthesis [9].

However, after IPIB irradiation there are always some microstructures formed on material surface, such as craters [10,11], cracks [12] and ripples [13]. In service process these microstructures where stress concentrates and erosion firstly occurs, may induce negative effects on material's performance and lifetime as well. To solve this problem, great efforts have been made to study the formation mechanism of these microstructures, and some fruitful achievements have been achieved [13–15]. As a frozen state of the extremely violent surface flow on the melt silicon caused by IPIB bombardment, craters were paid much attention. In general, the complexity of the crater formation mechanism involves thermal effect, shock effect and many other elements, whereas the materials' surface property plays a key role as well. However, for the purpose of potential industrial application, metal or alloy materials were frequently chosen as the research prototype. These materials contain a certain amount of impurities or grain boundaries, and the latter have turned out a promotion for crater formation [16]. On the other hand, the isotropy of these material properties limits the diversity of the IPIB-induced craters. As a result, the obtained craters always seem to be round and the puzzles from the materials cannot be bypassed in the mechanism analysis. Therefore, single crystal silicon has been irradiated with IPIB [17,18], intense pulsed electron beam [19,20] or laser beam[21], and some craters with novel shapes were observed. However, the influence from the native oxide layer was paid much attention in these works, which to some extent covered up the function of anisotropic characteristic of the material. As a result, the understanding of IPIB and target interaction mechanism is still elusive and far from well understood.

The aim of the current work is to investigate the dependence of the eventual crater shapes on material's anisotropic property and how it can affect the outcome of the super-fast ion beam irradiation scenario. For this purpose, a 3D Finite Element Method (FEM) model was built to simulate the thermal field induced on the IPIB-irradiated single crystal silicon, and corresponding experiments were conducted for verification.

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2. Simulation and experiment

2.1. Simulation method

To investigate the influence of the material's anisotropy on crater formation process, different radial directions from the crater centre, e.g., main axis direction (MAD) with the maximum thermal conductivity and non-main axis direction (NMAD) with the minimum thermal conductivity should be discriminated. Qualitatively speaking, due to the following two reasons, the crater shape after solidification will significantly be affected by the thermal field on the IPIB-irradiated single crystal silicon. On one hand, considering in terms of time sequence, the melting process of silicon should start earlier at MAD, and inevitably the flow there should start to move earlier and stop farther as well. On the other hand, in terms of the melt area, the faster heat conduction at MAD will result in larger range of the melt pond and thus farther crater boundary.

Basing on the above statement, the thermal field simulation should be conducted on both temporal and spatial dimensions. To start the simulation, two principals need to be made clear. Firstly, several simulation methods to study the IPIB-induced thermal field have been applied in previous works, such as Ref. [4,22]. They have been proved convincing to explain related experiments. Therefore, new development will not be focused on the modification of the heat conduction model describing IPIB-target interaction, except for some specific parameters of the target parameters. Secondly, as the driven force of crater's formation remains unsure, no matter central eruption or partial centralized ion beam deposition, it is dialectic and sufficient to consider the thermal field alone, rather than together with the flow field.

Thus, basing on our previous work [22], a 3D FEM model for thermal field evolution simulation was specifically developed for IPIB with maximum cross-sectional energy density of 1.5 J/cm^2 deposited in single crystal silicon (1 1 1). The 3D geometry of the studied object was a solid cylinder with 20 μm height and 30 μm diameter. The Fourier heat conduction equation was adopted as the governing equation:

$$\rho C_V \frac{\partial T}{\partial t} = \lambda \nabla^2 T + P \tag{1}$$

wherein ρ, C_V, and λ are the density, specific heat and thermal conductivity of the target, respectively, and all of them are temperature dependent. The latent heat of phase change was taken into consideration with equivalent specific heat within a 3 K temperature range. According to Refs. [23–25], the thermal conductivity anisotropy of single crystal silicon (1 1 1) target was defined with:

$$\lambda(\theta,\mathrm{T}) = \lambda(T)[1 + 0.2\cos(6\theta)] \tag{2}$$

here θ denotes the direction angle. To simplify the simulation, ratio of the thermal conductivity at MAD and NMAD was assumed temperature independent here, which may slightly affect the thermal field distribution values but can hardly change the tendency of the temperature evolution. The external heat source term P(x,y,z,t) induced by IPIB was defined as Ref. [22]:

$$P(x, y, z, t) = d(z)\cdot g(t)\cdot U(x, y) \tag{3}$$

Here P(x,y,z,t) is the power density distribution on the target induced by IPIB; U(x,y) is the cross-sectional energy distribution function, which can be set as $\exp(-(x^2 + y^2)/R^2)$ for simplification, wherein R stands for the parameter used to adjust the full width at half maximum of the Gaussian function to 20 μm, the size of a typical crater. Worth to mention, the origin of this 20 μm hot source could be attributed to the inhomogeneous anode surface emission, plasma instability during beam transportation, target surface nonuniformity, etc., where the exact mechanisms need further work to understand; d(z) is the depth-normalized energy loss distribution over the depth z, which can be readily obtained with Monte Carlo software SRIM [26]; g(t) is the time-normalized power density evolution function, which can be estimated with the IPIB current density measured by Faraday cup.

For initial condition, we took:

$$T(x,y,z,0) = T_0 \tag{4}$$

here T_0 is room temperature 298 K.

According to the evaluation results in Ref. [22], thermal radiation can be out of consideration in this process. In addition, as the air pressure in the vacuum chamber is quite low ($\sim 10^{-2}$ Pa), convective thermal transfer is not taken into consideration, neither. Therefore, the thermal conduction plays the most important part in the temperature evolution process and thermal insulation was taken as the boundary condition for this simulation.

As the estimated maximum temperature was far below the boiling point, sublimation and boiling effects were out of consideration in this model. The above equations were solved by Comsol Multiphysics, a finite element method (FEM) tool.

2.2. Experimental observation

The experimental research for single crystal silicon was conducted on IPIB accelerator TIA-450 in Shenyang, China. As shown in Fig. 1, the apparatus is mainly comprised of a Marx micro-second pulse generator, a Blumlein pulse forming line and a magnetically insulated diode (MID). To generate IPIB, the generator produces a high voltage microsecond pulse and then the pulse is compressed into a hundred of ns by the pulse forming line and applied on the MID. The MID anode is made of graphite, which produces explosive emission plasma under pulsed negative high voltage in Fig. 2. The ions in the plasma are accelerated and focused to form the IPIB by the second positive high voltage pulse. The general beam composition is ions of carbon (70%) and protons (30%), while the ion energy, pulse duration, current density and energy density are 250 keV, 200 ns, 180 A/cm^2, 1.5 J/cm^2, respectively.

The voltage and current density were measured by a voltage divider and a collimated Faraday cup with a biased magnetic field to cut off the electrons, respectively. Signals from detectors were recorded with a Tektronix TDS 2024 oscilloscope. The typical waveforms of diode working voltage and IPIB current density on the focusing point are shown in Fig. 2.

The single crystal silicon (1 1 1) samples with a dimension of 10 × 10 × 1 mm^3 were well polished and ultrasonically cleaned with acetone before irradiation. As shown in many previous works [5], multiple shots of IPIB can make the sample surface amorphous or bring new crystal orientations in the solidification and recrystallization. Therefore, the samples were irradiated with single shot of IPIB at various energy densities within 1–2 J/cm^2, which was measured with infrared imaging diagnostic method [27,28]. Finally the samples were examined with a Hitachi S-4800 scanning electron microscope (SEM) and optical microscope.

3. Results and discussion

As revealed in previous works [12,13], the crater shape of metal or alloy always tends to be round, even in single crystal metal [16]. To explain that, here the thermal conduction mechanism needs to be reviewed. In solids, thermal conduction is mediated by the combination of vibrations and collisions of molecules, propagation and collisions of phonons, and diffusion and collisions of free electrons. For metals or alloys, diffusion of uniformly distributed free electron takes the most part of the heat transfer at room temperature, which will probably limit the anisotropy effect. However, in semiconductors like silicon, the heat flux is carried almost entirely by phonon vibrations, and in different crystal directions, the periodical arrangement of atoms makes the atom distribution inhomogeneous. Therefore, there should be certain scientific basis and possibility that anisotropy effect plays a role in the crater information process. The simulation in this work evaluated the possibility that craters with 6-fold rotational symmetry are formed on single