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Channeling Contrast Simulation of Secondary Electron Images in Scanning Ion Microscopes

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Recent advances in focused ion beams (FIBs) allow us to fabricate nanostructures while simultaneously imaging them at high resolutions. In addition to topographic and material contrast, a large critical angle of several to ten degrees for ion channeling at tens-of-kiloelectron volt energy in a FIB can lead to a distinct crystalline-orientation contrast in polycrystalline material imaging. Previously, I reported a trajectory simulation of 30-keV He, Ne, and Ga ions in a body-centered cubic (bcc) crystalline tungsten (W) sample, a middle portion of which inclined at different angles against neighboring sides oriented toward the channeling direction [1]. The calculated backscattered ion and secondary electron (SE) yields suggested some deviations from the expected contrast variation predicted by a transparency model. Herein, I present further calculations of the SE profiles for platinum (Pt) with a face-centered cubic (fcc) structure irradiated with a Ne ion beam. The focus of this study was the contrast variation with tilt-angle of the beam and the crystal structure of the sample.

A rectangular cell with lattice constant a, base dimensions $10a\times2a$ and varying height (h=$10a$ and 15 nm) was taken as the simulation cell. The left and right sides of the top cell surface corresponded to a channeling direction [001] for an ion at normal incidence on the surface. The middle surface was inclined by angles of 30° and 45°, which respectively offered an unchanneled ion direction and another channeling direction [011]. The trajectory of an ion incident on the surface was then simulated by solving Newton's equations of motion and applying periodic boundary conditions to the sides of the cell, details of which are presented in a previous report [1]. By applying a semi-empirical model of SE emission [2] [λ_d=0.75 nm and ε=78 eV (W) and 60 eV (Pt)], the SE yield at each point across the left, middle, and right surfaces was calculated at intervals of a to simulate the line profile derived from the SE images. The SE profile enabled comparison of this trajectory simulation with a simple transparency model [3] based on an assumption that no channeled ions contribute to SE emission.

The transparency model provides simple evaluation of the image contrast between crystals of different orientations according to the probability of each ion colliding with any sphere (radius r_a) centered by lattice atoms along the line-of-sight channel. Line profiles of the probability is shown in Figs. 1(a)–1(c) at 30° inclination of the middle surface for an ion beam tilted by (a) 0°, (b) 30°, and (c) 45° against the surface normal. A Gaussian beam shape with standard deviation of 0.1 nm was assumed, which enabled the distinguishing of each atom on the left and right surfaces while a channeling condition of 0° tilt was kept. Upon beam tilting, most positions on the left and right surfaces were unchanneled and another channeling direction emerged on the middle surface. The calculated SE profiles in Fig. 1(d) correlate such changes to a general increase in the SE yield with increasing tilt angle, but the changes produced a gentle slope whose range was much wider than the beam size (i.e., 0.1 nm). The slope was induced by successive jumps of penetrating ions from one line to another along the atomic rows, resulting in the trajectories to be laterally distributed. Different crystal structures produced different contrast changes in the SE profile, as shown in Figs. 2(b) and 2(d) for simulation cells of bcc-structured W and fcc-structured Pt, respectively. In addition to unchanneled and violently-scattered profiles at the 30° inclination of the middle surface, the increase and decrease in the channeled profiles for bcc and fcc structures, respectively, were obtained at the 45° inclination. The profiles were also produced by the transparency model [Figs. 2(a) and 2(c)]. Since a square-shaped beam with an area of $a \times a$ was assumed in the figures, some changes with atomic rows on the middle surface was reproduced as previously found at the 45° inclination for W [1].

In summary, a trajectory simulation of a 30-keV Ne ion beam was performed to calculate the SE line profile of a crystalline material with two different orientations for ion channeling. The simulation reproduced contrast changes by tilting the ion beam against the surface. Nevertheless, the profile showed a much slower change than that of a transparency model owing to additional spread of the beam in the material. The profile also exhibited the contrast changes that depended on the bcc or fcc crystal structure.

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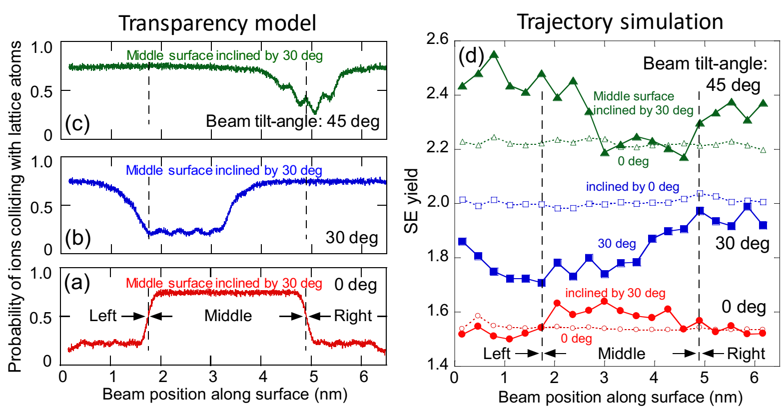

Figure 1. (a–c) Transparency model probability (r_a=0.06 nm) and (d) SE line profile on crystalline W (h=10a) irradiated with a 30-keV Ne$^+$ beam at different beam tilt-angles against the surface normal.

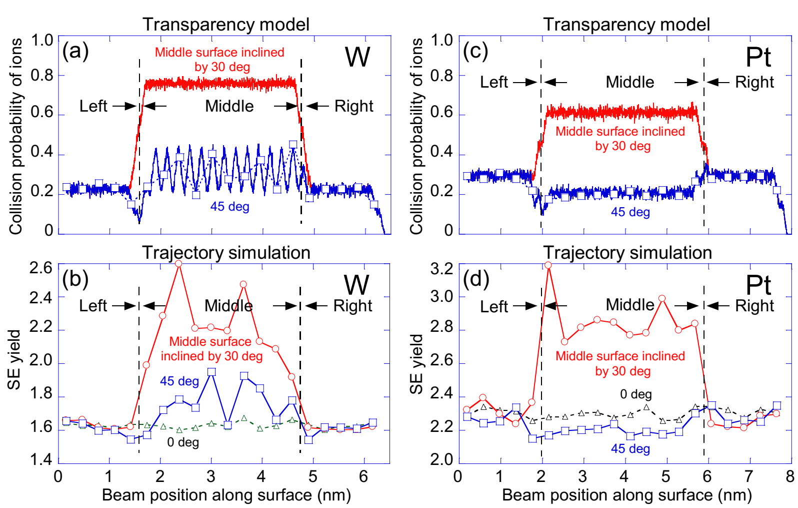

Figure 2. (a,c) Transparency model probability (r_a=0.06 nm) and (b,d) SE line profile for a 30-keV Ne$^+$ beam on (a,b) bcc W (h=15 nm) and (c,d) fcc Pt (h=15 nm)

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