東京大学大学院工学系研究科　総合研究機構

結晶界面工学研究室

Crystal Interface Laboratory, The University of Tokyo

Crystal Interface Lab. Seminar Series

Institute of Engineering Innovation

The University of Tokyo

Grain Boundary Segregation Analyzed by Reverse Process of Dynamic Scattering

by

Prof. Fu-Rong Chen

Dept. of Engineering and System Science, National Tsing Hua University, Hsin-Chu, Taiwan

Several approaches, such as the 1s state model, reversing multislice algorithms, or simulated annealing and maximum likelihood algorithms , have been proposed to remove the dynamical scattering effect and to retrieve the crystal potential from the complex exit wave. In my talk, I will present a new method to retrieve the potential map from the exit wave based on reversing multi-slice calculations. This algorithm uses a non-linear optimization scheme to find an optimum phase grating that satisfies two boundary conditions: knowledge of the entrance surface wave and the measured exit surface wave. The exit wave of a wedge shaped Au crystal and an Al (10%Cu) crystal were simulated to test this algorithm. Good agreement between the recovered crystal potentials and input parameters was found up to a thickness where phase reversal occurs because of dynamic scattering. After the phase grating is retrieved, the position of atom columns and their chemical composition can be quantified. Compositional maps $X_a(r)$ and $X_b(r)$ of binary alloys can be deduced from the crystal potential map V(r) using the linear relation $V(r) = X_a(r)V_a+X_b(r)V_b$, where V_a and V_b are the mean inner potentials of the element A and B, respectively. The reverse multi-slice algorithm is applied to analyze electron exit waves of an Al:Cu Σ5 bi-crystal and an InGaN/GaN quantum well that were reconstructed from focal series of 20 images each. The retrieved potential maps of the Al and Cu atoms allow us to analyze the site-specific Cu segregation to the boundary. The bounding energy of Al atoms at grain boundary to the segregatant Cu atoms is determined to be 0.02eV/ atoms. The retrieved Ga and In potential maps from the quantum well region enable to analyze the roughness of the interface. It is clear from both cases that chemical differences can be distinguished on a single atom level due to the different atomic number Z of the elements. Limitations of the algorithm due to systematic and statistical errors will be discussed.

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Organizer: Prof. Yuichi Ikuhara
TEL: 03-5841-7688
E-mail: ikuhara@sigma.t.u-tokyo.ac.jp

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