Theoretical Evaluation of Atomic-Resolution X-ray Analysis toward Quantification

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The latest aberration-corrected scanning transmission electron microscopes (STEMs) in combination with the large solid-angle silicon-drift X-ray detectors (SDDs) improve limited efficiencies of signal generation and collections. It is no longer dream to acquire atomic resolution X-ray maps and to achieve single atom sensitivity in X-ray analysis by using the latest aberration-corrected instruments. Obvious next challenge is quantification of such atomic-resolution X-ray maps. There are several attempts to perform quantification of the atomic resolution X-ray maps [e.g. 1, 2]. However, quantified results are deviated from expected values from the structures. For example, Ga composition does not reach to 100% at Ga only columns in a [100]-projected GaAs compound [1]. Clearly, X-ray signals are generated from the specific atomic column where the incident electron is focused but also surrounding columns. For appropriate quantification, it is essential to determine how much X-ray signals are generated from the target and neighboring columns. In this study, X-ray signal generation in an oriented crystalline structure is simulated theoretically toward quantitative analysis.

In order to simulate X-ray generation, first, it is required to know how the incident electron probe propagates in an oriented crystalline material. The electron propagation, called the electron wave function, can be simulated by multislice calculation. In this study, the xHREM code [3] was used to simulate the electron wave function, which actually represents electron propagation. Once the electron distributions are simulated, X-ray signals can be simulated at each sliced plane. X-ray spectra were simulated at each sliced layer by porting the X-ray generation engine of legacy Desktop Spectrum Analyzer (DTSA) codes [4]. An X-ray spectrum at a certain depth from the top surface of the specimen was obtained by adding individual spectra. Since the DTSA codes were used, X-ray absorption is also taken care of. X-ray maps were constructed by repeating this process at various positions. In this talk, the simulated X-ray signals will be quantitatively compared with experimental results from atomic-resolution X-ray analysis, and then quantification of such atomic-resolution X-ray analysis will also be discussed.

References

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