

# Quantitative measurement of intensity profiles of equal thickness fringes of Si and MgO crystals and estimation of crystal potential

Koji Nishio<sup>1</sup>, Toshiyuki Isshiki<sup>1</sup>, Eiji Okunishi<sup>2</sup>, Tetsuo Oikawa<sup>2</sup>,  
Masahiro Kawasaki<sup>2</sup>, Hisamitsu Endoh<sup>1</sup> and Makoto Shiojiri<sup>1,3</sup>

<sup>1</sup>Department of Electronics and Information Science, Kyoto Institute of Technology,  
Matsugasaki, Sakyo-ku, Kyoto 606-8585, Japan

<sup>2</sup>Application and Research Center, JEOL Ltd., Akishima, Tokyo 196-8558, Japan

<sup>3</sup>Department of Anatomy, Kanazawa Medical University, Uchinada, Ishikawa 920-0293, Japan

**Summary:** Exact measurement of intensity profiles of equal thickness fringes has been carried out in TEM images of Si and MgO crystals using an energy filtering TEM and an imaging plate. The intensities are measured in bright and several dark field images for [100] Si and [1 $\bar{1}$ 0] MgO, with and without a slit of  $\pm 5$  eV in energy width for incident electrons of 200 keV. Calculated diffraction intensities are compared with the experimental data and suitable complex potential is investigated.

## 1. Introduction

High-resolution transmission electron microscopy has been established as a method to analyze nano-structural materials with atomic scale resolution. The quantitative analysis of experimental data depends entirely on the simulation based on a dynamical theory of electron diffraction and an imaging theory of electron optics. Because these theories contain some approximations and there is a possibility that the simulation programs have bugs or errors, an accurate program objectively inspected is indispensable. Although mutual comparison of various programs may be effective to find out the bugs in them, the comparison with reliable experimental data and the subsequent feedback to the theories are still more important. In this paper, zero-loss filtered intensity profiles as well as unfiltered ones of equal thickness fringes of Si and MgO crystals are provided as the reliable data, following a previous report for a GaAs and an InP crystal [1]. The simulated results are checked with respect to the experimental data, the various crystal potentials being applied.

## 2. Experimental

Si single crystals prepared by cleaving a Si (001) wafer along the  $\{110\}$  planes and MgO single crystals, having the  $\{100\}$  surfaces, prepared by burning Mg in air were used. The crystal orientations, [100] for Si and [1 $\bar{1}$ 0] for MgO, were exactly settled using its diffraction patterns including Kikuchi lines. The edge of the specimen along the [001] axis has 90° wedge-shape, which has a merit that the thickness is deducible as a function of the distance from the edge. Zero-loss filtered images applying a slit of  $\pm 5$  eV in energy width for incident electrons and unfiltered images were observed under the zone axis condition at room temperature, with JEM-2010FEF and JEM-2010EF TEMs equipped with an  $\Omega$ -type energy filter, operated at 200 kV. The bright field and the 022 and 040 dark field images for Si, and the bright field and the 111, 002, 220, 113, 222, and 004 dark field images for MgO were recorded at a direct magnification of more than 200,000 on the imaging plates. The magnification of the images was calibrated using multi-beam lattice images recorded under the same condition without the objective aperture. The intensity of the equal thickness fringes was normalized with respect to the incident beam intensity which was measured in a vacuum region.

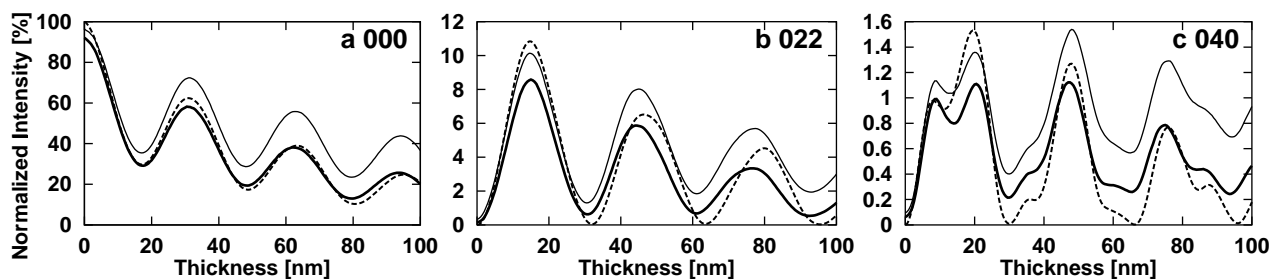
### 3. Results and Discussion

Figures 1 and 2 indicate the zero-loss filtered (thick solid lines) and unfiltered (thin solid lines) intensity profiles of equal thickness fringes of Si and MgO, respectively. Measurement with an energy filtering TEM enables us to cut the contribution of inelastically scattered electrons due to plasmon excitation out of the profiles. The ratio of the zero-loss filtered intensity to the unfiltered one tends to decrease with increase in thickness, although it is not always proportional to the thickness because of multiple scattering in crystal.

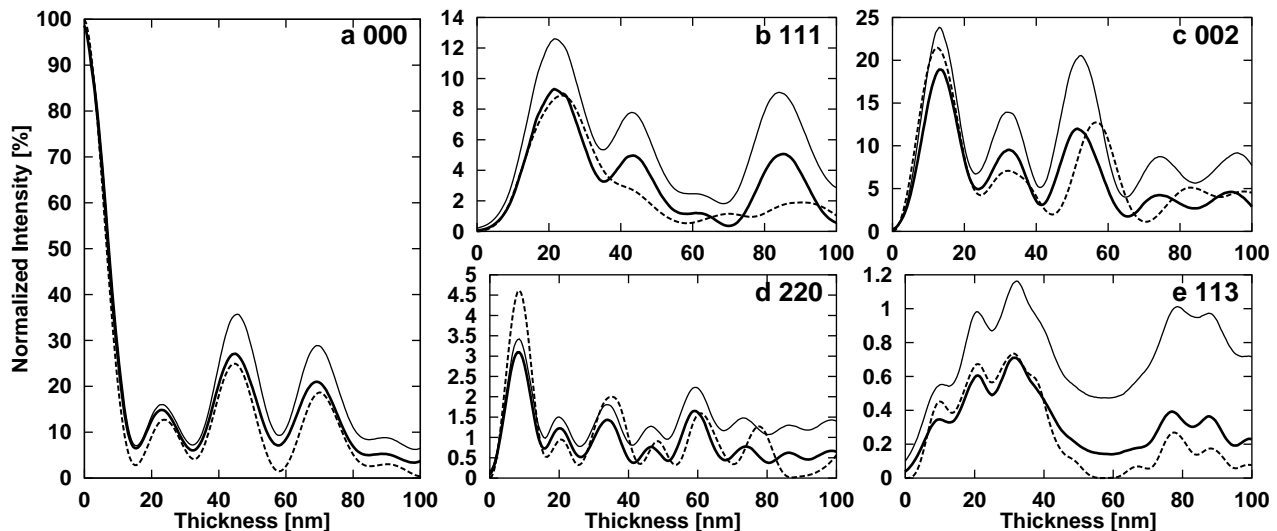
Comparison between the experimental profiles and the ones calculated with our multi-slice program [2] was carried out, where structural parameters such as the scattering factor, the temperature factor and the ratio of imaginary part of the complex potential to the real part were varied. It has been confirmed that the on-line version of EMS program [3] based on the Bethe method produces almost the same results as that by our program [4]. In the calculations for Si taking no account of inelastic scattering, the position of peaks almost agrees with the experimental one but the intensity of them disagrees. The agreement improves by introducing a complex potential of  $(1 + 0.04i)V_{re}$  and a temperature factor of  $4.5 \times 10^{-3} \text{ nm}^2$  (dashed lines in Fig. 1). In the calculations for MgO, the position as well as the intensity of peaks disagrees with the experimental one. The calculation with complex potential taking account of scattering factors for ions produces better correspondence (dashed lines in Fig. 2). The present experimental data have a possibility that the net charge of elements and the solid state effect as well as temperature effect and processes of inelastic scattering can be made clear [4].

### References

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**Figure 1:** Intensity profiles obtained from zero-loss filtered (thick solid) and unfiltered (thin solid) 000 (a), 022 (b), and 040 (c) images of Si and corresponding profiles calculated with a multi-slice program (dashed).



**Figure 2:** Intensity profiles obtained from zero-loss filtered (thick solid) and unfiltered (thin solid) 000 (a), 111 (b), 002 (c), 220 (d), and 113 (e) images of MgO and corresponding profiles calculated with a multi-slice program (dashed).