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Determination of a 3D Lattice Displacement Field by Iterative Phase Retrieval of Rocking Curves of HOLZ Reflections

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Kinematical diffraction intensity as a function of excitation error, or a rocking curve, observed from a crystal, which has a displacement field inhomogeneous along the incident beam direction, z, is obtained by an absolute square of lattice scattering amplitude $\phi_{\mathbf{g}}$ given by the following formula,

$$\phi_{\mathbf{g}} = \int_0^t e^{-2\pi i \mathbf{g}\cdot\mathbf{R}(z)} \cdot e^{-2\pi i s z} dz$$
$$= \int_{-\infty}^{\infty} A(z) e^{-2\pi i \mathbf{g}\cdot\mathbf{R}(z)} \cdot e^{-2\pi i s z} dz,$$

where t, s and $\mathbf{R}(z)$ indicate specimen thickness, excitation error and displacement vector of the strained lattice, respectively, and $A(z)$ is unity for $0 < z < t$ and zero for $z < 0$ or $z > t$. The z-axis is along the beam direction and its origin is set to be at the specimen surface. This formula shows that $\phi_{\mathbf{g}}$ is related to $A(z)e^{-2\pi i \mathbf{g}\cdot\mathbf{R}(z)}$ by Fourier transform. The Fourier iterative phase retrieval has been applied to reconstruct the phase of $\phi_{\mathbf{g}}$, and thus, phase factor $\alpha = -2\pi i \mathbf{g}\cdot\mathbf{R}(z)$ with an real space constraint of $A(z)$ [1]. In the present study, the z-dependence of the 3D lattice displacement field $\mathbf{R}(z)$ was determined by the Fourier iterative phase retrieval of rocking curve profiles of mutually independent reflections.

A $Si_{0.7}Ge_{0.3}$ layer of a 50 nm thickness was deposited on a silicon substrate of (110) plane by the molecular beam epitaxy technique. The specimen for the CBED experiment was prepared by ion thinning. Fig. 1 shows a cross section TEM image of the specimen used for the present study. The CBED experiment was conducted at an acceleration voltage of 200 kV by using a field-emission transmission electron microscope, JEOL JEM-2100F equipped with an energy filtering system, Gatan GIF with a 2k x 2k CCD camera.

Figs. 2(a) shows a CBED pattern taken from the Si substrate at a position close to the SiGe/Si interface, as indicated by the dot in Fig. 1. Figs. 2(b), 2(c) and 2(d) show rocking curve profiles of $1\bar{1}\bar{7}$, $\bar{6}4\bar{6}$ and 008 reflections, respectively. Figures 3(a), 3(b) and 3(c) show three components of the determined displacement field $\mathbf{R}(z)$ in the [001] direction (perpendicular to the interface), in the [230] direction (parallel to the incident direction) and in the [320] direction, respectively. The displacement in the [001] direction approximately show a mirror symmetry about the plane at $z = t/2$, indicating a bending displacement, whereas the displacement in the $[3\bar{2}0]$ direction show an inversion symmetry, indicating a lattice expansion in the [230] direction. These displacement features are consistent to the strain field expected by finite element simulations.

References

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[2] K. Saitoh et al. *J. Electron Microsc.* **59** (2010) 367.

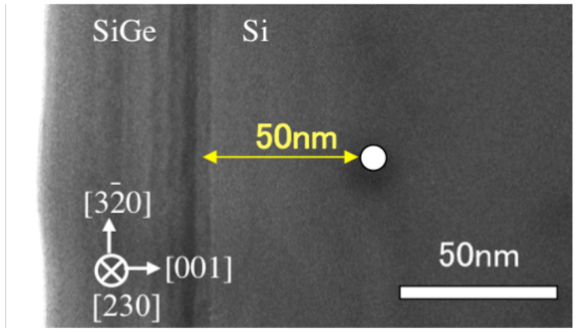

FIG. 1. Cross section TEM image of the specimen used in the present study. The white dot indicates the position at which CBED pattern of FIG.2(a) was taken.

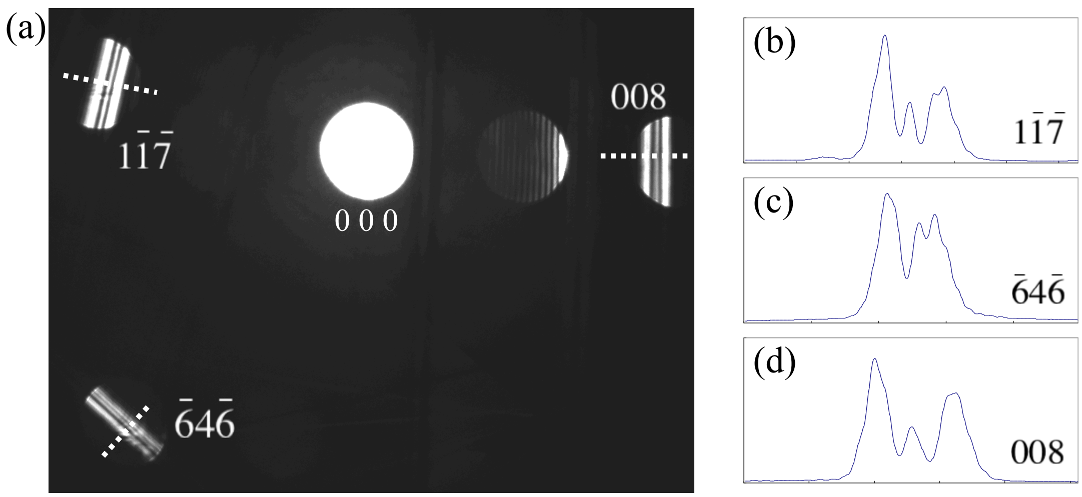

FIG. 2. (a) CBED pattern taken from the silicon substrate close to the interface. Rocking curves of $1\bar{1}\bar{7}$ (b), $\bar{6}4\bar{6}$ (c) and 008 (d) are taken along the white dashed lines.

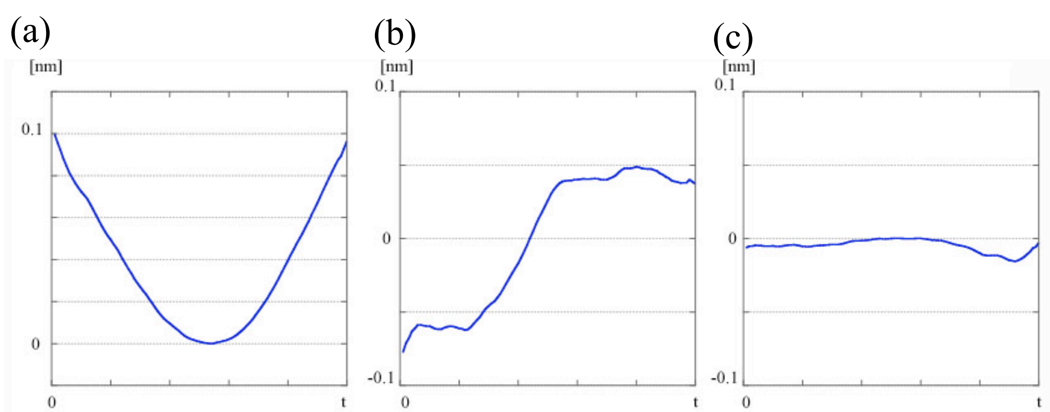

FIG. 3. Displacement fields **R**(z) in the [001] direction (perpendicular to the interface) (a), in the [230] direction (the incident direction) (b) and in the [$3\bar{2}0$] direction (c), reconstructed by the present study.

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