Determination of a 3D Displacement Field at a Vicinity of a GeSn/Ge Interface by the Phase Retrieval of Electron Rocking Curves

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Strain in materials is one of the important factors affecting physical properties of the materials such as carrier mobility, dielectric property, magnetism and so on. In semiconductor industry, strain engineering has been playing a primary role for the improvement of the device performance. Measurement of strain has also been very important as a key technique supporting the strain engineering. So far, the strain measurement by diffraction technique has been done mainly by measuring the positions of diffraction peaks and by fitting the experimental peak positions to simulated ones. This method implicitly assumes that strain in the volume contributing to diffraction intensities is uniform. Strain in real materials, however, is not always uniform and varies over the diffraction volume of the specimen. In the present study, we applied convergent-beam electron diffraction (CBED) to determine such non-uniform strain, whose lattice displacement vector varies along the incident direction of the electron beam.

Lattice scattering amplitude of reflection $g$ is given by the following formula,

$$\phi_g(s) = \frac{i\pi}{\xi_g} \int_{-\infty}^{\infty} A(z) e^{-2\pi i g \cdot R(z)} e^{-2\pi i s z} dz$$  \hspace{1cm} (1)

where $s$ and $z$ indicate extinction error and the real space coordinate along the electron beam propagation. $\xi_g$ and $R(z)$ indicates extinction distance and the displacement vector of the lattice, respectively. $A(z)$ is a hat-shaped function which expresses the inside or the outside of the specimen, that is, $A(z) = 1$ for $0 < z < t$ and $A(z) = 0$ for $z < 0$ and $t < z$. Eq. (1) indicates that $\phi_g(s)$ and $A(z)e^{-2\pi i g \cdot R(z)}$ are connected to each other by Fourier transform. We applied the Fourier iterative phase retrieval technique to restore the phase part of $\phi_g(s)$, and to determine the phase factor of the lattice displacement $2\pi i g \cdot R(z)$. In the present study, the modulus of $\phi_g(s)$ was measured from a rocking curve profile observed by a CBED pattern.

A Ge$_{92.9}$Sn$_{7.1}$ layer of 200 nm was deposited on a Ge (001) substrate by the chemical vapor deposition method in a ultra-high vacuum. Cross section samples for electron microscopy were prepared by mechanical polishing and ion-beam thinning. Rocking curves were obtained by the CBED technique at an incidence inclined by about 10 degree from the [110] direction. CBED experiment was conducted by using a transmission electron microscope operated at an acceleration voltage of 200 kV. CBED patterns were taken by using Gatan imaging filer with an energy window of 5 eV to remove inelastic scattering mainly by the plasmon loss.

Figure 1 shows a cross-section TEM image of the specimen. CBED patterns were taken from the positions indicated as 1 to 6 in the Ge substrate. Figure 2(a) shows a whole CBED pattern used in the phase retrieval, and Figures 2(b), 2(c) and 2(d) show enlarged disks of the $\overline{2}6\overline{8}$, 553 and $\overline{3}17$ reflections, respectively. Figures 3(a), 3(b) and 3(c) show rocking curve profiles of the $\overline{2}6\overline{8}$, 553 and $\overline{3}17$ reflections, respectively. Figures 4(a), 4(b) and 4(c) show phase profiles of $2\pi i g \cdot R(z)$ of the $\overline{2}6\overline{8}$, 553 and $\overline{3}17$ as a function of the $z$-coordinate, respectively. From these phase profiles, the lattice displacements in the [001], [110] and [110] directions are determined as shown in Figures 5(a), 5(b) and 5(c), respectively. It is clearly seen that the displacement field in the [001] direction is of mirror symmetry about the center of...
the specimen, which is consistent to the elasticity theory. The displacements field determined by the present method is quantitatively compared to the simulated values obtained by the finite element method.

FIG. 1. TEM image of a GeSn/Ge cross section.

FIG. 2. Whole CBED pattern (a) and reflection disks of 268 (b), 553 (c) and 317 (d).

FIG. 3. Rocking curve profiles of 268 (a), 553 (b) and 317 (c).

FIG. 4. Retrieved phase profiles of 268 (a), 553 (b) and 317 (c).

FIG. 5. Displacement field at a vicinity of a GeSn/Ge interface determined by the present method.