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Hole Accumulation in Ge/Si Core/Shell nanowires Studied by Electron Holography

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Due to the large valence band offset (≈500meV) between Ge core and Si shell, hole accumulation in the Ge core of undoped Ge/Si core/shell nanowires (NWs) has been reported: this effect has potential applications for high mobility devices [1]. While most experiments have focused on the *p*-type depletion-mode field-effect device behavior and transconductance measurements [1-2], this present study of the Ge/Si core/shell system concentrates on the location of charge accumulations as well as corresponding charge densities. The observations were made with a Philips CM200 FEG TEM operated at 200kV.

Figure 1(a) shows a HRTEM image of a Ge/Si core/shell NW in a {110} projection: the diameter of the Ge core here is around 10nm. The corresponding inset Fast Fourier Transform (FFT) shows a {110}-type growth direction. Fig. 1(b) is a plan-view image showing a NW sample where the Ge crystal core has a diameter of ~30nm, as well as a thin amorphous Si shell and SiO_2 wrapped around for protection. This NW had also grown along a {110} direction, as shown by the corresponding FFT. The core region shows primarily {111} and {100} facets, with some sidewall imperfections and a slight misorientation from {110}. Fig. 1(c) is an ADF STEM image of the core/shell NW showing a brighter core region. The intensity across the NW, as indicated by the white box, was averaged over 50 pixels, and the result is shown by the red squares in Fig. 1(d). The blue line with circles shows a calculation for a hexagonal prism Ge core having {111} and {100} facets [3], and a cylindrical Si shell, as sketched in Fig. 1(e). In comparison, the green line with triangles shows the calculation for cylindrical Ge core and Si shell. The calculations are based on the fact that the STEM intensity is proportional to projected thickness and Z^n, where Z is corresponding atomic number and n is set as 1.3 to match the experimental data. The hexagonal prism core model shows a better match with the experimental profile although there is a slight difference at the interface between the core and shell, as well as at the shell surface region, which is possibly due to interface diffusion or surface roughness.

A typical hologram of a Ge/Si core/shell NW is shown in Figure 2(a). After the hologram was reconstructed, the upper part of the phase image, which was free of diffraction contrast, was selected for phase line profile across the NW. The experimental phase data is shown by the green dotted lines in Fig. 2(b). The core and shell regions were smoothed separately with polynomials, as shown by the blue squares and red triangles, respectively. The thin black line is a calculation based on the model shown in Fig. 1(e). The phase difference between smoothed experimental data and calculation is presented in Fig. 2(c). This shows positive phase shift inside the core region, and small peaks around the interface between core and shell, suggesting possible hole accumulation inside the core close to the interface region, which is expected according to the band diagram of the Ge/Si core/shell system shown in Fig. 2(c). Since the location and height of the peaks are very sensitive to the model, further work will concentrate on simultaneously obtaining STEM images and holograms from specific nanowires, since the former can provide accurate projected thickness needed for the reconstruction of the latter.

References

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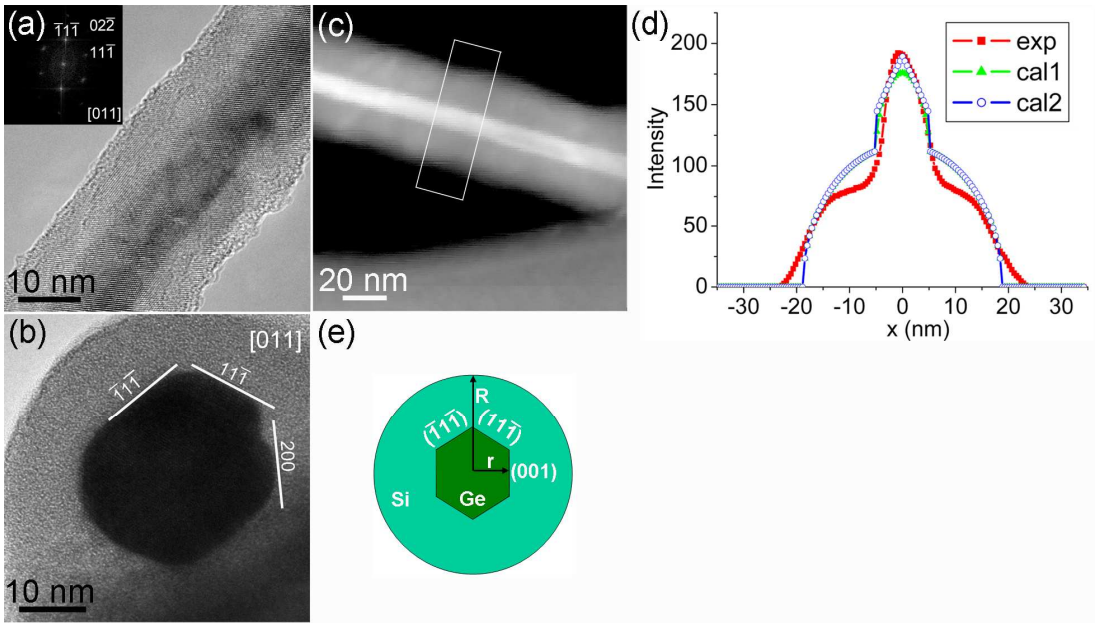

FIG. 1. (a) TEM image of Ge/Si core/shell nanowire grown along {110}. (b) Plan view of a Ge nanowire grown along {110}. (c) STEM image of Ge/Si core/shell nanowire with the area for line profile shown in white box. (d) Intensity profile of experimental STEM image and profiles calculated from cylindrical and hexagonal prism core models. (e) The hexagonal prism core model.

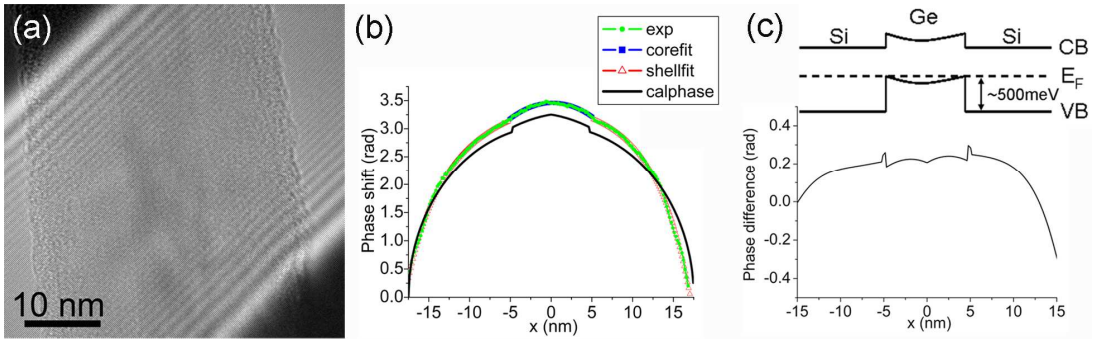

FIG. 2. (a) Off-axis electron hologram of Ge/Si core/shell nanowire. (b) Experimental phase shift across nanowire which is smoothed with polynomials and compared with calculation from model. (c) Phase difference between experimental and calculated phase shifts. The top inset is the band diagram of Ge/Si core/shell system.

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