

Molecular dynamics simulations of (Si, Ge) quantum dots to quantify the shape analysis by electron holographic phase measurement

K. Scheerschmidt¹, C.L. Zheng², H. Kirmse², I. Häusler² and W. Neumann²

1. Max Planck Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

2. Humboldt-Universität zu Berlin, Institut für Physik, D-12489 Berlin, Germany

schee@mpi-halle.de

Keywords: holography, molecular dynamics, mean inner potential, shape reconstruction

Electron microscope (EM) techniques provide very powerful tools to investigate nanostructures in solids: Structure, shape, extension and strain of, e.g., quantum dots (QDs) have strong influence on the confinement of electrons and determine the optoelectronic properties in device applications. Conventional EM, however, needs additional data to separate the different effects, which can be provided by the wave phase extracted from electron holograms. By electron optical arguments the phase shift $\Delta\phi$ of a crystal is proportional to the mean inner potential V_o , the interaction constant C_E ($0.00729V^{-1}nm^{-1}$ at 200kV), and the sample thickness t : $\Delta\phi(x, y) = C_E \cdot V_o \cdot t(x, y)$. Thus, the mean inner potential may be determined, e.g., from the gradient of the phase shift at wedge shaped samples [1, 2]. On the other hand, if V_o is known, the 2D map $\Delta\phi(x, y)$ of the shift of the wave phase can be transformed into a thickness map $t(x, y)$ for surface morphology reconstruction.

However, at least two problems arise: The mean inner potential is not well defined, as already discussed very early [3], and the phase shift is not only proportional to the mean inner potential, it is modified by defects, strain, composition changes, shape, and surface structure, too. In addition, the model of scattering itself also influences V_o : the simple isolated atom approximation [4] has to be replaced by evaluating the charge density (cf. [5, 6] and references therein).

Molecular dynamics (MD) using the bond order potential (BOP, cf. [7, 8] and references therein) provides a possibility to model both, the relaxation of nanostructures with the resulting EM-phase, and the evaluation of V_o by scanning the BOP itself. Fig. 1 shows a relaxed pyramidal QD model in different views within a super cell of 23 nm to guarantee sufficient extension for MD-relaxation and multi-slice wave simulation, the latter shown by amplitude and phase of the scattered wave in (c). The remaining strains, cf. [001] view in (b), yield to the oscillating amplitude, whereas the simulated wave phase reveals the QD-shape as demonstrated by the respective profile.

In Fig. 2 different models to calculate V_o as function of the Ge concentration are shown. The BOP data are extracted by scanning MD-relaxed half spaces of (Si, Ge) with different Ge concentration, cf. Fig. 2a. However, the results, shown in (b), need further scaling of the absolute value, when compared with isolated atom approximation and interpolated DFT data. Nevertheless, the green triangular dots and squares demonstrate clearly the small influence of the relaxation to V_o .

Fig. 3 demonstrates the experimental EM shape analysis of (Si, Ge) islands grown by liquid phase epitaxy on (001)-Si, thinned from the back side of the substrate to preserve the islands. In order to get a large area phase mapping, parts of the electron holograms were recorded in Lorentz mode, amplitude and phase information of electron exit wave were extracted as usual by holographic reconstruction using reference holograms. The hologram itself is shown in (a), reconstructed amplitude in (b), wrapped and unwrapped phases in (c) and (d), respectively. Amplitudes and phases in (e) are comparable to the simulated ones shown in Fig. 1c, but they have to be discussed in terms of V_o . Thus the resulting 3D-shape in (f) depends finally on the model used for V_o , nevertheless it demonstrates that mainly the correct height of the QD may be revealed.

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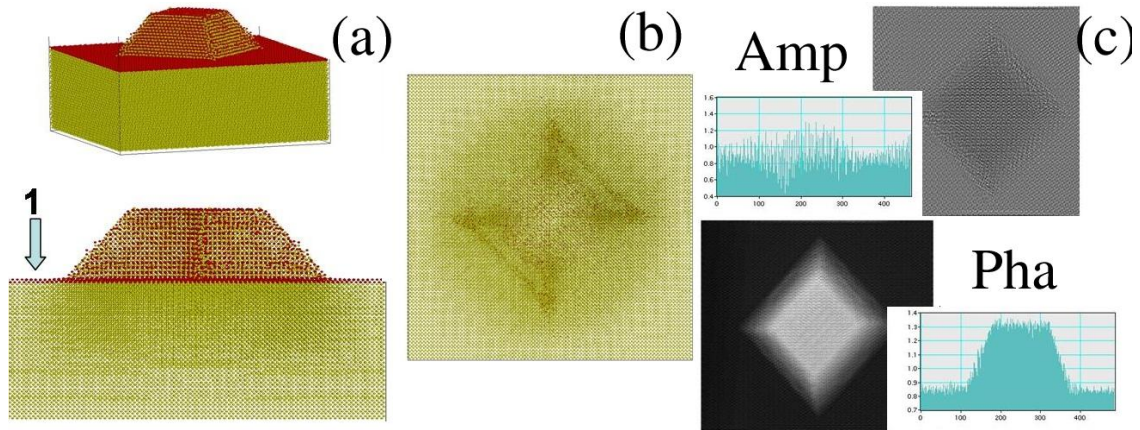


Figure 1. {110}-(Si,Ge)-pyramide, free-standing on (001)-Si with a monoatomic Ge-wetting layer: (a) super cell of 23nm box length in perspective and [100] view. (b) [001] view of the relaxed model showing strains in the pyramid and the substrate. (c) Modulus and phase of the simulated wave for the model (a) after tilting the super cell to [-1, 12, 120] zone axis (as in experiment for special two beam incidence with high composition sensitivity) and applying multi-slice 200kV. The line scan with 0.5π phase difference reveals the height assumed in (a).

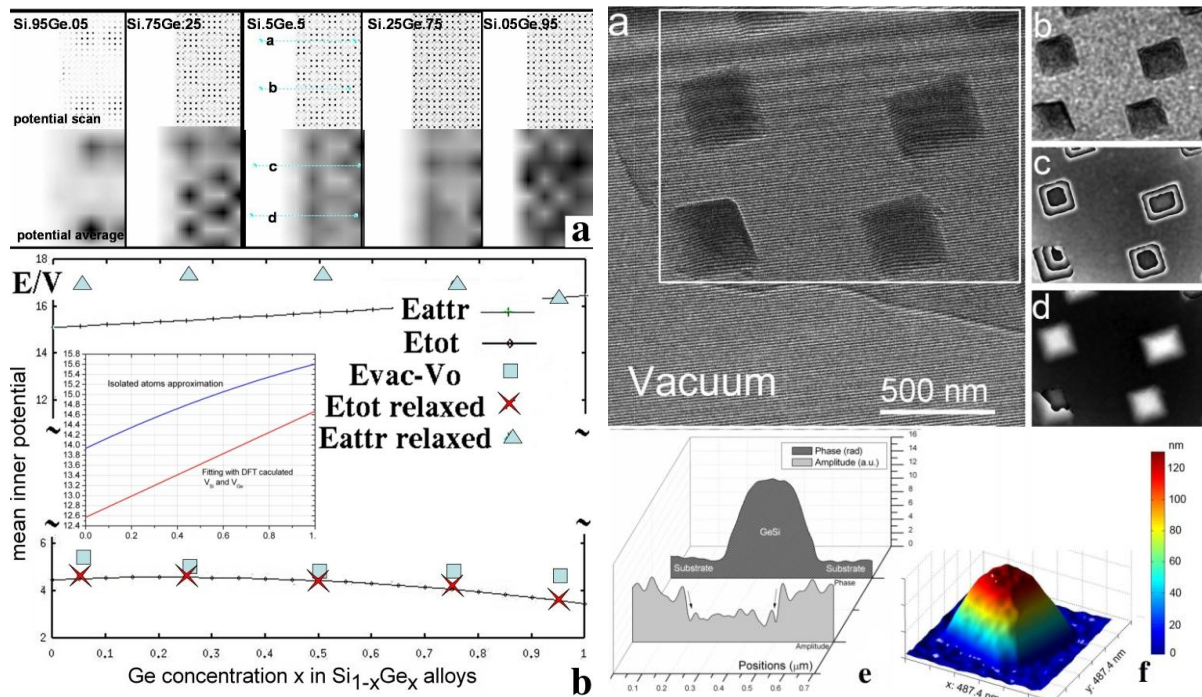


Figure 2. (left panel). Mean inner potential E (in V) of (Si,Ge) compounds as a function of the Ge concentration x for different scattering models: (a) Scan of the bond order potential [7] after relaxation using classical molecular dynamics for vacuum super cells of 23nm box length half filled with (Si,Ge) of different x . (b) Total energies vs. all attraction terms, i.e. σ -, π -bonds and promotion energy. Isolated atom approximation (Doyle-Turner, insert blue) with atomic form factor of Si (5.828\AA) and Ge (7.378\AA) vs. linear fitted DFT data (insert red), i.e. Si (12.57 V) and Ge (14.67 V) using data of [1, 2, 4]. **Figure 3. (right panel):** Reconstruction of the 3D-shape of a (Si,Ge) island grown on (001) oriented Si substrates from holographic phase analysis with scattering potential as given in Fig. 2: (a) Hologram, (b) reconstructed amplitude, (c) 2π -raw phases, (d) unwrapped phase image, (e) scan of modulus and phase of one island, and (f) (Si,Ge) island as reconstructed using the phases of (d).