Molecular Dynamics Simulations of (Si, Ge) Quantum Dots to Quantify the Shape Analysis by Electron Holographic Phase Measurement

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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 ($0.00729 V^{-1}nm^{-1}$ 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 using the bond order potential (BOP, cf. [7] 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, Fig. 2 the remaining strains and Fig. 3 the EM-phase multi-slice simulated. In Fig. 4 for different models V_o as function of Ge concentration are shown. The BOP data on the right need further scaling of the absolute value, but demonstrate the small influence of the relaxation. Thus the theoretical phase in Fig. 5 evaluated from Fig. 3 shows that mainly the correct height of the QD may be revealed.

Figs. 6 and 7 demonstrate 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 3D result in Fig. 7 will be discussed in terms of V_o.

[1] M. Gajdardziska-Josifovska, M.R. McCartney, et al., *Ultramicroscopy* **50** (1993) 285
[2] P. Kruse, M. Schowalter, et al., *Ultramicroscopy* **106** (2006) 105
[3] M. von Laue, Materiewellen und ihre Interferenzen, Geest & Portig, Leipzig 1948
[4] P.A. Doyle, P.S. Turner, *Acta Cryst.a* **A24** (1968) 390
[5] M. O'Keeffe, J.C.H. Spence, *Acta Cryst.* **A50** (1994) 33
[6] M.Y. Kim, J.M. Zuo, J.C.H. Spence, *phys. stat. sol (a)* **166** (1998) 445
[7] K. Scheerschmidt, V. Kuhlmann, *Int. J. Mat. Res.* **98** (2007) 11

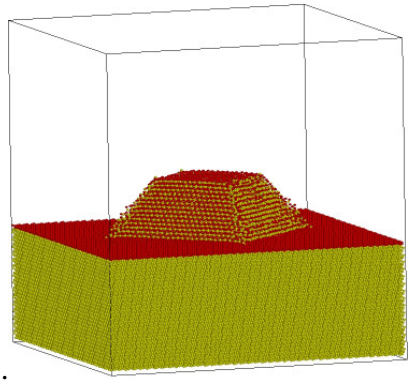

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FIG. 1: {110}-SiGe-pyramide, free-standing on (001)-Si with monoatomic Ge-wetting layer (super cell of 23nm box length).

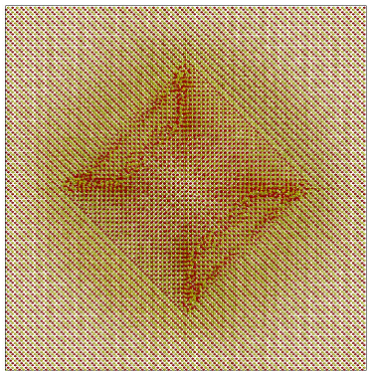

FIG. 2: [001] view of the relaxed model showing the strains in the pyramide and the substrate.

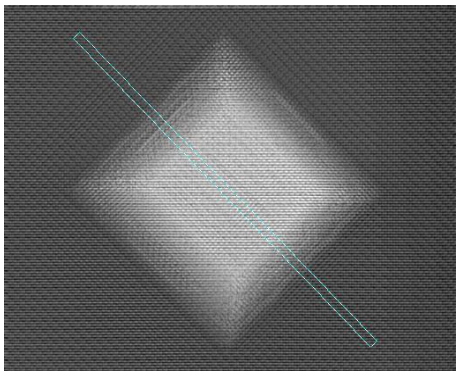

FIG. 3: Simulated wave phase for the model of Fig. 1 after tilting the supercell to [-1,12,120] zone axis applying multi-slice 200kV.

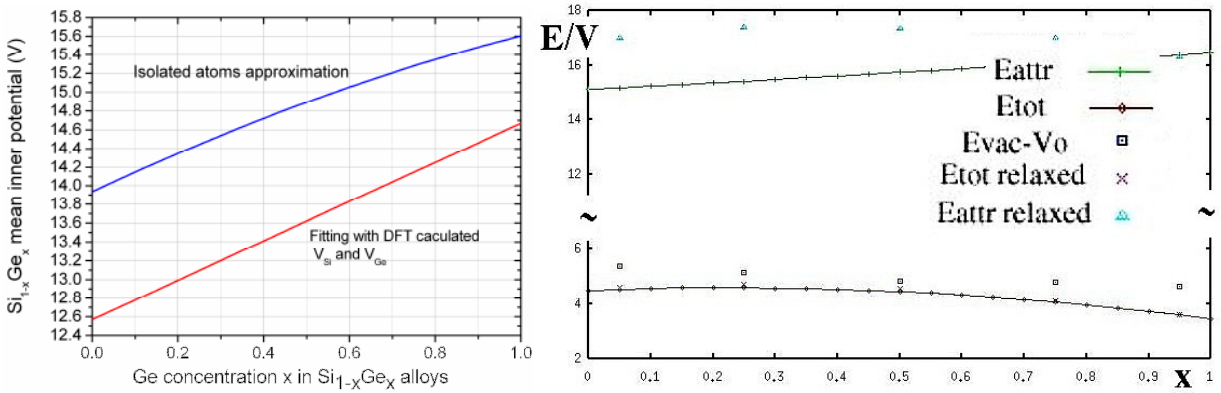

FIG. 4: Mean inner potential E (in V) of (Si,Ge) compounds as a function of the Ge concentration x for different scattering models: Isolated atom approximation (Doyle-Turner, left side, blue) with atomic form factor of Si (5.828Å) and Ge (7.378Å). Linear fitted DFT data (left side, red), i.e. Si (12.57 V) and Ge (14.67 V) [1]. Energies (total vs. all attraction terms, i.e. sigma-, pi-bonds and promotion energy) of the bond order potential scanned in vacuum super cells of 23nm box length half filled with SiGe before and after relaxation using classical molecular dynamics (right side).

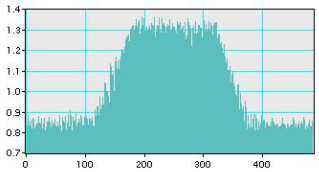

FIG. 5: Line scan from Fig. 3 with 0.5π phase difference revealing the height assumed in Fig.1

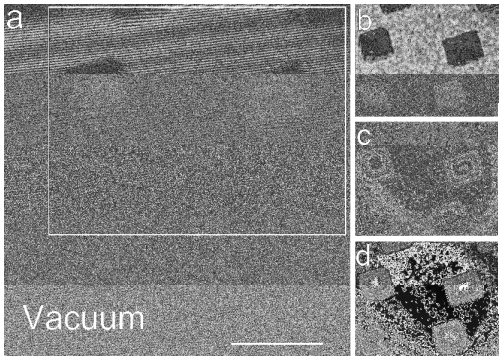

FIG. 6: Hologram (a), amplitude (b), 2π– raw phases (c) and unwrapped phase image (d) of (Si,Ge) islands grown on (001) oriented Si substrates.

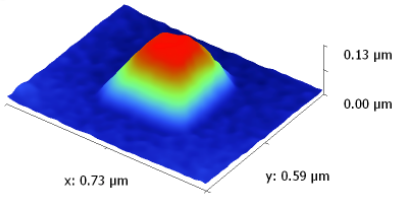

FIG. 7: 3D-shape of a (Si,Ge) island as reconstructed using the phases of Fig. 6d.