Electron Imaging based on Charge Density Potentials and Frozen Lattices

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The quantitative analysis of electron microscope images requires image simulations of the object wave function (exit wave) based on well relaxed structure models and a suitable description of the electron scattering. The elastic interaction between electrons and an object can be simulated with good accuracy using the multi-slice formulation of the dynamical theory of electron interferences. Thereby the concept of structure factors is applied - scattering potentials according to Doyle-Turner (TDscf) or Weickenmeier-Kohl - or the scattering potential V(r) is given by solving the Poisson equation for the charge density. In order to calculate both the scattering potentials and the relaxed structure models molecular dynamics (MD) simulations have been performed, e.g. to study atomic processes related to the reordering at interfaces and the relaxation of nanostructures [1]. From MD-relaxed structures, e.g. for 4 substitutional defects of Ge in Si ($Si_{4S(Ge)}$) as shown in FIG. 1, exit waves are simulated using TDscf and compared with simulations using potentials based directly on the charge density [2]. In addition, the influence of the thermal diffuse scattering is included using the frozen lattice model [3].

Ab initio density functional calculations of V(r) may be carried out in the local density approximation (LDA) [2], for small structures considered here the code ABINIT [4] was applied. Consisting of the Hartree energy for the valence electrons, the contribution of all effective nucleus potentials, and the exchange correlation effects, the charge density of the ground state yields directly the scattering potential. Simulations on the first principle level may include quantum effects properly and describe electronic properties completely, however, they are computationally too expensive for large systems because the diagonalization of the Hamiltonian scales as $O(N^3)$. Empirical MD enable larger structure relaxations, but the inter-atomic forces used are accurate only if the influence of the local environment according to the electronic structure is included. This requires better approximations, such as the analytic bond order potentials (BOP) based on the tight binding approximation (TB), as it preserves the essential quantum mechanical nature of atomic bonding, yet abandons the electronic degree of freedom. The analytic BOP achieves O(N) scaling by diagonalizing the orthogonal TB-Hamiltonian approximately and is recognized as a fast and accurate model for atomic interaction [5] especially in higher order approximation as BOP4+ [2].
FIG. 2 shows the amplitudes and phases of the exit wave in [110] projection calculated for a 2x2x2 supercell of the $Si_{4S(Ge)}$ example. The supercell (1.536nm x 1.086nm) is sliced into 8 different slices of 0.192nm thickness, the exit wave is calculated for a thickness of 6.144 nm (4x8 = 32 slices). The simulations using the DTscf (FIG. 2a) are compared with calculations for potentials derived from LDA charge densities (FIG. 2c) and those using scanned BOP4+ (FIG. 2b). The structure factor model is represented always by spherical symmetrical scattering potentials, whereas for the other approximations the phase grating is influenced by the angular behavior of the bond structure. The different potential models do not modify the exit wave as strong as the phase grating. The detailed investigation of the contrast effects (especially why additionally phase and position shifts and contrast reversals occur, and why the defects occur in the amplitudes of LDA but in the phases of DTscf and BOP4+), and the application to large supercells containing lattice defects will be the matter of work in progress.

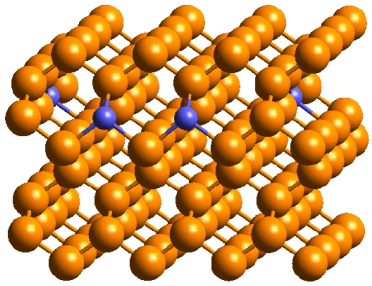

FIG 1. Si structure with 4 substitutional Ge defects $Si_{4S(Ge)}$ as used for molecular dynamics simulations and DFT and BOP electron density calculations.

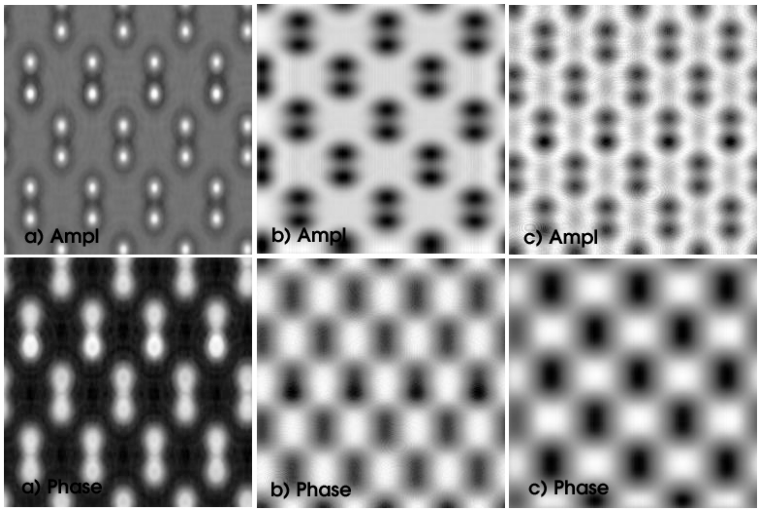

FIG. 2. Amplitudes and Phases of simulated exit waves of the $Si_{4S(Ge)}$ model: a) DTscf, b) BOP4+, c) LDA

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