Substitution of Atomic Scattering Amplitudes in TEM Interpretation by Analytic Bond Order Potentials

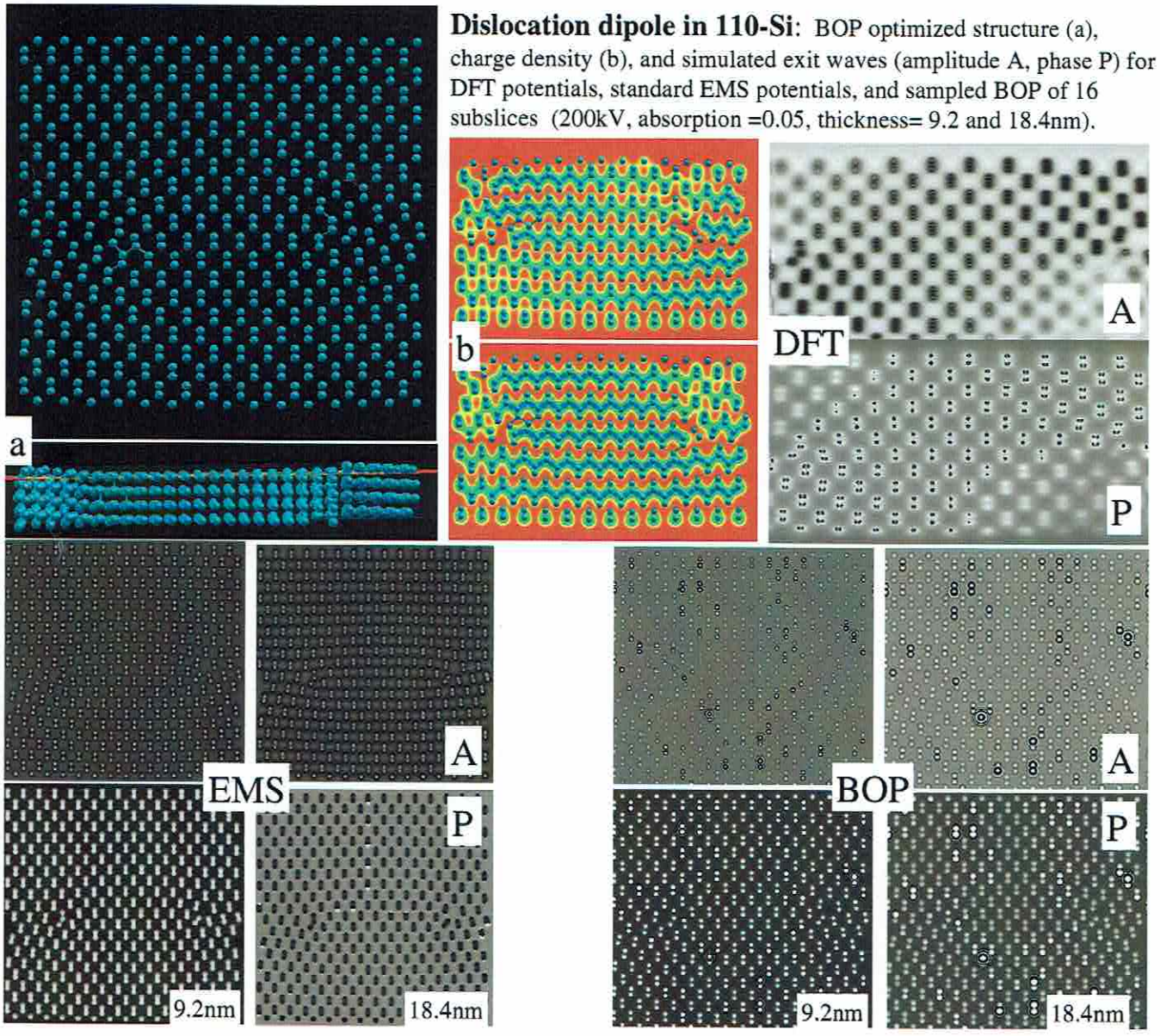
Kurt Scheerschmidt and Volker Kuhlmann

Max Planck Institute of Microstructure Physics, Weinberg2, D-06120 Halle, Germany

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 using scattering amplitudes (SCA) according to Doyle-Turner or Weickenmeier-Kohl. In a direct way the scattering potential V(r) may be 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 such MD-relaxed structures exit waves are simulated using SCAs and compared with simulations using potentials based directly on the charge density [2,3]. In addition, the influence of the thermal diffuse scattering is included using the frozen lattice model [4].
The direct ab initio density functional calculations of V(r) may be carried out in the local density approximation (LDA) or all electron methods. 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 [5,6] especially in higher order approximation as BOP4+ [7].
FIG. 1 shows the amplitudes and phases of the exit wave in [110] projection calculated for a 16x9x4 supercell with a dislocation dipole relaxed using elastic boundary conditions. The supercell is sliced into 8 different slices of 0.096nm thickness, the exit wave is calculated for thicknesses of 9.2 nm and 18.4nm. The simulations using the SCA within the EMS package are compared with calculations for potentials derived from LDA charge densities in the DFT approximation and those using scanned BOP4+. Whereas the scattering amplitudes are spherical symmetric the electron density due to the bonds creates small contrast effects which may be reflected similarly in the DFT and the BOP approximation. The differences due to the approximation level will be discussed in detail using such t-periodic defects as the dislocation dipoles or small defects like interstitial or vacancy cluster. Larger, non-periodic defects, however, may be simulated only using the BOP-approximation.

Correspondence: schee@mpi-halle.de

[1] Scheerschmidt, K.: Empirical Molecular Dynamics: Possibilities, Requirements and Limitations, in: Theory of Defects in Semiconductors, Drabold, D. A., Estreicher, S. (Eds.), Topics in Applied Physics 104, Springer 2006, Chapter 9, pp 213-244.
[2] K. Scheerschmidt and V. Kuhlmann, Proc. Int. Conf. DFTEM2006, Wien, 2006, submitted
[3] K. Scheerschmidt, V. Kuhlmann, A. Rother, and S. Gemming, Proc. 16th Intern. Microscopy Congress, Sapporo, Japan, 2006, Vol.2, p.739
[4] K. Scheerschmidt, Microscopy Conference 2005, 6. Dreiländertagung Davos 2005, PSI Proceedings 05-01,pp.23-24.
[5] M.W. Finnis: Interatomic Forces in Condensed Matter, Oxford Series on Materials Modelling (Oxford University Press, Oxford, 2003).
[6] D.G. Pettifor, M.W. Finnis, D. Nguyen-Manh, et al., Mat. Sci. Eng. A, 365 (2004) 2.
[7] V. Kuhlmann, Thesis, Halle 2007; V. Kuhlmann and K. Scheerschmidt, Phys. Rev. B 2007, in print



Dislocation dipole in 110-Si: BOP optimized structure (a), charge density (b), and simulated exit waves (amplitude A, phase P) for DFT potentials, standard EMS potentials, and sampled BOP of 16 subslices (200kV, absorption =0.05, thickness= 9.2 and 18.4nm).