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Ab-initio simulation of the object exit wave of ferroelectrics

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Ferroelectrics are unique in that, below Curie temperature, they posses a permanent electric polarization along a given axis. High Resolution Electron Holography reveals the electric polarization down to atomic resolution in $BaTiO_3$. To interpret these findings accurately and, at the end, quantitatively, it is indispensable to model the potential distribution in the unit cell, which gives rise to the phase modulation of the object exit wave analyzed by holography.

Simulations with parametrized atomic potentials cannot provide the needed data about the electric potential distribution (e.g. [1]). For accurate potential calculations, we chose the following way: In a first step, a structure optimization within the framework of DFT (Density Functional Theory) was carried out with the software package ABINIT [2]. The obtained structural parameters were compared with X-ray diffraction measurements. An excellent agreement could be verified. The electron density is then calculated using the all-electron full-potential local-orbital calculation scheme. The calculations were scalar-relativistic and the Perdew-Wang parametrization of the local-density-approximation exchange-correlation functional was used [3]. Finally the natural unit cell was determined using a Bader analysis [4]; the dipole moment of that unit cell was found in good agreement with experimental data. In a second step, the Coulomb potential distribution in the unit cell is determined by solving the Poisson equation for the resulting charge density distribution. The charge density distribution is periodic in real space. Hence the solution of the Poisson equation in Fourier space provides the periodic part of the potential, whereas the potential wedge produced by the electric polarization is a harmonic function and can be determined via the dipole moment of the unit cell. The calculated potential is depicted in FIG. 1, clearly revealing the dipole character. In a last step, the potential distribution is used for computing the object exit wave attainable in High Resolution Electron Holography neglecting inelastic scattering, particularly addressing the question of the existence of periodic boundary conditions and well-confined potentials normally applicable in such simulations.

The final comparison of the simulated images with the experimentally recorded ones shows similar features; accuracy is not yet satisfactory, possibly due to inadequate consideration of additional effects, e.g. scattering on thermally elongated atoms in the simulation, relativistic effects and inelastic scattering, which are presently also under our consideration.

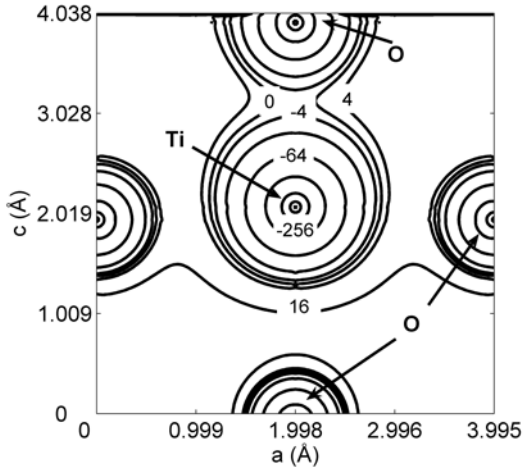

FIG. 1 Potential map of a BaTiO3-crystal in a (010) plane containing Ti and O. The contour lines are drawn at $U = -4^n\ V\ n \in \{-2,-1,1,..,7\}$. The dipole character of the distribution, pointing from top to bottom, is clearly revealed.

[1] A. Weickenmeier, H. Kohl (1991), *Computation of Absorptive Form Factors for High-Energy Electron Diffraction*, Acta Cryst. A47, 590-597

[2] The ABINIT code is a common project of the Universite Catholique de Louvain, Corning Inc., and other contributors.

[3] J. P. Perdew and Y. Wang, Phys. Rev. B **45**, 13244 (1992).

[4] R. Bader, *Atoms in Molecules: A Quantum Theory* (Oxford University Press, New York, 1990)

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