Chemical bonding effects in HRTEM images

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We present HRTEM image simulation taking into account charge redistribution caused by chemical bonding. Conventional image simulation is based on scattering factors that are obtained by relativistic Hartree-Fock calculations and fitted to analytical functions. One example are the scattering factors from Doyle and Turner [1] where the atomic potential is fitted to four Gaussians, so it can easily be documented by listing the eight fitting parameters. The potential of the solid used in the conventional simulation is calculated by adding these isolated atom potentials. Main assumptions by using Doyle and Turner scattering factors for image simulation are:

1. isolated atoms
2. spherically symmetric atom potentials
3. neutral atoms

This model is reasonable for most materials because they have much more core electrons than valence electrons and only the latter are strongly influenced by chemical bonding.

A more accurate way to obtain projected potentials of light element materials for TEM image simulation is to use quantum chemistry methods like density functional theory (DFT). These methods iteratively solve the quantum many body problem of interacting electrons and cores in a solid. For selected oxides the influence of chemical bonding on HRTEM images has been explored by Deng and Marks [2]. Here, we study the influence of chemical bonding effects on HRTEM images in exclusively light element materials like graphene or boron nitride. The future aim is to study defects and adsorbates on graphene.

1. P.A. Doyle and P.S. Turner, Acta Cryst. (1968). A**24**, 390
2. B. Deng and L.D. Marks, Acta Cryst. (2006). A**62**, 208-216

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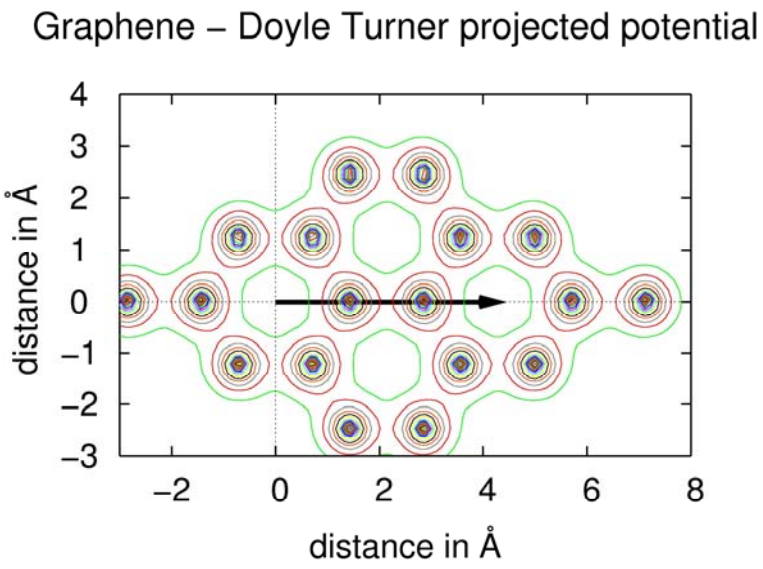

Figure 1. Projected potential of graphene calculated as sum over Doyle Turner potentials of 18 carbon atoms. Arrow indicates direction of the line scans in figure 2.

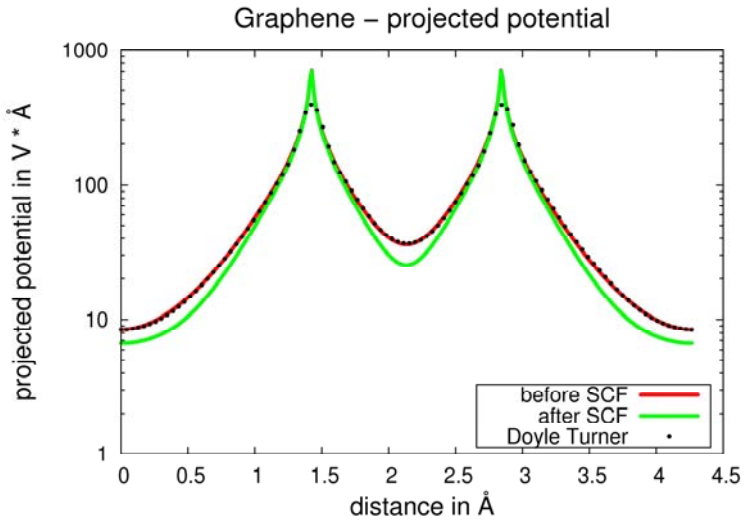

Figure 2. Comparison between the projected potential obtained by DFT and Doyle Turner. The Doyle Turner potential is calculated from the model shown in figure 1. "before SCF" and "after SCF" are from the DFT software. The first one is the starting potential, the second one shows the projected potential after the calculation converged. The direction of the line scans is indicated by the arrow in figure 1.

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