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IT-2-O-1857 Towards a quantitative exit wave function: the influence of phonon scattering

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To provide the utmost quantitative information about the atomic structure of the specimen is the ultimate challenge sought by modern high-resolution transmission electron microscopy. At the specimen exit surface, quantitative structural information is embedded in the object complex wave function, which can be recovered, with atomic resolution, from a focal (or tilt) series of aberration corrected HRTEM images [1]. Nonetheless, the quantitative information that is obtained from the exit wave is often in disagreement with imaging simulations. This disagreement is in effect a contrast mismatch, or Stobbs factor, which accounts for a reduction of the experimental image contrast by a factor of three with respect to the calculations [2]. The scattering of phonons following the electron beam-specimen interaction is amongst the possible causes of the Stobbs factor [3].
In this contribution, we discuss the role of phonon scattering in the quantification of the exit wave function of a single layer of graphene. For this idealized object, the contribution of the thermal phonon scattering to the total elastic scattering can be directly investigated by quantifying the exit wave function at different temperatures. For the imaging simulations, the influence of thermal motion upon modeling of the elastic scattering is studied quantitatively, using both the absorptive potential and frozen phonon approaches, addressing the role of the Debye-Waller factor in predicting the thermal displacement of graphene atoms. Experimentally, the exit wave function is recovered in the linear imaging approximation, in both heating and cooling conditions, as well as at room temperature.
To conclude, we present, and discuss, the comparison between the quantitative exit wave functions, obtained in both calculated and experimental approaches.

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