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Thermal scattering (due to phonon excitation) plays an important role in transmission electron microscopy and convergent-beam electron diffraction patterns. It makes the dominant contribution to Z-contrast (high-angle annular dark field) measurements in scanning transmission electron microscopy. Recent experimental advances have put Z-contrast imaging on an absolute scale [1] and structures can be solved and the atoms in a column counted to an accuracy of ±1 atom [2]. The results in Ref. [2] relied on simulations of thermal scattering using the frozen phonon model. Within this semi-classical model “the electron sees a snapshot of the atom frozen midvibration” [3]. Each electron “sees” a different configuration, and the contributions of different electrons are summed incoherently in the detector plane. Furthermore the frozen phonon model does not contain within its conceptual framework the momentum or energy transfer one would normally associate with inelastic scattering (in this case phonon excitation).

The correct model for thermal scattering is based on many-body quantum mechanics, as expressed by the equations of Yoshioka [3], with phonon excitation treated as a quantum excitation of the crystal during which the incident electron is inelastically scattered. We use an approximation similar to the Born-Oppenheimer-type approximation used in molecular physics for the many body wave function to derive a model for electron diffraction and imaging which can explicitly calculate the elastic component and the many inelastic components of the scattered electron wave. Our model predicts the scattered probability distributions for a single electron, including multiple elastic and inelastic phonon scattering to all orders. This is an advantage over other approaches based on the Yoshioka formalism in which, to allow for tractable calculations, the single inelastic scattering approximation is made.

Our model leads to a scattering intensity which is numerically similar to that calculated using the frozen phonon model and we provide a perspective on why this is the case, albeit that the two models have quite different conceptual underpinnings. Therefore our model underpins the integrity of the recent progress in the use of quantitative Z-contrast imaging to solve structures.

We will present several examples of how (crystalline) structures can be solved using quantitative Z-contrast imaging.


JANA2006 as a unique tool to refine nuclear and/or magnetic structures using ToF data
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Powgen represents a departure from previous designs for a time-of-flight powder diffractometer at a spallation neutron source and may be considered as a third-generation design. The geometric design of the instrument allows for all detected scattered neutrons to be focused onto a single diffraction profile yielding high count rate while preserving good resolution dΔd = 0.0015 at a d = 1 Å. The settings differ in the center wavelength, λcenter of neutron band chosen, each band being of ~1 Å width with Powgen chopper system operating at 60Hz. Full diffraction profiles need to be fitted using a peak shape based on convolution of back-to-back exponentials with a pseudo-Voigt. The use of a cold cryogenic moderator (and to lesser extent supermirror guide) yields significant differences in the d-space dependencies of the exponential rise (α) and decay (β) terms as well as the correction needed for reflection position, compared to the standard dependency functions modeled in GSAS [2]. Therefore, alternate functions for α, β, and...