Thermal diffuse scattering in low energy electron transmission using a time-dependent wave function propagation approach

Rudinsky, S.[1], Sanz, A.S.[2] and Gauvin, R.[1]

[1] McGill University, Canada, [2] Universidad Complutense de Madrid, Spain

Thermal diffuse scattering (TDS) has an important effect on the experimental data that can be acquired from scattering experiments. Simulations must therefore take TDS in to account when reproducing and being compared to such scattering phenomena. In the case of techniques such as X-ray diffraction, the Debye method is often used to account for TDS through modulation of the diffraction peaks [1]. In this case, the Debye-Waller factor modulates the intensity while an absorbing function is applied to convolve the peaks. In electron diffraction, the frozen phonon model coupled with wave function propagation techniques such as multislice are typically used to simulate high energy diffraction patterns [2]. However, such propagation algorithms assume the paraxial approximation in which the beam can be considered to enter the sample at normal incidence and the entirety of the wave function probability density is transmitted at each slice. This results in a 2D projection of the wave function at the exit or any thickness of the specimen. While these assumptions are acceptable at accelerating voltages in the 100 keV range, at lower accelerating voltages, other methods must be devised which incorporate TDS.

Here, the frozen phonon model is incorporated into a time-dependent wave function propagation scheme which solves the Schrodinger equation numerically [3]. An electron probe transmitted through a thin aluminum single crystal at 1keV is simulated in 2D. A Gaussian wave packet is used as the initial wave function of the particle and the split-operator method is used to propagate the wave function through the material [4]. The Einstein model is used to replicate phonon excitation and Monte Carlo integration is taken over 100 realizations at various vibration amplitudes corresponding to varying specimen temperatures. It is shown that modulation of the intensity peaks in the near-field diffraction pattern arises naturally without the requirement of a Debye-Waller factor and that changes in the spatial dispersion of the wave function can be observed over all spatial dimensions. Figure 1 shows the diffraction pattern of a static crystal compared to those obtained with TDS at vibration amplitudes corresponding to 26.7, 241.4, and 670.6 K. The effect of temperature of the material is linked to the amount of incoherence observed in the diffraction pattern by the increase in noise observed between the characteristic peaks and the reduction of their overall intensity. Overall, it is shown that the frozen phonon model at low accelerating voltages can be used to display the effects of TDS without the need of artificial modulations arising from the Debye method.

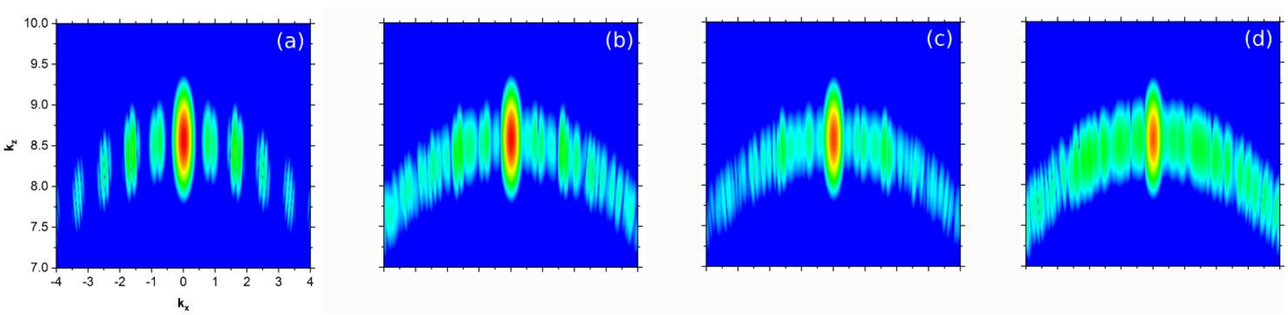

Figure 1: Averaged near-field diffraction patterns of (a) a static lattice and at (b) 26.7, (c) 241.4, and (d) 670.6 K.

REFERENCES

[1] B. Warren, X-ray diffraction, Dover Publications, 1969.

[2] R. F. Loane, P. Xu and J. Silcox, "Thermal vibrations in convergent-beam electron diffraction," *Acta Crystallographica Section A,* vol. 47, pp. 267-278, 1991.

[3] S. Rudinsky, A. Sanz and R. Gauvin, "A novel quantum dynamical approach in electron microscopy combining wave-packet propagation with Bohmian trajectories," *Journal of Chemical Physics,* vol. 146, p. 104702, 2017.

[4] M. Feit, J. Fleck and A. Steiger, "Solution of the Schrödinger equation by a spectral method," *Journal of Computational Physics,* vol. 47, pp. 412-433, 1982.