Simulation of Dynamical Scattering Effect in Electron Diffraction Patterns

Electron diffraction(ED) structure determination has been successfully applied to macromolecular structures since 2013 [1] using standard macromolecular X-ray crystallographic(MX) techniques [2]. ED is an appealing technique because it works with crystals grown to only a few hundreads of nm. Besides, ED patterns may provide higher resolution than cryo-EM data [3]. However, theoretical works [4, 5] suggest that dynamical diffraction effects are too prominent for crystals larger than a few tens of nanometer to use standard MX techniques. In this work, simulations of ED patterns are performed with the multislice algorithm(MS) [6, 7, 8] to explain the discrepancies between theory and experiment. As proof of concept, simulations are performed on small molecules such as biotin.

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