

Diffuse Scattering from Nanoparticles

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Diffuse scattering is often treated as background and is usually removed from empirical fittings. However, structural disorders in the crystalline sample cause diffuse scattering, which transfer elastic scattering from Bragg peaks to Bragg tails. In this work, we aim to correlate structural changes with intensity spectrum through modeling. Debye scattering equation is applied to generate intensity profiles from the structures of nanocrystal generated in classical molecular dynamics simulations. Two types of diffuse scattering, Huang diffuse scattering due to structural disorders and thermal diffuse scattering due to thermal vibration, are then analyzed and compared.