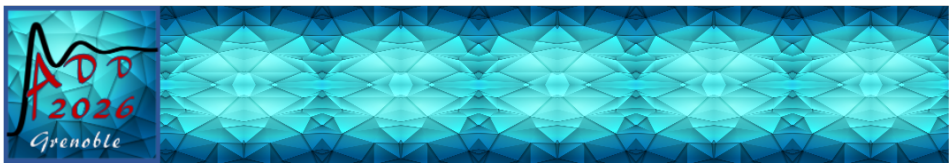

Abstract ID : **28**

Fast Simulation of Disordered Crystals Using Gaussian Copulas

Content

Substitutional disorder is ubiquitous in crystalline materials, from proteins to metal-organic frameworks, yet generating physically realistic disordered structures remains computationally challenging. We present a novel algorithm that employs Gaussian copulas to rapidly generate realizations of disordered crystal structures consistent with experimentally observed diffuse scattering patterns. The method works by first generating correlated Gaussian random variables with a carefully chosen covariance matrix, then applying thresholding to transform these into discrete site occupancies. For binary disorder with equal probabilities, the relationship between Gaussian and binary correlations follows the analytical arcsin law, enabling straightforward implementation. The approach directly utilizes pairwise correlations obtained from 3D-ΔPDF refinement of diffuse scattering data, providing and provides both a generation method for the real structure in real space and a simple check whether correlation matrix from 3D-ΔPDF is admissible.

Our algorithm offers significant computational advantages over traditional Monte Carlo and Reverse Monte Carlo simulations, requiring only the generation of Gaussian random variables and a single FFT operation for periodic systems. We demonstrate the method on experimental diffuse scattering from various crystals. The technique naturally extends to non-equal probability distributions and multi-state disorder through modified thresholding schemes. By bridging mathematical techniques from signal processing and statistical modeling with crystallographic applications, this work provides crystallographers with a practical, efficient tool for modeling disordered materials that is implementable in just a few lines of code.

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