Optimization challenges in fitting stochastic models for atomic positions in nanoparticles

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Given a material, what is the arrangement of atoms inside it? Traditional crystallographic methods base the answer to this question on models for the material with atomic positions arranged in an infinitely periodic lattice. These models are helpful for the study of bulk materials, but do not well-approximate atomic positions in nanoparticles and other materials in which the atomic positions are disordered. Furthermore, the number of atoms, atomic positions and other structural features characteristic of an ensemble of nanoparticles may be best described by a stochastic model. In this talk we discuss stochastic models for nanoparticles. We show how the atomic pair distribution function (i.e., distribution of interatomic distances) is connected to structural features of nanoparticles such as lattice parameters. Finally, we present the optimization challenge associated with finding the most likely set of atomic positions in an ensemble of nanoparticles given measured pair distribution functions, and discuss the use of R in addressing this challenge.

References

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