

Robust recognition and exploratory analysis of crystal structures via Bayesian deep learning

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Due to their ability to recognize complex patterns, neural networks can drive a paradigm shift in the analysis of materials science data. Here, we introduce ARISE, a crystal-structure identification method based on Bayesian deep learning. As a major step forward, ARISE is robust to structural noise and can treat more than 100 crystal structures, a number that can be extended on demand. While being trained on ideal structures only, ARISE correctly characterizes strongly perturbed single- and polycrystalline systems, from both synthetic and experimental resources. The probabilistic nature of the Bayesian-deep-learning model allows to obtain principled uncertainty estimates, which are found to be correlated with crystalline order of metallic nanoparticles in electron-tomography experiments. Applying unsupervised learning to the internal neural-network representations reveals grain boundaries and (unapparent) structural regions sharing easily interpretable geometrical properties. This work enables the hitherto hindered analysis of noisy atomic structural data from computations or experiments.

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