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Crystal structure prediction supported with diffraction data NAOTO TSUJIMOTO, DAIKI ADACHI, Department of Physics, The University of Tokyo, SYNGE TODO, Department of Physics, The University of Tokyo and Institute of Solid State Physics, The University of Tokyo, RYOSUKE AKASHI, Department of Physics, The University of Tokyo, SHINJI TSUNEYUKI, Department of Physics, The University of Tokyo and Institute of Solid State Physics, The University of Tokyo — Atomistic computer simulation is of growing importance in the study of unidentified crystals, although prediction or determination of complicated structure is still a challenging problem due to its many degrees of freedom. Here we propose to utilize experimentally available data of powder diffraction to support and accelerate the structure simulation. In so-called direct-space methods for structure determination from powder diffraction, simplified interatomic potential energy or some other physical constraints are often used in combination with the cost function defined by diffraction data (R.Černý and V. F. Nicolin, Z. Kristallogr. **222**, 105 (2007)). On the other hand, we formulate a cost function called "crystallinity" to support simulation with accurate interatomic potential energy. Since the crystallinity here is defined as the sum of the diffraction intensities only at the peak positions detected in experiments, this method is applicable to low-quality diffraction data such as those obtained at high pressures. We apply this method to well-known polymorphs of SiO_2 with up to 96 atoms in the simulation cell to find that it reproduces the correct structures efficiently with information of a very limited number of diffraction peaks.

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