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ASSESSMENT OF PHASE FIELD CRYSTAL CONCEPTS USING LONG-TIME MOLECULAR DYNAMICS

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Accelerated molecular dynamics is used to compute the one-particle probability density in a complex defect consisting of a Lomer dislocation with an equilibrium distribution of vacancies in the core, and the results are considered within the framework of the Phase Field Crystal (PFC) model. The computed one-particle density shows numerous spatially-localized peaks with integrated densities smaller than unity (less than one atom on average) which correspond to a superposition of just a few specific, well-defined atomic configurations with well-defined energies and energy barriers between them. There is no clear path for reconstructing the actual atomic structures from the one-particle density in the absence of knowledge of the multi-particle correlations. The potential energy computed using the one-particle density differs from the actual atomistic energy by nearly 40eV and is distributed among the partially occupied atomic peaks. These results demonstrate, in one non-trivial case, that the PFC model cannot predict the atomistic defect structures, energies of those structures, nor kinetic barriers between those structures. The PFC model thus appears to be limited in its ability to predict atomic defect properties at the quantitative level needed for application to problems in materials science.