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Glass Transition and Structure in the Phase Field Crystal Model
JOEL BERRY, MARTIN GRANT, McGill University, KEN ELDER, Oakland University — The dynamics of the glass transition and structure of the disordered phase are studied using the Phase Field Crystal (PFC) model in two and three dimensions. It is shown that a kinetically driven glass transition is produced in 3D for sufficiently large cooling rates. Analysis of free energy barriers indicates that the glass phase is more accessible from the liquid than the crystalline phase, but will not be stable for long times unless a critical cooling rate is exceeded. Below the critical cooling rate an equilibrium BCC structure is established. A Vogel-Fulcher type divergence in the density autocorrelation function is produced as the glass transition temperature is approached, signifying fragile glass forming behavior. As well the structure factor of the glass phase shows the characteristic split second peak. Notable differences between results in 2D and 3D will be discussed, as well as results for pure and binary systems.

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