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Limit of validity of Ostwald's rule of stages in a model of solution crystallization[1] LESTER HEDGES, STEPHEN WHITELAM, Molecular Foundry, Lawrence Berkeley National Laboratory — Many systems take "nonclassical" crystallization pathways, forming ordered solids via intermediates that do not share the architecture of the stable material. We possess only rules-of-thumb to explain such dynamics. Chief among them is Ostwald's rule of stages, which states that the phase that first emerges is the one closest in free energy to the parent phase. Although widely applicable, the rule breaks down in many experiments and computer simulations. It is therefore clear that the rule is without firm theoretical foundation, but it is not clear when it should apply. To this end we test Ostwald's rule of stages in a lattice model of solution crystallization. We find that rule holds in certain regions of parameter space and breaks down in others. We argue that its breakdown can be predicted using simple arguments. In addition, we find that crystallization pathways depend qualitatively on both the thermodynamic landscape prescribed by inter-particle interactions and on the relative rates of particle rotations and translations.

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