

Starting is the hardest part: Nucleation dynamics and phase transformations

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In the classical sense, nucleation is a mechanism of phase transformation in which a new phase comes into existence by overcoming a size-dependent free energy barrier that scales as the ratio of the macroscopic interfacial tension cubed to the square of the chemical driving force. In the corresponding atomistic perspective, the assembly of the nascent phase occurs through the addition of individual species (i.e. ion-by-ion), until the particle obtains such a size that the energy penalty due to the creation of a new interface is overcome by the favorable change in free energy associated with the formation of the bulk mineral phase. While such processes remain amongst the most difficult to examine, both experimental and theoretical techniques are making significant strides forward. Although “non-classical” aggregation-based mechanisms of mineral formation are becoming increasingly recognized in prominent geochemical systems, recent work both reinforces and challenges classical models of phase transformation.

This session invites experimental and theoretical contributions which inform on all aspects of mineral nucleation, growth, aggregation transformation, and reactivity at all stages of growth. Particular focus will be centered on understanding mechanistic aspects of new phase formation at various time and length scales, and the influence of impurities (both inorganic and organic), mineral and organic surfaces (topology, interfacial energy, and crystal chemistry), and chemical driving force on the thermodynamics and kinetics of nucleation and phase transformation.