Transient Melting and Freezing Under Thermal Gradient: a Non-Equilibrium Simulation Study

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Transient melting and growth of solids is an ubiquitous phenomenon in Nature, which is becoming increasingly relevant in the processing of nanomaterials and in energy storage applications. Nanoscale transient melting is attracting interest in nanoparticle heating processes driven by high power lasers. The nanoparticles can undergo melting and freezing processes, and when they are embedded in a solid matrix they can induce local melting processes too. Furthermore, when considering multicomponent systems, the intense thermal gradients generated around the particles, 10^{6-8} K/m, can potentially drive strong thermodiffusion responses.

The classical approach to study heat transport with a concomitant phase change relies on the solution of the heat diffusion equation, the so-called Stefan problem, which introduces a number of simplifications: constant density and thermal conductivity in the bulk phases as well as neglecting the molecular structure of the solid/melt interface. However, intense thermal gradients can induce significant changes in these local properties at nanoscale distances, adding additional challenges for the continuum approach to be deployed at the nanoscale. Here, we will discuss non-equilibrium molecular dynamics simulation methods to investigate these transient processes in the presence of large thermal gradients. The simulations can be used to test the accuracy and limitations of the continuum method, as well as a route to quantify the dynamics of the transient process.

References:

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