Phase-field modeling for the morphological evolution of three-dimensional crystals

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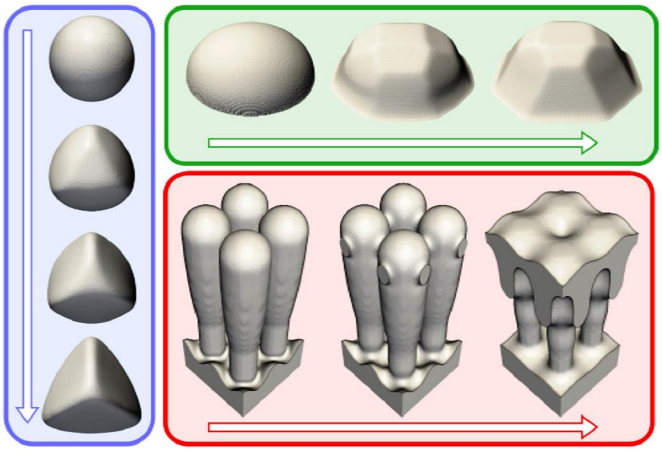
The fine control of the crystal morphologies during growth and processing is nowadays important in order to provide optimized structures for several technological applications. Simulations can be very helpful to predict crystal shapes and to analyze the mechanisms involved in the morphological changes, allowing the experimental activity to be focused on selected conditions. However, managing the evolution of faceted, three-dimensional shapes in a suitable simulation framework is far from trivial.
We present a phase-field (PF) modeling of surface diffusion [1] able to describe the morphological evolution of three-dimensional structures when driven by surface energy minimization. A convenient and general description of the surface-energy anisotropy is introduced, allowing us to manage faceted shapes also in the "strong anisotropy" regime [2]. We show how parameters can be tuned in order to obtain the desired morphologies and several illustrative applications to semiconductor structures are described. Complex time evolutions, even involving topological changes, can be readily tackled in the considered PF framework and a specific example is reported. Moreover, we apply the developed PF method to describe the morphological changes of technology-relevant microstructures during annealing experiments, also predicting a coalescence mechanism occurring for closely spaced crystals. This evolution has been confirmed by dedicated experiments, demonstrating the predicting power of our approach and leading to a promising structure for the high-quality integration of semiconductor heterostructures [3].



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