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Nucleation of crystal surfaces with corner energy regularization

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Abstract: The thermodynamics of strongly anisotropic crystalline surfaces is analogous to that of a binary mixture exhibiting phase separation. On a metastable planar surface, formation of stable orientations requires a nucleation process, in which the energy associated with the presence of corners must be considered. In this context, a nucleation event corresponds to the formation of a critical shape for the crystalline surface before the system enters the growth regime. We first derive the Euler-Lagrange equation for crystal surface nucleation, in two dimensions, and show that the saddle-point condition corresponds to a vanishing chemical potential along this critical surface. We then perform numerical simulation of the equation of motion for the crystal surface and show that, as compared with saddle point nucleation, ridge crossing is dynamically favoured.

Key words: A1. Nucleation; A1. Interfaces; A1. Growth models; A1. Crystal morphology

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I. INTRODUCTION

The problem of determining the equilibrium shape of a crystallite is well understood in the sharp-interface framework, in which the crystal surface is assimilated to a smooth line and atomistic details such as steps and adatoms are not considered. This shape is spherical (or circular in two dimensions) in the absence of anisotropy. If the surface free energy is anisotropic, the shape deviates from a sphere: low-energy directions are preferred and occupy