Equilibrium Shapes of Micro/Nano- Solid Particles on Substrates

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We present a new approach for predicting stable equilibrium shapes of crystalline islands on flat substrates, as commonly occur through solid-state dewetting of thin films. The new theory is a generalization of the widely used Winterbottom construction, i.e., an extension of the Wulff construction for particles on substrates). This approach is equally applicable to cases where the crystal surface energy is isotropic, weakly anisotropic, strongly anisotropic and ``cusped''. We demonstrate that, unlike in the classical Winterbottom approach, multiple equilibrium island shapes may be possible when the surface energy is strongly anisotropic. We analyze these shapes through perturbation analysis, by calculating the first and second variations of the total free energy functional with respect to contact locations and island shape. Based on this analysis, we find the necessary conditions for the equilibria to be stable to two-dimensional perturbations and exploit this through a generalization of the Winterbottom construction to identify all possible stable equilibrium shapes. Finally, we propose a dynamical evolution method based on surface diffusion mass transport to determine whether all of the stable equilibrium shapes are dynamically accessible. Applying this approach, we demonstrate that islands with different initial shapes may evolve into different stationary shapes and show that these dynamically-determined stationary states correspond to the predicted stable equilibrium shapes, as obtained from the generalized Winterbottom construction.

References:

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