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Modeling Patterning of Heteroepitaxial Overlayers from Nano to Micron Scales

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Thin heteroepitaxial overlayers have been proposed as templates to generate stable, self-organized nanostructures at large length scales, with a variety of important technological applications. However, modeling strain-driven self-organization is a formidable challenge due to a large span of length and time scales involved. In this talk, I will present a method for predicting the patterning of ultrathin films on micron length scales with atomic resolution [K.R. Elder *et al.*, Phys. Rev. Lett. **108**, 226102 (2012)]. It is based on the Phase-Field Crystal model, which allows one to reach diffusive time scales for relaxation of the system. We make quantitative predictions for the type of superstructures (stripes, honeycomb, triangular) and length scales of pattern formation of both compressively strained and tensile overlayers on metal-metal systems, including Cu on Ru(0001), Cu on Pd(111), and Ag on Cu(111). Our findings are in excellent agreement with previous experiments and call for future experimental investigations of such systems.