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Harnessing Surface Dislocation Networks for Molecular Self-Assembly¹

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The controlled fabrication of functional wafer-based nano-arrays is one of the ultimate quests in current nanotechnologies. Well-ordered misfit dislocation networks of ultrathin metal films are viable candidates for the growth of two-dimensional ordered cluster arrays in the nanometer regime. Such bottom-up processes can be very complex, involving collective effects from a large number of atoms. Unraveling the fundamental forces that drive these self-assembly processes requires detailed experimental information at the atomic level of large ensembles of hundreds to thousands of atoms. The combination of variable temperature measurements from our home-built STM correlated with 2D Frenkel-Kontorova models based on first-principle interaction parameters is used to explain how uniform arrays can form with the strain in the thin film as the driving force responsible for the surface self-assembly process. This process is generally applicable to assemble many molecular species thus opening avenues towards complex self-assembled structures based on a lock-and-key type approach. Moreover, when increasing the molecular coverage and/or decreasing the strain in the thin film the intermolecular interactions will eventually dominate the elastic effects and dictate the self-assembly process via molecular structure and functionality. We will show that controlling this delicate balance leads to a richness of structures, ranging from disperse ordered arrays of molecular clusters to patterned self-assembled monolayers (SAMs) of functionalized fullerenes and methanethiol.

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