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Pentacene thin films on vicinal Ag(111) surfaces[1] FATIH DANISMAN, Middle East Technical University, ILKER DEMIROGLU, ERSEN METE, SINASI ELLIALTIOGLU — Here we present a structural study of pentacene thin films on different vicinal Ag(111) surfaces by helium atom diffraction measurements and density functional theory (DFT) calculations. Our helium atom diffraction results suggest a step flow growth mechanism evidenced by initial slow specular reflection intensity decay rate as a function of pentacene deposition time. This is in agreement with our previous helium diffraction results on flat Ag(111) surfaces with a small miscut angle. In parallel with the experimental findings, our DFT calculations predict the step edges as the most stable adsorption site on the surface. Isolated pentacene molecules adsorb on the step edges in a tilted configuration with a binding energy of 0.615 eV. In addition a complete monolayer with tilted pentacene on the step edges is found to be more stable than one with all lying flat molecules. Hence our results suggest, in agreement with prvious predictions, that step edges can trap the pentacene molecules and act as nucleation sites for the growth of ordered thin films with a crystal structure similar to that of bulk pentacene.

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