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Pentacene thin films on flat and vicinal Au(111) surfaces M. FATIH DANISMAN, Middle East Technical University, ERSEN METE, Balikesir University, EROL ALBAYRAK, Ahi Evran University — Here we present a structural study of pentacene thin films on flat and vicinal Au(111) surfaces by He atom diffraction measurements and dispersion corrected density functional theory (DFT) calculations. Though experimentally investigated parameter space was limited, no significant difference between the films prepared by different deposition energies was observed. Completion of monolayer coverage was confirmed by simultaneous helium scattering and quartz crystal resonance frequency shift measurements during pentacene film growth on the gold electrode of a quartz resonator. Monolayer films were found to adopt a (6x3) unit cell which was also observed for pentacene monolayers on Ag(1 1 1). However no ordered multilayer film structure could be observed which is in contrast with the previous Ag(1 1 1) studies. DFT calculations were performed with and without dispersion correction. Adsorption site of isolated pentacene molecules, crystal and electronic structure of monolayers and multilayers (up to 4 ML) were studied. The most stable monolayer structure was found to be the (6x3) unit cell in agreement with the experimental findings.

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