

Structure and growth of dotriacontane films on SiO₂ and Ag(111) surfaces: synchrotron X-ray scattering and molecular dynamics simulations

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Abstract

We report synchrotron X-ray scattering experiments and molecular dynamics simulations of the structure and growth mode of dotriacontane (n-C₃₂H₆₆ or C₃₂) films adsorbed on Ag(111) and SiO₂-coated Si(100) substrates. On the SiO₂ surface, the X-ray measurements confirm a structural model of the solid film inferred from high-resolution ellipsometry measurements in which one or two layers of C₃₂ adsorb with the long axis of the molecule oriented parallel to the interface followed by a monolayer in which the molecules have a perpendicular orientation. At higher C₃₂ coverages, preferentially oriented bulk particles nucleate consistent with a Stranski–Krastanov growth mode. On the Ag(111) surface, we again observe one or two layers of the “parallel” film but no evidence of the perpendicular monolayer before nucleation of the preferentially oriented bulk particles. We compare the experimentally observed structures with molecular dynamics simulations of a multilayer film of the homologous C₂₄ molecule.