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Computational diffusion model of reconstructed regions in Ag/Si epitaxial growth JOSEPH DRISCOLL, KELLY ROOS, Bradley University, D. WALL, M. HORN-VON HOEGEN, F.-J. MEYER ZU HERINGDORF, Department of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen, 47057 Duisburg, Germany — The thermal decay of Ag islands, grown epitaxially in a Stranski-Krastanov mode on Si(001) and Si(111) surfaces, has been studied experimentally with photoemission electron microscopy (PEEM). In a range of elevated temperatures the islands decay mainly by dissociation of Ag atoms from island edges, rather than by direct desorption into the gas phase. On the surrounding surface, the Ag atoms are subject to thermally-activated diffusion and desorption. The Ag surface concentration decreases with distance from the island edges. Where the local concentration is above a critical value, coverage-dependent reconstructed overlayers form surrounding the islands. The spread of the overlayers, relative to the position of the decaying island, depends on competition between diffusion and desorption. Previous quasi-static models [1] have shown that the observed reconstructed regions are related to the atomistic parameters describing surface diffusion, and have been applied to extract diffusion coefficients from the experimental data. Here we present results from a dynamic diffusion model that captures many of the qualitative and quantitative time- and temperature-dependent phenomena observed in the experiments.

[1] K.R. Roos et. al. PRL 100, 016103 (2008); D. Wall et. al. NJP 12 (2010) 103001

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