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Early stages of growth and surface alloying of group-14 elements on ruthenium

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As has been recently revealed, group-14 adatoms exhibit distinct growth characteristics on Ru(0001) at submonolayer coverages, despite a similar configuration of valence electrons. More specifically, Pb and Sn atoms tend to agglomerate and form dense islands of the c(2×4) or c(2×8) symmetry, respectively, with local coverage of 1/2 ML already for much lower deposition doses [1-3]. In contrast, Ge atoms preferably self-assemble into the dilute ($\sqrt{21}\times\sqrt{21}$) structure with adatom density of 1/7 ML [4]. To trace the observed differences, we employed ab-initio DFT simulations and followed the early stages of growth of all group-14 elements on Ru(0001) in a systematic manner by examining the potential energy surfaces for successive adsorption of up to several atoms within a large surface unit cell (cf. left figure). This way the effective lateral interactions between adatoms were recognized and their most favorable dimer and trimer configurations were identified, which can be interpreted as initial building blocks of the resultant adsorbate structure. Moreover, the DFT-derived many-body interaction energy terms between adatoms were implemented in large-scale kMC simulations of the nucleation process of various group-14 elements on Ru(0001) to verify their tendency towards self-assembling in an ordered (dense or dilute) overlayer.

In addition, we investigated co-adsorption of immiscible Sn and Pb metals, so as to establish conditions for the existence of their two-dimensional ordered alloys on Ru(0001) reported experimentally [1]. Several models of binary film formation, reflecting the experimental procedure of subsequent deposition of fixed doses of compositionally minor and major elements, were considered. We found the general preference for mixing of Sn and Pb atoms within the first wetting adlayer, and identified the favorable morphology of Sn-Pb surface alloys in terms of their stoichiometry, lateral symmetry, as well as the optimal adatom arrangement within the surface unit cell [5]. In particular, the hexagonal-like ($\sqrt{7}\times\sqrt{7}$) alloy structure with Sn:Pb = 3:1 composition ratio was predicted to occur at nominal Sn and Pb coverages of around 0.40 ML and 0.15 ML, respectively (cf. right figure), in accordance with experiment [1].

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