Mechanistic insights into thermal processes of metal deposits on h-BN/Rh(111): A comparison of Au and Rh

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A hexagonal boron nitride (h-BN) monolayer has a periodically undulating structure on Rh(111) due to the lattice mismatch and the relatively strong interaction with rhodium. The corrugated h-BN "nanomesh" is in turn a good template for metal nanoparticles [1-3]. Here the thermal properties of Au and Rh deposits are compared on hexagonal boron nitride (h-BN) "nanomesh" prepared on Rh(111), applying STM, XPS, low energy ion scattering (LEIS), LEED, and DFT. Besides similarities, notable differences have also been revealed (Fig. 1) [3]. At room temperature, both metals essentially follow Volmer-Weber (3D) growth. Upon subsequent annealing, agglomeration (sintering), intercalation, and desorption are competing surface processes for both metals. For the more reactive Rh, we suggest an additional encapsulation mechanism: between 600 K and 750 K, fragments of decomposed h-BN diffuse locally from the bottom onto the metal clusters covering them partially. STM data indicates that agglomeration of gold nanoparticles proceeds faster compared to rhodium. At higher temperatures (~1050 K–1100 K), all non-desorbing gold atoms diffuse below h-BN, even for large initial coverages. On the other hand, for larger Rh deposits (≥5 ML), the outermost layer always contains Rh. Accumulation of gold at the interface between h-BN and Rh(111) significantly enhances the thermal stability of h-BN, attributed to the lower reactivity of Au in the decomposition of h-BN compared to Rh(111). At elevated substrate temperatures, intercalation of individual adatoms takes place during deposition, which requires higher temperatures for rhodium due to its slower diffusion and higher probability of nucleation.

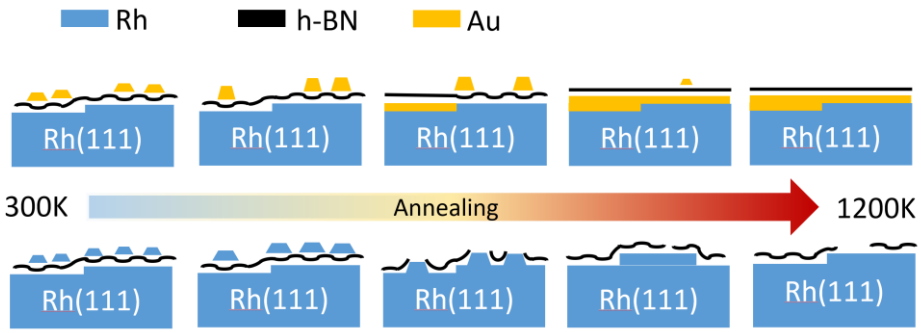

Fig. 1. Thermal processes of Rh and Au deposits on hexagonal boron nitride nanomesh

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