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Room-Temperature Epitaxy of Metal Thin Films on Tungsten Diselenide

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ABSTRACT

The orientation of selected metals (Pd, Ni, Al, and Co) deposited on WSe_2 by physical vapor deposition was examined using transmission electron microscopy and selected area electron diffraction. We discovered that Ni demonstrates room-temperature epitaxy, similarly to other face centered cubic (FCC) metals Au, Ag, and Cu. These epitaxial metals exhibit the following orientation relationship, where M stands for metal: $M(111) \parallel WSe_2(0001)$; $M[2\bar{2}0] \parallel WSe_2\ [11\bar{2}0]$. Hexagonally close-packed Co, and FCC Pd and Al, were not epitaxial on deposition; however, Pd became epitaxial after annealing at 673 K for 5 h. To uncover critical variables for epitaxial growth, we correlated our experimental work and reports from the literature on Cu, Ag, and Au with density functional theory calculations of the energetics of metal atoms on the surface of WSe_2 and thermodynamic calculations of metal-W-Se phase equilibria. Furthermore, we compared the findings to our previous work on metal/MoS_2 systems to draw conclusions more generally applicable to epitaxial growth of metals on transition metal dichalcogenides (TMDs). We observed that epitaxy of metals on TMDs can occur when there is a match in crystallographic symmetry, even with a large lattice mismatch, and it is favored by metals exhibiting a low diffusion barrier on the TMD surface. However, reaction processes between the metal and WSe_2 can prevent epitaxy even when the other factors are favorable, as