Structural Phenomena at the 3D/2D Interface: Epitaxy of Metals on Transition Metal Dichalcogenides

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Of the many emerging 2D materials, transition metal dichalcogenides (TMDs) are interesting for electronic and photonic devices because many of them are semiconducting when only a few layers thick, and they can be transferred onto flexible substrates. Successful application of these materials relies on building a fundamental understanding of the interfaces between TMDs and other materials, such as metals. Although metal/TMD epitaxy has been reported in literature, it has been observed in only a few systems to date. Much remains to be learned about this interesting phenomenon, which could offer new insights into quasi-van der Waals epitaxy for the development of novel heterostructures and for electrical contacts that may be altered or improved through epitaxy.

This work investigates a series of transition metals deposited on TMDs (MoS_2, WSe_2) at room temperature to identify metals exhibiting epitaxy on TMDs and to determine factors controlling this growth. Each metal/TMD system was analyzed by transmission electron microscopy and selected area electron diffraction to identify phases present and their crystallographic orientation. Annealed samples (4 h @ 400 ^{o}C) were also examined to determine if thermal processing induced structural or chemical changes.

On MoS_2, many FCC metals from our work (Ag, Al, and Pd) and literature (Au, Pt, and Pb) - along with an HCP metal (Zn) from our work—were epitaxial with the following relationships: $(111)_{FCC} \parallel (001)_{TMD}$ and $\langle 110 \rangle_{FCC} \parallel \langle 110 \rangle_{TMD}$ or $(0001)_{HCP} \parallel (0001)_{TMD}$ and $\langle 11\bar{2}0 \rangle_{HCP} \parallel \langle 11\bar{2}0 \rangle_{TMD}$. In all cases, the close-packed plane with hexagonal symmetry grows on the basal plane of MoS_2, although lattice mismatches range from 9.4-18.6%. Like all tested BCC metals (Mo and Mn), the FCC Ni and HCP Ru and Re metals were not epitaxial on MoS_2, despite providing similar symmetry and lattice mismatches. We have discovered a strong correlation between activation energy to surface diffusion available from DFT calculations [1] and metal epitaxy on MoS_2. Our work also suggests that additional variables, such as homologous temperature, correlate almost as well.

In expanding the study to include metal/WSe_2 systems, a number of interesting differences were observed. Some metals were epitaxial on WSe_2 but not on MoS_2. Conversely, FCC Pd was epitaxial on MoS_2 after deposition, but it was epitaxial on WSe_2 only after annealing. More modeling of the surface of WSe_2 is needed to better understand these differences. Our ongoing work opens pathways for fundamental studies of Schottky barrier heights and the effect of atomic arrangement at the contact interface on this important parameter.

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Supplementary Information

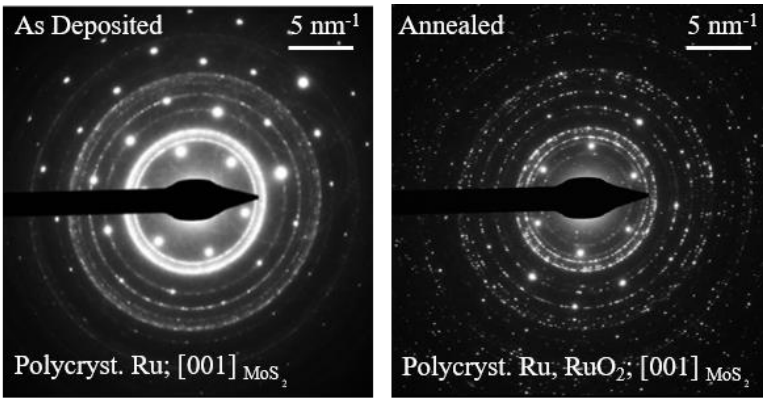

Figure 1 Selected Area Electron Diffraction Ru/MoS_2

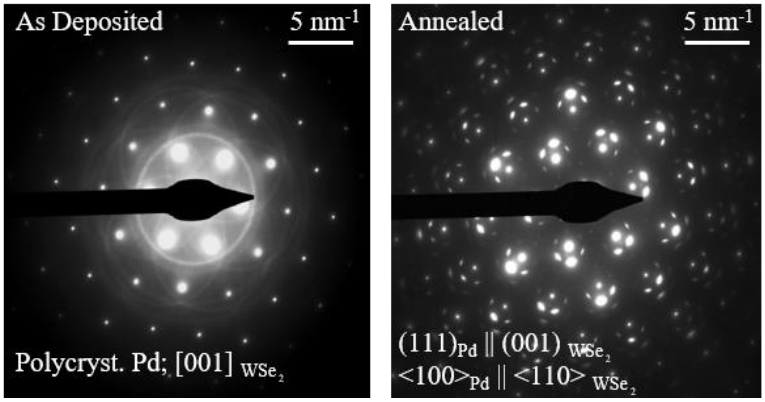

Figure 2 Selected Area Electron Diffraction Pd/WSe_2