TEM-STEM Studies of Gold Nanoparticles in Twisted MoS_2 Bilayers

Robert Sinclair[1], Yi Cui[1], Pawel Czaja[1,2] and Yi Cui[1]
[1]*Department of Materials Science and Engineering, Stanford University, Stanford, CA 94305, United States*
[2]*Institute of Metallurgy and Materials Science, Polish Academy of Sciences, 30-059 Krakow, Poland*

The development of 2D materials such as graphene and metal dichalcogenides has been the subject of much recent research. For possible device applications, their interaction with metal contacts will be critically important. While the epitaxial growth of a pure metal such as FCC gold on hexagonal molybdenum disulfide (MoS_2) is well understood, the intercalation of metals between two 2D layers is not, and this could have interesting consequences. Accordingly we have deposited Au nanoparticles onto thin MoS_2 substrates by electron beam evaporation, applied a second MoS_2 layer with various MoS_2-MoS_2 twist angles, annealed the samples and examined them by TEM and STEM techniques.

We have found, by through-foil transmission electron microcopy (TEM), that annealing epitaxial gold nanoparticles sandwiched between mechanically twisted MoS_2 bilayers results in morphology changes of the gold into nanodiscs and reorientation of the Au-MoS_2 alignment. At low twist angles, the gold re-orients half-way between the orientation of the encapsulating bilayers, while for larger twists, the re-orientation shows a milder sinusoidal variation with increasing twist ("twisted epitaxy") [1]. This behavior is shown to be consistent with density functional theory (DFT) calculations of the interfacial energies. Application of STEM techniques (e.g. 4D-STEM) allows further analysis of the exact atomic arrangements.

These new findings therefore open up several possibilities for further investigation, in terms of both the systems involved and any influence on physical properties. This paper will discuss progress along these lines [2].

[1] Y. Cui et al. *Science* **383** (2024) 212-219
[2] This work was partly supported by Office of Basic Energy Sciences of the U.S. Department of Energy (DOE), Division of Materials Science and Engineering. Pawel Czaja acknowledges receipt of a Fulbright Fellowship. The authors also appreciate the use and support of the Stanford Nano Shared Facilities (SNSF).