Atomistic Studies of Silver Nanorods on β-MoTe$_2$ Substrates

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Noble metals deposited onto transition-metal dichalcogenides (MX$_2$)[1] represent convenient model systems to investigate microscopic features of surface processes like nucleation, growth, diffusion and reactivity. STM is in principle capable of revealing the microscopic details of such processes. Dependent on deposition parameters and on the surface corrugation of the substrate noble metals tend to nucleate either as irregular amorphous grains or as epitaxially grown elongated grains of regular shapes. In the presence of larger disc-like surface defects, where entire X-M-X triple layers were removed, the adatoms also tend to diffuse into the van der Waals (vdW) gaps of the substrate. In such cases, the electronic structure of the topmost chalcogen layer above an intercalated region is greatly modified with regard to that of the bare substrate and often reveals in STM images an enhanced contrast, which can even reveal intercalated superstructures[2,3].

Silver, thermally deposited onto β-MoTe$_2$, first tends to form elongated tapes along the substrate [010] direction[4], followed by the formation of epitaxially grown nanorods, very similar in their appearance to those formed by gold[5]. The particles are regularly only a few atomic layers high and show incomplete topmost adlayers (Fig.1). According to the established epitaxial relationship between the deposit and the substrate[6], i.e. (112)[1-10]Ag || (001)[010]β-MoTe$_2$, the misfit between the (112) silver and the (001) β-MoTe$_2$ contact planes is determined by their corresponding surface ridges and groves, i.e. 3 x d_{111} (0.7077 nm) and d_{011} (0.2889 nm) of silver are locked-in to d_{100} (0.6330 nm) and d_{010} (0.3469 nm) of β-MoTe$_2$, respectively. STM images with atomic resolution, like the one shown in Fig.2, reveal details of the substrate and the silver nanorods.

It is shown that the interfaces between the nanorods and the β-MoTe$_2$ substrate are locked-in by adjusting the interatomic distances in the deposit to those of the substrate. Thus, a tensile stress along the [0-11] direction and a corresponding compressive stress along the perpendicular [1-1-1] direction of the silver nanorod are performed. The terminating atoms at the surfaces and edges of the nanoparticles are displaced from their expected bulk positions. Incomplete silver adlayers are bent by a tensile strain, while the first subsurface layers experience a compressive strain, often accompanied by a surface reconstruction in regions close to the incomplete adlayers. The observations are in agreement with recent calculations[7], where a stress and strain variation in the two topmost layers of a reconstructed (111) gold surface was predicted.

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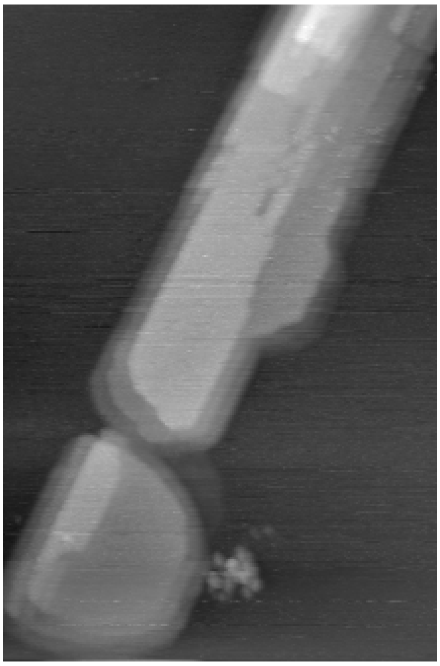

Fig.1: STM of a silver nanorod on β-MoTe$_2$ with steps between adjacent layers [150 nm x 100 nm, CCM, U_g = 0.1 V, I_t = 1 nA, t = 600 μs, W tip].

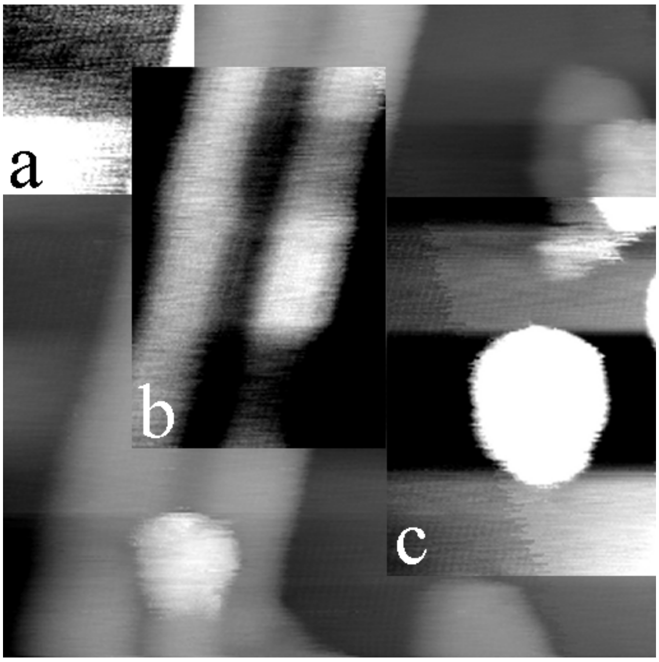

Fig.2: STM image with atomic resolution of the β-MoTe$_2$ substrate (a), a silver nanorod (b) and a round-shaped silver grain above the edge of an intercalated region (c) [50 nm x 50 nm, CCM, U_g = 10 mV, I_t = -1 nA, t = 500 μs, W tip].