Functionalized graphene as a system for hydrogen storage

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Hydrogen is well known as a possible clean fuel for the future since the only waste product is water. Nevertheless, one of the main problems dealing with hydrogen as a widespread energy carrier is its storage. In this respect, graphene has recently attracted attention as a promising medium due to its small weight, chemical stability, and attractive physico-chemical properties for hydrogen adsorption. The hydrogen storage capacity of graphene can be further increased by chemical functionalization of the surface with different types of metals. One of the most promising materials for this purpose is titanium. Calculations show that each adsorbed titanium atom can bind up to $4 \sim 5$ H_2 molecules, with related gravimetric density of 7.8 wt% [1]. In this work, we investigated the deposition of titanium on graphene and its potential for hydrogen storage.

For this study we used epitaxial monolayer graphene grown on SiC(0001). Different quantities of titanium were deposited on this surface. The characteristics of the growth process and the amount of coverage were determined by scanning tunneling microscopy (STM) in ultra high vacuum (UHV). As shown in Fig. 1a, the titanium atoms form small islands (diameter $\sim$ 10 nm) with a size distribution given in the inset. The Ti-covered graphene was exposed to molecular hydrogen (5 min at 1×10^{-7} mbar deuterium). The sample temperature was then increased up to 550 ºC with a constant heating rate of 10 K/s while measuring the mass-sensitive desorption. The desorption spectra are shown in Fig. 1b. Two desorption peaks at 210 ºC and 290 ºC are clearly visible. Their intensity increases with increasing Ti coverage [2]. We verified that without Ti there was no desorption detectable. Our data demonstrate suitability of functionalized graphene for hydrogen storage applications, since the binding is stable at room temperature and desorption occurs at moderate temperatures.

To decrease the size of the Ti-islands and increase their density and therefore the active surface for hydrogen adsorption, we will show first promising results of reducing the mobility of the titanium by defects induced in the graphene layer by ion bombardment.
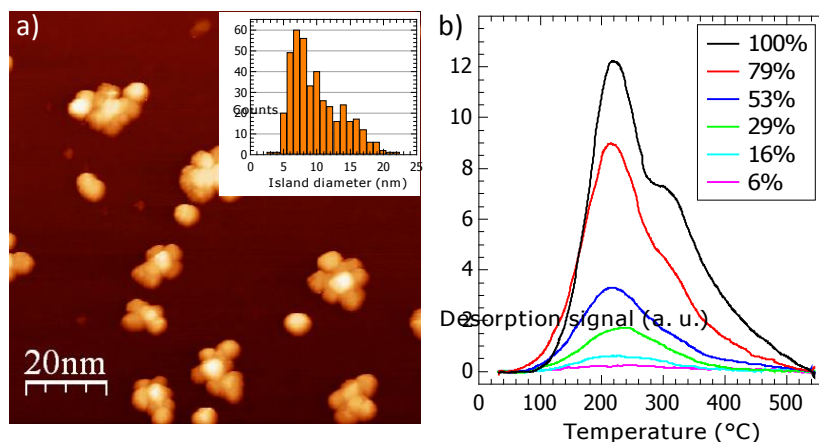

Fig. 1:a) 100 x 100 nm² UHV-STM image of a graphene surface with a titanium coverage of 16% (V = 2 V, I = 280 pA). The titanium atoms form small islands with a size distribution as shown in the inset. b) Desorption spectra measured for different coverages of titanium. The amount of stored hydrogen increases with Ti-coverage.

[1]   E. Durgun *et al.*, Phys. Rev. B **77**, 085405 (2008).
[2]   T. Mashoff *et al.*, Appl. Phys. Lett. **103**, 013903 (2013).