FUNCTIONALIZATION OF TUNGSTEN DISULFIDE NANOPARTICLES BY PLASMA AND ION BOMBARDEMENT

Alex Laikhtman

Physics Department and the Faculty of Sciences, Holon Institute of Technology (HIT), Holon, Israel
alexl@ht.ac.il

Inorganic nanotubes and inorganic fullerene-like nanoparticles of WS_2 are exploited as porous media for hydrogen storage. A new approach of using hydrogen activated by radiofrequency plasma dramatically increased the efficiency of its absorption on the nanoparticles surface as compared to hydrogenation by high pressure molecular unactivated hydrogen. The chemical configuration of the absorbed hydrogen is of primary importance as it affects its absorption stability and possibility of release. For this purpose, we applied both the experimental analysis methods by using various spectroscopy and microscopy techniques and the theoretical model. In all plasma-hydrogenated samples of WS_2 nanoparticles molecular form of the absorbed hydrogen (H_2) was clearly identified: in the frame of this study we did not find any experimental evidence for intercalation of atomic hydrogen. In addition, it was shown that hydrogen is generally stable under high vacuum conditions at room temperature, which implies its stability at the ambient atmosphere. A model based on the density functional theory (DFT) was developed to simulate the absorption of hydrogen in the WS_2 nanoparticles. The DFT model considers various absorption sites and defines the preferential locations of the absorbed hydrogen in several WS_2 structures. It demonstrates good concordance between theory and experiment and providing tools for optimization of hydrogen exposure conditions and the type of substrate materials.

Another possible application of WS_2 nanoparticles is based on the fact that they conserve their semiconductor and diamagnetic behavior of bulk WS_2 material. Implantation of metal atoms like Ga, Nb, Cl, Re, etc. into the crystal structure of these nanoparticles can change their electronic (semiconductor to metal transfer), magnetic (diamagnetic to paramagnetic transfer), and optical properties, surface characteristics, and chemical behavior. These parameters are of extreme interest during the last few decades as could be useful in many nanotechnology applications, like photovoltaics and optoelectronics, catalysts and sensors preparation, and even tribology and lubrication. For example, doping of WS_2 fullerene-like nanoparticles with Re atoms resulted in their improved lubrication properties due to increase in electrical conductivity which led to electrostatic mutual repulsion. Focused ion beam (FIB) etching was previously used for ion implantation into different materials with the objective to apply this technology as an alternative method for fabricating semiconductor devices. FIB-induced implantation of Ga to WS_2 NP may considerably affect their electronic and electrical properties.