Implantation of Gallium into Layered WS_2 Nanostructures is Facilitated by Hydrogenation

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Implantation of atoms into solid materials provides a way to modify their properties. Doping of layered MoS_2 and WS_2 nanoparticles with alkali metal atoms, Re, Nb, and possibly other elements is a promising technique to change the electronic (semiconductor to metal), magnetic (diamagnetic to paramagnetic), and optical properties, the surface characteristics, and the mechanical and chemical behavior of these materials. The modified materials could be used in nanotechnology applications, catalysts, and sensors, as well as in tribology and lubrication. However, the implantation processes often have a damaging effect on the materials structure. In this contribution, experimental results and theoretical simulations for the implantation of Ga into WS_2 nanoparticles exposed to focused Ga^+ ion beams (FIB) with various doses are reported [1]. The higher ion doses produce a drastic change of the morphology and the near-surface structure of the bombarded region, and some Ga is retained in the material, whilst in case of lower ion doses the damage is found to be small, and only minor implantation of Ga is detected. Nonetheless, in a second set of FIB experiments, the WS_2 nanoparticles had been previously hydrogenated by their exposure to a radiofrequency (RF) hydrogen plasma [2]. In that case, substantial Ga implantation occurs without destructive effects on the WS_2 nanostructures. We decided to apply this hydrogen plasma pretreatment based on the previously observed effect of interlayer expansion in the WS_2 nanoparticles due to hydrogenation [1], which was confirmed and explained by density functional theory (DFT) calculations [2, 3]. Herein, Density Functional Theory (DFT) – and beyond – calculations relevant to the implantation process have been exhaustively performed to complement the FIB experiments. This large battery of first-principles atomistic simulations successfully explains the decisive effect of hydrogenation in facilitating Ga implantation.

References

[1] J. I. Martínez, et al., Small, DOI: 10.1002/smll.202312235 (2024; in press).
[2] A. Laikhtman, et al., J. Phys. Chem. C 121 (2017) 11747.
[3] J. I. Martínez, et al., Phys. Chem. Chem. Phys. 20 (2018) 12061.

Figures

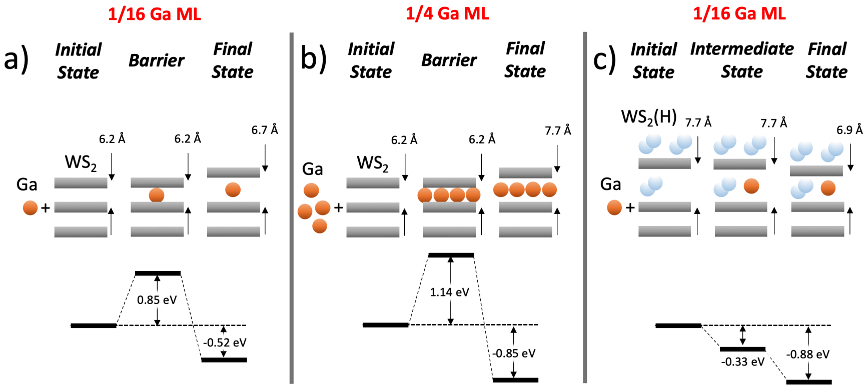

Figure 1: Schematic view of the process of implantation of Ga between layers L1 and L2 of pristine WS_2. (a) and (b) concentration of implanted Ga atoms of 1/16 and 1/4 ML, respectively. (c) implantation of 1/16 ML of Ga in hydrogenated WS_2.