Advanced Electron Microscopy Study of Gadolinium based compounds encapsulated within WS_2 Nanotubes

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Abstract The hollow interiors of nanotubes could host the growth or filling of foreign elements or compounds to obtain hetero-structures. The growth of these materials in the confined one dimensional space lead to novel properties. Capillary filling serves as a method to enable filling of carbon nanotubes and inorganic nanotubes including those of BN and WS_2.[1, 2] In this work, considering the biocompatibility of WS_2 and paramagnetic property of gadolinium (III) compounds, capillary filling is employed to obtain $GdX_3@WS_2$ nanotubes (X=Cl, Br, I). Gadolinium based compounds find important applications in medical imaging and diagnosis. Thus the precise determination of the structure and composition is detrimental in its further application. In the present case the morphology, structure and chemical composition of the synthesized GdI_3 filled WS_2 NTs is investigated using aberration corrected scanning/transmission electron microscopy and associated spectroscopic techniques (Electron Energy Loss Spectroscopy (EELS) and Energy Dispersive X-Ray Analysis (EDS)). The three-dimensional morphology is investigated using Scanning Transmission Electron Microscopy (STEM) tomography but obtaining three dimensional compositional information is non-trivial due to the presence of multiple high atomic number elements. Therefore, EDS-STEM tomography[3] is employed to map the chemical composition in three dimensions. In order to reduce the beam induced effects on the specimen, tomography experiments were carried out at 80 kV in the present case. In view of the long duration of electron beam exposure necessary to perform EDS-STEM tomography, electron irradiation studies are carried out to optimize the EDS-STEM tomography conditions. The experimental observations are adequately supported by carrying out Molecular Dynamics Simulation in order to elucidate the difference in behavior of the various halides (GdI_3 vs $GdCl_3$ vs $GdBr_3$) towards their affinity to fill the interior of the WS_2 Nanotubes.[4]

References

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Figure

a) Volume rendering of EDS-STEM tomograms of $GdI_3@WS_2$ nanotube. b) Vertical orthoslice of the nanotube. c) and d) Orthoslices along the nanotube cross section. Greyscale images represent HAADF. The elements are color coded as blue for W, yellow for Gd, green for S and red for I.