Experimental and Computational Study on the Mechanism of Hydrogen on $MoSe_2$ Growth and Etching in CVD

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Molybdenum diselenides have great attractive to electronic, photoelectric devices for its outstanding electric properties. It is necessary to provide large-scale and high crystalline monolayer $MoSe_2$. Typical synthesis for high quality TMDC is CVD. In CVD, the hydrogen helps growth of MoSe2 by reduction of MoO_3 precursor, but also it etches grown-$MoSe_2$ domain.

Here, we have investigated that the existence of MoO_x prevents $MoSe_2$ monolayer to be desorbed by hydrogen etching. Pure $MoSe_2$ monolayer and $MoSe_2$ monolayer with oxide seeds ($MoSe_2$+Ox) are treated under H_2 condition. It is obtained using SEM and AFM analysis that the shape of pure $MoSe_2$ are changed but $MoSe_2$+Ox are not changed much after H_2 treatment. As we have computationally calculated, H prefers to adsorb to MoO_x than atoms in $MoSe_2$ layer, so that MoO_x hinders etching of $MoSe_2$. It also demonstrates that hydrogen supports the growth of $MoSe_2$ by reducing precursor rather than etching nuclei in nucleation steps. Our research offer insight into the $MoSe_2$ growth mechanism and pave a way to synthesize high quality $MoSe_2$ for electronic devices.