In-situ observation of symmetrical phase transition in $MoSe_2$ on graphene substrate

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Recently, tuning the electronic properties of atomically thin semi-conducting materials has become one of the exciting challenges. The modification of atomic structures by introducing ordered atomic defects has been demonstrated as a powerful strategy to control their band structures [1]. Inversion domain boundary (IDB) in transition metal selenides, such as $MoSe_2$, is one of the interesting ordered defect structures, which locally introduces 1D metallic channels in 2D atomic layers [2]. Understanding the mechanism of formation, elimination and migration of IDBs will be thus a key to control the electronic property of 2D layers.

In this work, we studied the formation and behavior of defect structures in $MoSe_2$ by *in-situ* aberration corrected transmission electron microscopy (AC-TEM) which enables simultaneous visualization and modification of atomic structure in 2D layers by electron irradiation. $MoSe_2$ monolayer grown on a CVD graphene was used in order to study the dynamics of $MoSe_2$ on the vdW substrate. First, the IDBs are successfully formed in a free-standing $MoSe_2$ monolayer (Figure 1) as previously observed in the literatures [3]. However the IDB formation was not observed in $MoSe_2$ supported on graphene but only the vacancy line (VL) defects are formed under the same condition (Figure 2) [4]. Although both the IDBs and VLs are Se deficient line defects, the formation of IDBs requires local symmetrical phase transition 2H to 2H'. The energy we supplied by the electron irradiation was not sufficient to promote a symmetrical phase transition in $MoSe_2$ layers on graphene substrate. We performed the *in situ* AC-TEM experiments at 400°C and 600°C using a dedicated heating sample holder to trigger the symmetrical phase transition. In this presentation, we demonstrate direct observation of formation, migration and elimination of IDBs in $MoSe_2$ occurring on graphene surface at different conditions and their mechanisms will be discussed.

References

[1] Lin et al., 2D Materials, 3 (2016) 022002
[2] Barja et al., Nat.,Phys., 12 (2016) 751
[3] Lehtinen et al., ACS Nano,3(2015)3274
[4] C. Alvarez, H. Okuno et al., submitted.

Figures

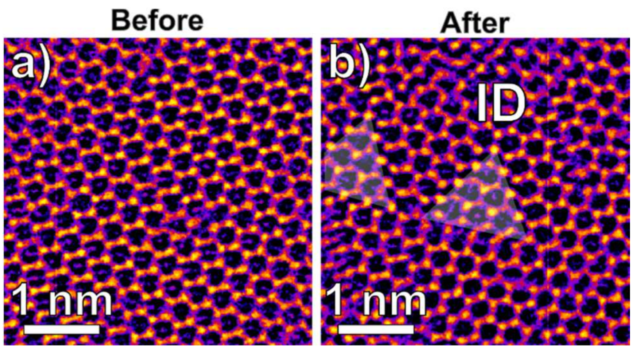

Figure 1: Inversion domain (ID) in free-standing $MoSe_2$ monolayer created after electron irradiation, following a local symmetrical phase transition.

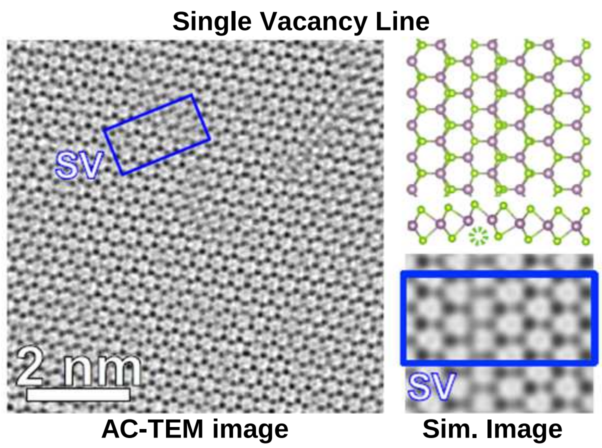

Figure 2: AC-TEM image with DFT model of single vacancy lines created in $MoSe_2$ monolayer on graphene substrate after the electron irradiation under the same condition as in Figure 1, whereas the vdW stacking of 2 monolayers was transferred together.