Atomic defects and doping of monolayer NbSe2

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Abstract

We have investigated the structure of atomic defects within monolayer $NbSe_2$ encapsulated in graphene [1] by combining atomic-resolution transmission electron microscope (TEM) imaging, density functional theory (DFT) calculations and strain mapping using geometric phase analysis (GPA). We demonstrate the presence of stable Nb and Se monovacancies in monolayer material and reveal that Se monovacancies are the most frequently observed defect, consistent with DFT calculations of their formation energy. We reveal that adventitious impurities of C, N and O can substitute into the $NbSe_2$ lattice stabilizing Se divacancies. We further observe evidence of Pt substitution into both Se and Nb vacancy sites. This new knowledge of the character and relative frequency of different atomic defects provides the potential to better understand and control the unusual electronic and magnetic properties of this exciting two-dimensional material.

References

[1] Cao, Y.; Mishchenko, A.; Yu, G. L.; Khestanova, E.; Rooney, A. P.; Prestat, E.; Kretinin, A. V.; Blake, P.; Shalom, M. B.; Woods, C.; Chapman, J.; Balakrishnan, G.; Grigorieva, I. V.; Novoselov, K. S.; Piot, B. A.; Potemski, M.; Watanabe, K.; Taniguchi, T.; Haigh, S. J.; Geim, A. K.; Gorbachev, R. V. Nano Lett., 2015, 15 (8), pp 4914–4921.

Figures

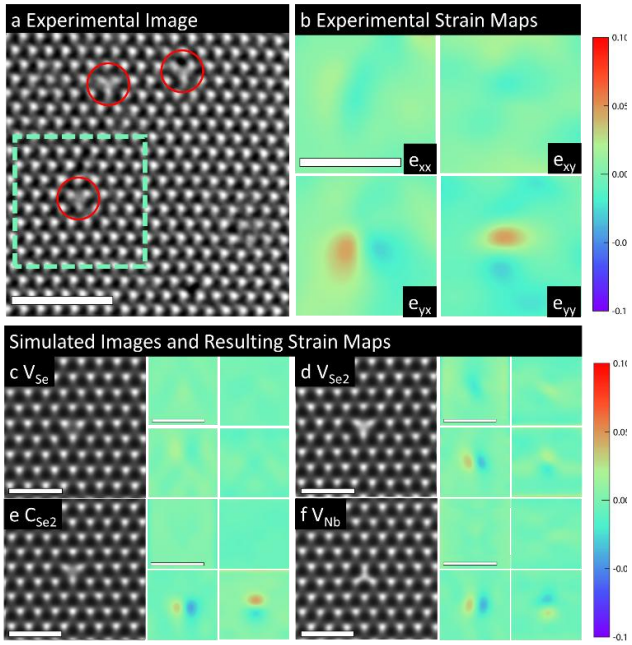

Figure 1: GPA of high-resolution TEM images of point defects are compared to image simulations of DFT-relaxed models for identification (Scale 2nm)

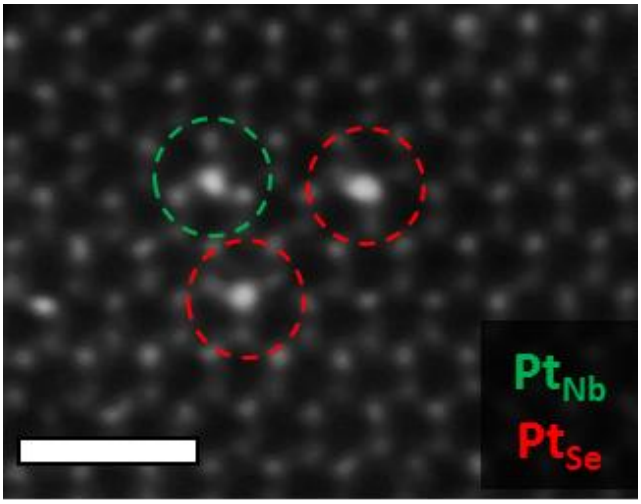

Figure 2: Scanning TEM High-angle annular dark field (HAADF) imaging of Pt substitutions into Atomic sites of $NbSe_2$. (Scale 1nm)