Detailed Atomic Reconstruction of Extended Line Defects in Monolayer MoS_2

Hwanyeol Park
Sungwoo Lee[1], Shanshan Wang[2], Euijoon Yoon[1], Jamie H. Warner[2], and Gun-Do Lee[1],*

[1]Department of Materials Science and Engineering, Seoul National University, 151-742 Seoul, South Korea
[2]Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

**E-mail: gdlee@snu.ac.kr*

Abstract

We study the detailed bond reconstructions that occur in S vacancies within monolayer MoS_2 using a combination of aberration-corrected transmission electron microscopy, density functional theory(DFT), and multislice image simulations. Removal of a single S atom causes little perturbation to the surrounding MoS_2 lattice, whereas the loss of two S atoms from the same atomic column causes a measurable local contraction. Aggregation of S vacancies into linear line defects along the zigzag direction results in larger lattice compression that is more pronounced as the length of the line defect increases. For the case of two rows of S line vacancies, we find two different types of S atom reconstructions with different amounts of lattice compression. Increasing the width of line defects leads to nanoscale regions of reconstructed MoS_2 that are shown by DFT to behave as metallic channels. These results provide important insights into how defect structures could be used for creating metallic tracks within semiconducting monolayer MoS_2 films for future applications in electronics and optoelectronics.

References

[1] Shanshan Wang, Gun-Do Lee, Sungwoo Lee, Euijoon Yoon, and Jamie H. Warner. Detailed Atomic Reconstruction of Extended Line Defects in Monolayer MoS_2. ACS Nano 2016, 10(5), 5419-5430.

Figures

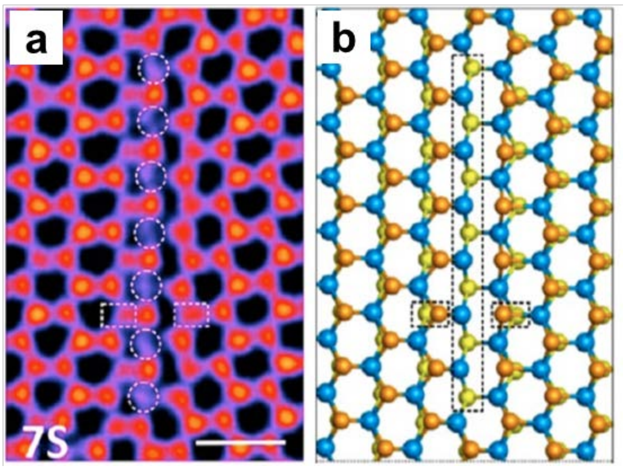

Figure 1: (a) AC-TEM image showing one sulfur vacancies line (1SVL) having numbers of 7 single S vacancies aligning in the same line and (b) DFT-calculated atomic model based on (a).

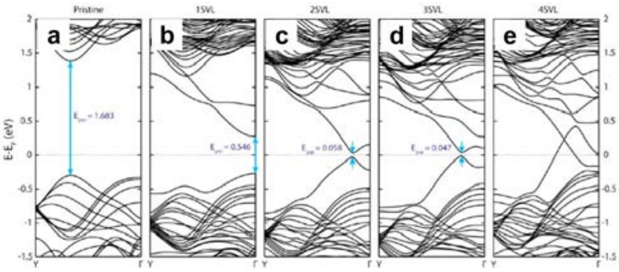

Figure 2: (a-e) DFT-calculated band structures of pristine, 1SVL, 2SVL, 3SVL, and 4SVL, indicating a gradual band gap decrease as the line defect broadens with the electronic property alteration from semiconductor to metal.