Detailed Atomic Reconstruction of Extended Line Defects in Monolayer MoS$_2$

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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