Electron-irradiation induced sulphur displacement cross section in MoS_2

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Atomic-resolution imaging of 2D materials allows investigating electron-irradiation effects with unprecedented accuracy, as has been demonstrated for graphene [1,2] and MoS_2 [3]. While the measured displacement cross section in graphene can be explained by a knock-on process caused by elastic scattering of electrons from carbon nuclei of the material at its ground state, the situation with semi-conducting MoS_2 is more complicated. Specifically, Kretschmer et al. [3] showed that there is a peak in the displacement cross section at energies close to 30 keV, which the authors explained to arise from an excited state knock-on event whose probability increases with decreasing electron energy. They also predicted that at energies above 80 keV the cross section should again increase due to displacements from the ground state. However, experimental data at the higher energy range is still lacking. Very recently, Yoshimura et al. established a more elaborate theoretical model [4] based on quantum electrodynamics to calculate from first principles the probabilities of excitations and displacement events related to them. However, their results only agree with the experimental data of Kretschmer et al. if single and double excitations do not contribute to observed displacements, but only higher ones. Overall, it is clear that more experimental data is needed to be able to properly test these theoretical models. Here, we combine aberration-corrected scanning transmission electron microscopy and computational assisted image analysis to extend the experimental data set for MoS_2 between 55 and 90 keV. Several hundred image sequences were recorded to provide statistically significant data. Examples of the first two frames from one recorded image sequence are shown in Figure 1, where a sulphur vacancy (red circle) was created in the second frame. Our results hint at another peak at electron energies close to 70 keV, and a significant increase at higher energies.

References

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Figures