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Atomic Resolution Investigation of Ultra-Low Energy Ion-Implanted Monolayer TMDs Using Scanning Transmission Electron Microscopy

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The modification of monolayer-thick transition metal dichalcogenides (TMDs) on the atomic scale is a crucial step towards the development of photonic devices with new functionalities [1]. Monolayer TMDs can be easily incorporated into electrically driven devices, which in turn can be coupled to optical microcavities or photonic circuits [2]. Ultra-low energy ion implantation [3] allows for highly pure, clean and selective substitutional incorporation of dopants [4] and is compatible with standard semiconductor processing. Additionally, post-growth doping of TMDs offers an expanded selection of possible dopants compared to the popular method of doping via CVD growth [5].

Here, we present results of ultra-low energy (10-25 eV) ion implantation of monolayer TMDs, modified using the ADONIS mass-selected ion beam deposition system at the University of Göttingen [6]. Transition metal (Cr) and chalcogen (S, Se) dopants are introduced into the MoS_2 and $MoSe_2$ crystal lattice. Atomic resolution high angle annular dark field (HAADF) scanning transmission electron microscopy (STEM), together with core-loss electron energy loss spectroscopy (EELS) analysis, is used to identify the sites of individual dopants in the host lattice and examine the atomic structure of the defects and dopants in the monolayers. Low loss EELS is used in conjunction with low temperature photoluminescence to study excitonic behaviour at the implantation sites.

Analysis of experimental HAADF STEM data is carried out using the TEMUL Toolkit Python library [7], based on Atomap [8], to determine the percentage of ions that cause substitutional implantation, create adatoms, and create vacancies. We introduce the Model Refiner class from the TEMUL Toolkit Python package, which automatically identifies and fully characterises each atomic site in the experimental HAADF STEM image. We report that accurate atom statistics can be obtained from non-ideal STEM imaging conditions through post-processing and avoidance of contaminated areas when extracting atom sites.

This work constitutes a proof-of-principle study concerning the possibility and procedure of incorporating non-classical single photon emitting diodes into monolayer TMDs [9]. The development of such devices has far-reaching implications for quantum science and technology, with applications in the fields of quantum cryptography and quantum metrology [10, 11].

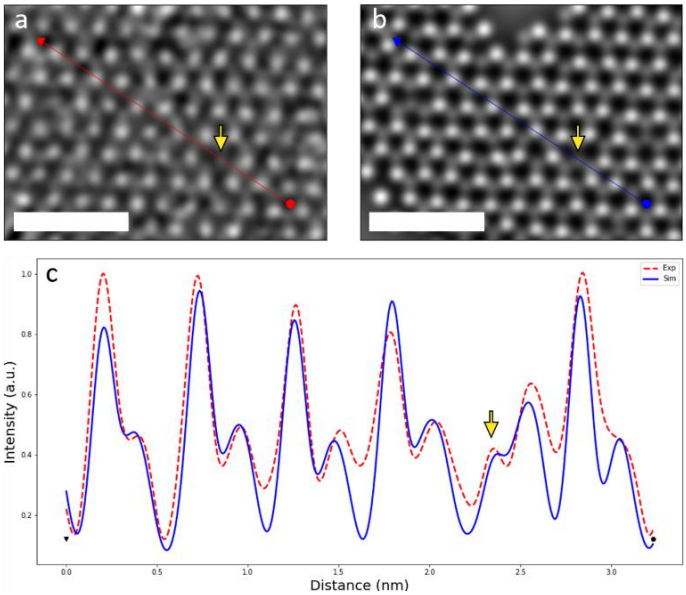

Figure 1. Intensity profile comparison between a) the double Gaussian filtered experimental image of Cr-implanted MoS2 and b) the simulated image of the same region. The average intensity was calculated across ten pixels perpendicular to each point on the red and blue lines in a) and b). The intensity profiles are plotted in c). The atom site highlighted by the yellow arrows is a transition metal site with lower intensity (~0.40) than its nearest neighbours in the transition metal sublattice and is potentially the site of substitutional implantation of a chromium atom into a molybdenum site. This site has been modelled as a single chromium atom in the simulation. The line profile comparison was created using a function from the TEMUL Toolkit. Scale bars in a) and b) are 1 nm.

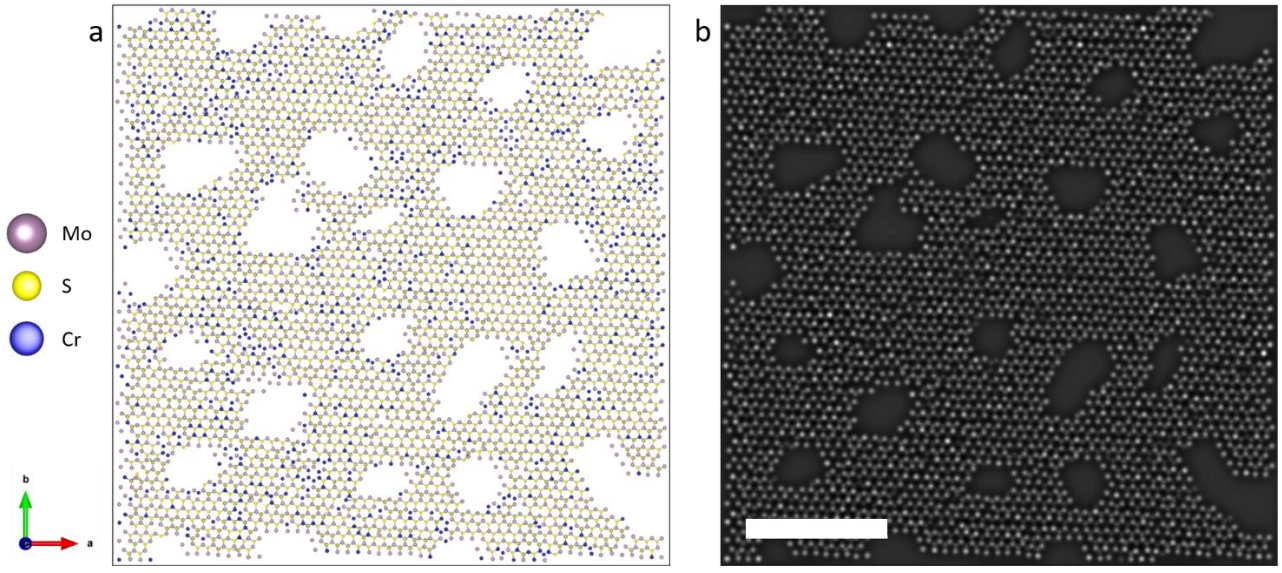

Figure 2. a) Refined atomic model of an entire HAADF STEM image of Cr-implanted MoS2. The model was created using the Model Refiner class from the TEMUL Toolkit and visualised using VESTA. b) Simulated HAADF STEM image created using the model. Scale bar is 4 nm.

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