Understanding atom-by-atom the dynamics and the properties fo the evolution of point and extended defects in single-layer 2H-MoTe2 by Cc/Cs-corrected 40 kV high-resolution TEM

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To understand the dynamics of structural transformations on the level of a single atom, a new type of transmission electron microscope operating at electron energies between 80 keV and 20 keV has been developed which allows to undercut the knock-on damage thresholds even of low-Z-number materials, to increase the contrast and to compensate for the reduced resolution at lower electron energies by a new spherical and chromatic aberration corrector for the objective lens. Sub-Angstroem resolution is achieved down to 40 keV in a wide field of view of 4000x4000 pixels [1, 2], making the tool predestined for in-situ studies of the dynamics in low-dimensional materials at the atomic level. In this contribution we apply our newly developed Cc/Cs-corrected SALVE (Sub-Angstrom Low-Voltage Electron microscopy)[1-3] instrument to study the evolution and dynamics of the growth of extended defects in single-layer 2H-$MoTe_2$ at 40kV accelerating voltage. Due to the unprecedented resolution of our microscope at 40kV together with first-principles calculations, we reveal atom-by-atom the dynamics of one-dimensional and two-dimensional defect structures. We show that the formation process of one-dimensional defect structures originate from single point defects and the two-dimensional defects arise from double vacancies with two missing tellurium atoms in-column.

Moreover, we report about the atom-by-atom transformation of an area in single-layer $MoTe_2$ from the semiconducting 2H to the distorted and metallic 1T' phase, starting with a single vacancy line of missing Te atoms like it is shown in figure 1. We find that the size of the transformed area is defined by the length of the single vacancy line and we can explain the driving force for the transformations.

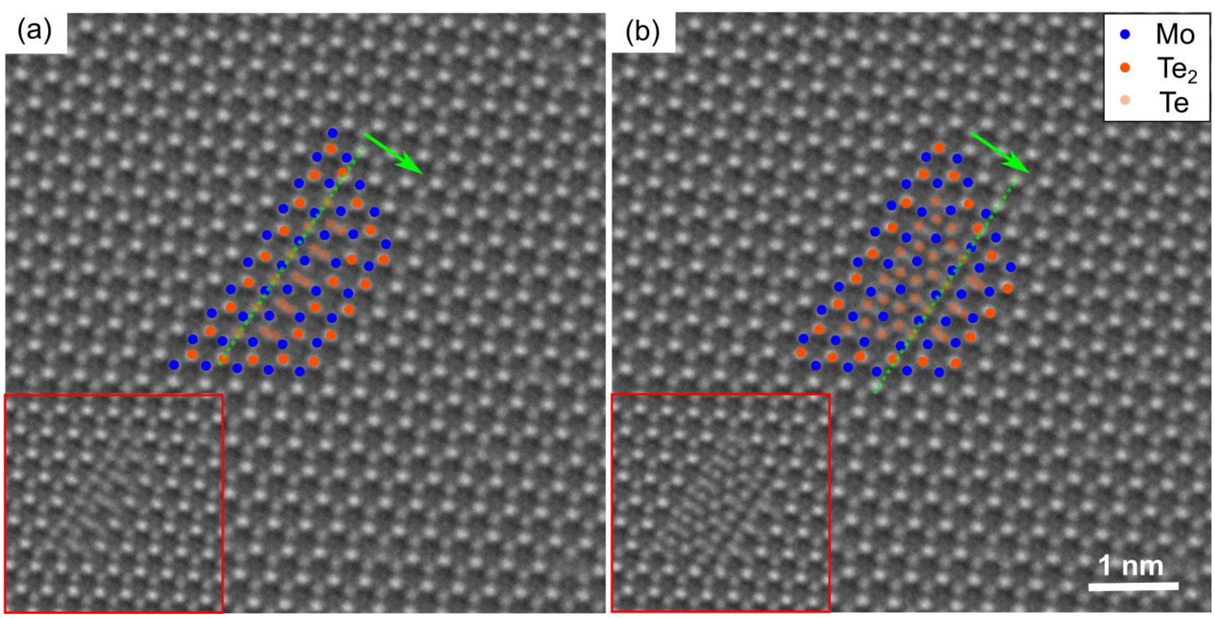

Figure 1: Cc/Cs-corrected high resolution TEM images of 2H-$MoTe_2$ at 40 kV. (a) shows a one-dimensional single vacancy line marked with the green dashed line. The atoms are marked in the interesting area with different colors for better visualization. However, the insets show the defect structures without marking of atoms. Due to

strain, the vacancy line moves and a transformation into the metallic 1T' $MoTe_2$ is taking place along the moving direction indicated by the green arrow in (b).

[1] U. Kaiser, J. Biskupek, J.C. Meyer, J. Leschner, L. Lechner, H. Rose, M. Stöger-Pollach, A.N. Khlobystov, P. Hartel, H. Müller, M. Haider, S. Eyhusen and G. Benner Ultramicroscopy 111 (2011) 1239.

[2] M. Linck, P. Hartel, S. Uhlemann, F. Kahl, H. Müller, J. Zach, and M Haider, M. Niestadt and M. Bischoff, J. Biskupek, Z. Lee, T. Lehnert, F. Börrnert, H. Rose, and U. Kaiser, Phys. Rev. Lett. 117 (2016) 076101.

[3] www.salve-project.de

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