doi:10.1017/S1431927620021339
Microsc. Microanal. 26 (Suppl 2), 2020

Investigation of Structural Phases in $Mo_{1-x}W_xTe_2$ in STEM

Yueming Guo[1], Sergei Kalinin[1], Hui Cai[1], Kai Xiao[1], Sergiy Krylyuk[2], Albert Davydov[2] and Andrew Lupini[1]

[1]Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States, [2]National Institue of Standards and Technology, Boulder, Colorado, United States

The transition metal dichalcogenide (TMD) alloys, $Mo_{1-x}W_xTe_2$, can host various phases at different temperatures and compositions. For example, with $x < 0.10$, $Mo_{1-x}W_xTe_2$ can crystallize to a 1T' semimetal, 2H semiconductor and a Td phase at high (900 °C), room and low (250 K) temperatures, respectively [1]. Both the 1T' and Td phases in $MoTe_2$ have been identified as topologically nontrivial [2]. At room temperature, the crystal structure of the ternary system transforms from 1T' to Td as the W concentration (x) increases from 0 to 1 [1]. The various structural phases hosted by this TMD show promise for a variety of applications and, in particular, phase change memory devices. Disorder brought by composition fluctuations can play an important role in the performance of such devices. It is therefore necessary to understand the distribution of substitutional atoms in the $Mo_{1-x}W_xTe_2$ alloys. We characterized the concentration and the distribution of the W atoms in 2H $Mo_{0.91}W_{0.09}Te_2$, as well as lattice defects, by using aberration-corrected scanning transmission electron microscopy (STEM) with atomic resolution. During the acquisitions of STEM images, it is probably inevitable that the high-energy electrons cause radiation damage to the samples, which introduces extra lattice defects, such as vacancies and dislocations. In the meantime, the W atoms can migrate into neighboring sites through interstitial sites or vacancies. These structural variations can be recorded sequentially using short image acquisition times, which results in noisy data. However, by using machine learning algorithms [3], we can analyze the trajectories of the moving atoms from the noisy datasets and deduce various physical properties of the system, potentially extrapolating backwards in time to the pristine configuration before any radiation damage. Such data analysis will make the STEM experiments more relevant for finding the spatial distribution of substitutional atoms in the pristine structure. In addition, composition fluctuations limit the phonon correlation length, which will affect the lifetime of charge carriers and heat dissipation. The phonon modes can be characterized locally by using vibrational electron energy loss spectroscopy (EELS) in STEM, which may provide insights into the relationship between composition fluctuations and phonon correlation length [4].

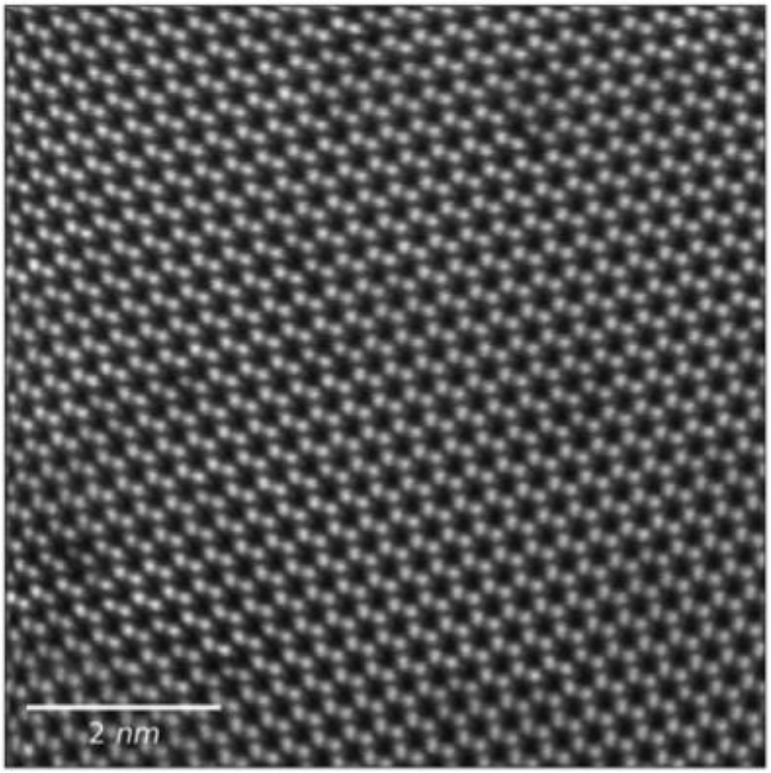

Figure 1. A STEM image of few-layered MoTe2.

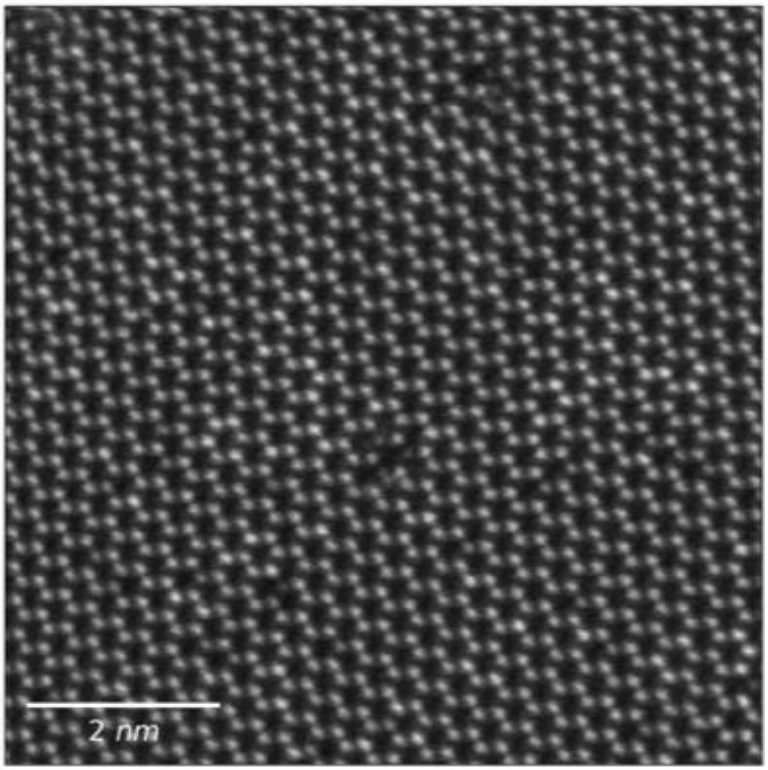

Figure 2. A STEM image of few-layered Mo(1-x)Mo(x)Te2, where the nominal composition is about x = 0.09.

https://doi.org/10.1017/S1431927620021339 Published online by Cambridge University Press

References

[1] S. M. Oliver *et al.*, *2D Mater.* **4** (2017) 045008.
[2] Deng, K., Wan, G., Deng, P. *et al. Nature Phys* **12**, (2016) 1105–1110.
[3] M. Ziatdinov *et al.*, ACS Nano **12**, (2017), 12742-12752.
[4] This effort is based upon work supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), Materials Sciences and Engineering Division and was performed at the Oak Ridge National Laboratory's Center for Nanophase Materials Sciences (CNMS), a U.S. Department of Energy, Office of Science User Facility.