doi:10.1017/S143192762001541X
Microsc. Microanal. 26 (Suppl 2), 2020


# Atomic Electron Tomography: Past, Present and Future

Jianwei Miao[1], Xuezeng Tian[1], Dennis Kim[1], Jihan Zhou[1], Yongsoo Yang[1], Yao Yang[1], Yakun Yuan[1], Colin Ophus[3], Andreas Schmid[3], Shize Yang[4], Fan Sun[5], Christopher Ciccarino[6], Blake Duschatko[6], Juan-Carlos Idrobo[7], Prineha Narang[6], Hao Zeng[5] and Peter Ercius[3]

[1]University of California Los Angeles, Los Angeles, California, United States, [2]Korea Advanced Institute of Science and Technology, Daejeon, Ch'ungch'ong-bukto, Republic of Korea, [3]Lawrence Berkeley National Laboratory, Berkeley, California, United States, [4]Arizona State University, Tempe, Arizona, United States, [5]University at Buffalo, Buffalo, New York, United States, [6]Harvard University, Cambridge, Massachusetts, United States, [7]Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States,

Crystallography has been fundamental to the development of many scientific fields. By measuring the 3D arrangement of atoms with high precision, coupled with quantum mechanical calculations such as density functional theory, we can understand and engineer new materials with applications from electronics and energy conversion to disease fighting drugs. But, the limitation of this powerful technique is that we can only know the periodically averaged structure. Crystallography is blind to defects and aperiodicities in the atomic arrangements, which are often crucial to a material's performance. Although cryo-electron microscopy can determine the 3D structure of biomolecules at near-atomic resolution, it requires the averaging of many copies of the biomolecules with identical or similar conformations. The development of powerful ultra-high resolution imaging methods such as scanning probe microscopy and aberration-corrected electron microscopy allow us to *see* individual atoms without the constraint of periodic averaging. However, *seeing* atoms is not the same as knowing their 3D coordinates with sub-angstrom resolution, which is required for accurate prediction of properties using quantum mechanics. However, we are now on the cusp of a solution to this problem. By combining the atomic resolution electron imaging methods with powerful tomographic reconstruction, it is now possible to obtain the 3D atomic structure of crystal defects and non-crystalline systems. Many challenges had to be overcome for atomic electron tomography (AET) to succeed, but over the past years several such structures have begun appearing heralding a revolution in structure science that may be comparable to that of x-ray crystallography a century ago. Here, we review the major advances and the interdisciplinary science enabled by this groundbreaking methodology that is expected to transform our understanding of structure - function relationships in materials science, chemistry, condensed matter physics, nanoscience and nanotechnology in the 21$^{th}$ century.

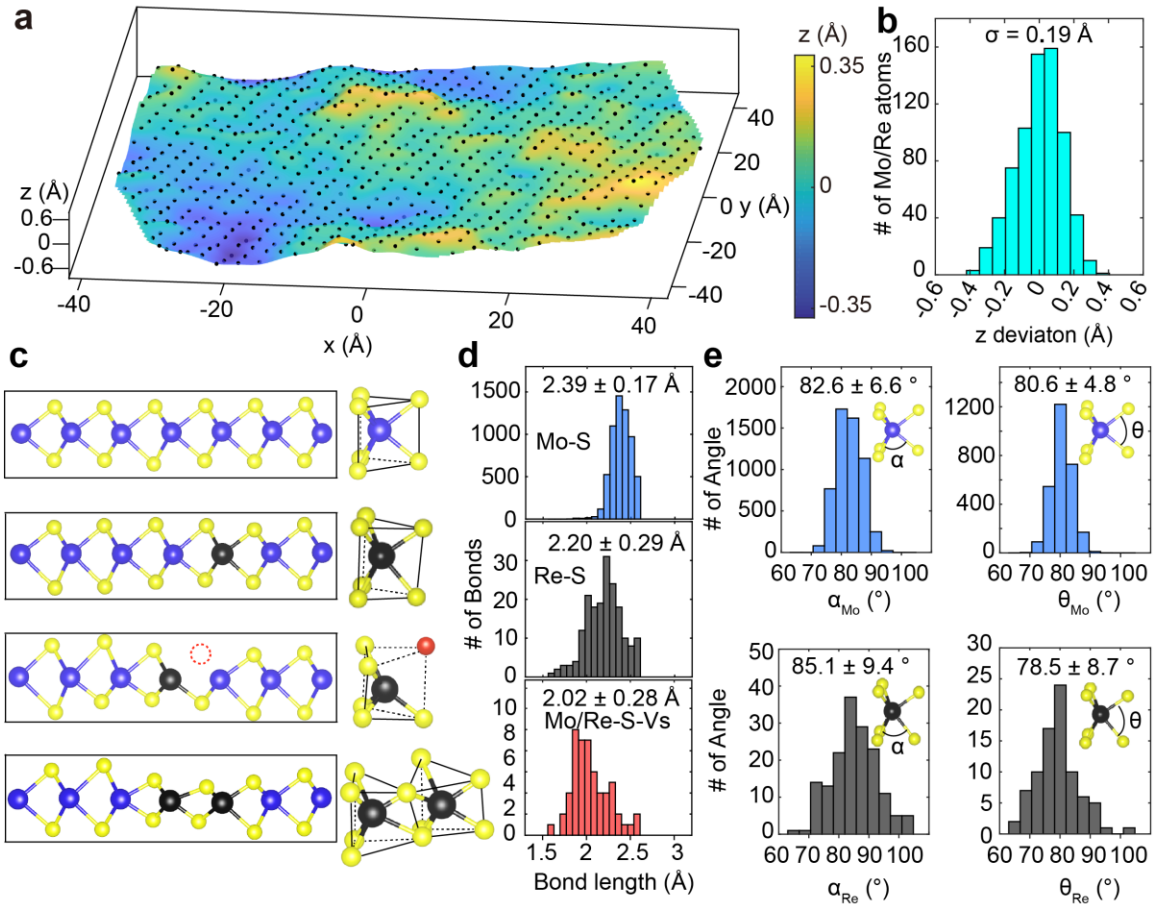


**Figure 1.** Scanning atomic electron tomography reveals 3D atomic coordinates in Re-doped MoS2 and 3D bond distortion induced by single dopants. a, 3D atomic-scale ripples in a Re-doped MoS2 monolayer, where the dots represent the Mo/Re atoms. The total number of Re, Mo, S atoms and S vacancies in the data set is 21, 686, 1381 and 15, respectively. b, Histogram of the distribution of the z coordinates of the Mo/Re atoms with a standard deviation of 19 pm. c, Magnified views of four configurations cropped from the 3D coordinates showing the 3D bond distortion: MoS2 (top), MoS2 with a single Re dopant (2nd panel), MoS2 with a Re-vacancy pair (3rd panel) and MoS2 with double Re dopants (bottom), where the red circle and sphere represent a S vacancy. In each case, the 6 coordinating S atoms (yellow spheres) are shown in the right panels. d, Statistical distributions of the Mo-S and Re-S bond length as well as the shortened bond length if there is a S vacancy in the opposite S layer. For reference, the Mo-S bond length of a perfect 1H structure is 2.36 Å. e, Statistical distributions the two angles between the M-S bonds (top) and Re-S bonds (bottom) in the same and opposite atomic layer. For reference, the corresponding angles of a perfect 1H structure are 83.8°and 79.1°. (From ref. 8)

References

1. Miao, P. Ercius and S. J. L. Billinge, *Science* **353**, aaf2157 (2016).
2. C. Scott *et al. Nature* **483**, 444–447 (2012).
3. C. Chen *et al. Nature* **496**, 74–77 (2013).
4. Xu *et al*. *Nature Mater*. **14**, 1099-1103 (2015).
5. Pryor Jr. *et al*. *Sci. Rep*. **7**, 10409 (2017).
6. Yang *et al*. *Nature* **542**, 75-79 (2017).
7. Zhou *et al. Nature* **570**, 500-503 (2019).

https://doi.org/10.1017/S143192762001541X Published online by Cambridge University Press

8. Tian *et al.*, *Nature Mater*. in press, arXiv:1901.00633.
9. This work was supported by STROBE: A National Science Foundation Science & Technology Center under Grant No. DMR 1548924, the Office of Basic Energy Sciences of the U.S. DOE (Grant No. DE-SC0010378) and the NSF DMREF program (DMR-1437263). ADF-STEM imaging was performed at the Molecular Foundry, which is supported by the Office of Science, Office of Basic Energy Sciences of the U.S. DOE under Contract No. DE-AC02—05CH11231. Part of this research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.