doi:10.1017/S1431927621006383
Microsc. Microanal. 27 (Suppl 1), 2021

Atomic electrostatic maps of sulfur vacancies in MoS_2 by differential phase contrast

Sebastian Calderon[1], Rafael Ferreira[1], Deepyanti Taneja[2], Jayanth Raghavendrarao[2], Langyan Zhou[2], Deji Akinwande[2] and Paulo Ferreira[3]

[1]International Iberian Nanotechnology Laboratory, Braga, Portugal, [2]The University of Texas at Austin, United States, [3]International Iberian Nanotechnology Laboratory, United States

Recent developments in differential phase contrast (DPC) STEM have allowed us to obtain information beyond the structural features of a material. This technique has proven to be a powerful tool for acquiring information not only about heavy and light elements simultaneously but also about the atomic electrostatic field and total charge distribution in materials, in a way no other technique has permitted. This information is retrieved by measuring the centre of mass of the diffraction disk using a segmented or pixelated detector to collect its intensity distribution. In the case of a pixelated detector, quantification capability is much more accurate compared to a segmented detector, due to detailed information recorded from the diffraction disk in large pixel arrangements [1]. However, the speed and sensitivity of segmented detectors have shown remarkable results in mapping the electrostatic field and charge distribution in materials such as GaN [2] and graphene [3]. In this report, we apply the DPC-STEM technique to an investigation the atomic electric field of monolayer MoS2. The electrostatic maps of pristine regions and areas containing the presence of sulphur vacancies were recorded at 60 kV and 200 kV, supported by multislice computer simulations.

STEM images were acquired in a double-corrected FEI Titan-Themis TEM/STEM, operated at 60 kV and 200 kV. Annular dark-field and DPC images were obtained simultaneously from a sample of exfoliated MoS2, transferred to an ultra-flat SiNx grid. A segmented annular detector was used to image the in-plane displacement of the transmitted electrons, which is proportional to the projected electric field, while the images proportional to the potential and charge distribution were calculated according to [4-6].

We demonstrate the capacity of DPC-STEM to map the atomic-level electrostatic field in monolayer MoS2, providing information about the local chemical state of monolayer MoS2 in the presence of sulphur vacancies. The results show detailed information about the projected charge distribution and projected electric field at the sulphur atomic positions.

Acknowledgements

The authors would like to acknowledge that this project has received funding from the EU Framework Programme for Research and Innovation H2020, scheme COFUND – Co-funding of Regional, National and International Programmes, under Grant Agreement 713640. This work was supported by FCT, through IDMEC, under LAETA, project UIDB/50022/2020. RMR acknowledges the FCT grant UIDB/FIS/04650/2020-2023. D.A acknowledges the Presidential Early Career Award for Scientists and Engineers (PECASE) through the Army Research Office (W911NF-16-1-0277), and a National Science Foundation grant (ECCS-1809017).

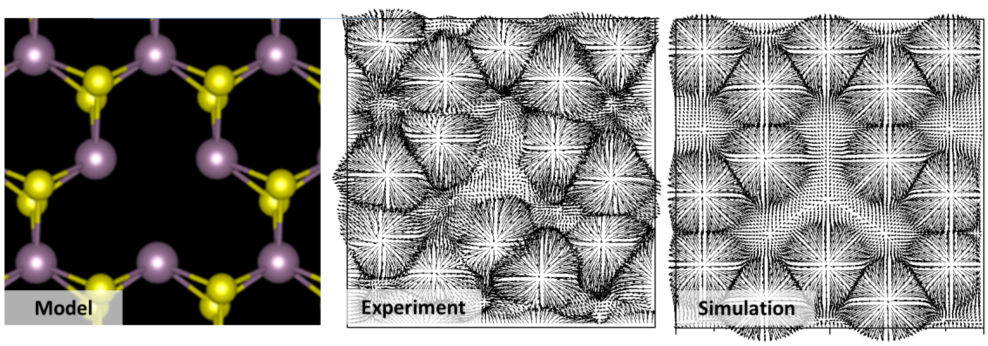

Figure 1. Probe-convolved atomic electric field vector map for experimental results and computer-simulated monolayer MoS2.

References

[1] K. Müller-Caspary, F.F. Krause, F. Winkler, A. Béché, J. Verbeeck, S. Van Aert, A. Rosenauer, Ultramicroscopy. 203 (2019) 95–104. doi:10.1016/j.ultramic.2018.12.018.

[2] N.R. Lugg, T. Seki, R. Ishikawa, S.D. Findlay, Y. Kohno, Y. Kanitani, S. Tanaka, S. Tomiya, Y. Ikuhara, (2018). doi:10.1021/acsnano.8b03712.

[3] R. Ishikawa, S.D. Findlay, T. Seki, G. Sánchez-santolino, Y. Ikuhara, N. Shibata, Y. Kohno, Nat. Commun. (n.d.) 8–13. doi:10.1038/s41467-018-06387-8.

[4] Ivan Lazić, Eric G.T. Bosch, Sorin Lazar, Ultramicroscopy, Volume 160, 2016, Pages 265-280,

[5] Shibata, N.; Seki, T.; Sánchez-Santolino, G.; Findlay, S. D.; Kohno, Y.; Matsumoto, T.; Ishikawa, R.; Ikuhara, Y. Nat. Commun. 2017, 8, 15631.

6] Gabriel Sánchez-Santolino, Nathan R. Lugg, Takehito Seki, Ryo Ishikawa, Scott D. Findlay, Yuji Kohno, Yuya Kanitani, Shinji Tanaka, Shigetaka Tomiya, Yuichi Ikuhara, and Naoya Shibata, ACS Nano 2018 12 (9), 8875-8881

https://doi.org/10.1017/S1431927621006383 Published online by Cambridge University Press