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Structural Analysis of MoS_2 and other 2D layered materials using LEEM/LEED-I(V) and STM MAXWELL GRADY, ZHONGWEI DAI, University of New Hampshire, WENCAN JIN, JERRY DADAP, RICHARD OSGOOD, Columbia University, JERZY SADOWSKI, Center for Functional Nanomaterials, Brookhaven National Laboratory, KARSTEN POHL, University of New Hampshire
— Layered two-dimensional materials, such as molybdenum disulfide, MoS_2, are of interest for the development of many types of novel electronic devices. To fully understand the interfaces between these new materials, the atomic reconstructions at their surfaces must be understood. Low Energy Electron Microscopy and Diffraction, LEEM/μLEED, present a unique method for rapid material characterization in real space and reciprocal space with high resolution. Here we present a study of the surface structure of 2H-MoS_2 using μLEED intensity-voltage analysis. To aid this analysis, software is under development to automate the procedure of extracting I(V) curves from LEEM and LEED data. When matched with computational modeling, this data provides information with angstrom level resolution concerning the three dimensional atomic positions. We demonstrate that the surface structure of bulk MoS2 is distinct from the bulk crystal structure and exhibits a smaller surface relaxation at 320K compared to previous results at 95K. Furthermore, suspended monolayer samples exhibit large interlayer relaxations compared to the bulk surface termination. Further techniques for refining layer thickness determination are under development.

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