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Atomic structure of the CoS_2(100)-(1×1) Surface Z.X. YU, M.A. VAN HOVE, S.Y. TONG, Department of Physics and Materials Science, City University of Hong Kong, D. WISBEY, N. WU, P.A. DOWBEN, W.N. MEI, Department of Physics and the Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln, Y.B. LOSOVYJ, Center for Advanced Microstructures and Devices, Louisiana State University, M. MANNO, L. WANG, C. LEIGHTON, Department of Chemical Engineering, University of Minnesota — Atomic structure and top-layer relaxation of the CoS_2(100) surface are studied by using the quantitative low energy electron diffraction (LEED). From the LEED images, we observed a clear 1×1 pattern with 4-fold symmetry. Over 18 beams of intensities versus energy curves are acquired from the LEED spots. With a series of trial model structures, theoretical intensities computed from full dynamical method are used to compare with experimental data by means of the Pendry R-factor. The clearly favored structural model from the LEED analysis is the 1S-terminated surface, in which the S-S dimmers remain intact and keep a complete S-Co-S sandwich structure. We also find that sub-surface Co and the third layer S atoms relax downward and upward by 0.10 Å, respectively. These results could be compared with other theoretical and experimental studies. *This work was supported by RGC grant No. 8730017 of Hong Kong, Nebraska Research Initiative, the UNL NSF "QSPINS" MRSEC (DMR 0213808) and the UMN NSF MRSEC (DMR-0212302).

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