

Abstract Submitted
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Atomic structure determination of the (001) surface of the semimetal Bi by STM and LEED J. SUN, J. WANG, Dept. of Physics, Univ. of New Hampshire, J. WELLS, NTNU, Trondheim, Norway, PH. HOFMANN, Institute for Storage Ring Facilities, University of Aarhus, Denmark, K. POHL, Dept. of Physics, Univ. of New Hampshire — The Bi surfaces differ from the semimetal bulk due to the metallic surface states, induced by the symmetry breaking and strong spin-orbit interaction. All Bi surface states studied are spatially confined to the first layer. Bi(001) is a notable exception with deeply penetrating states, which could have a significant effect on the bulk properties of nanostructures. This work presents surface morphology observation by STM and atomic structure determination by LEED, which are expected to be closely related to the electronic properties. STM shows an unreconstructed surface and wide terraces with double-layer step heights of about $3.76 \pm 0.02 \text{ \AA}$. We also identify the short termination by obtaining unstable single step heights via special sputtering operations. In the LEED analysis, the termination with an intact bilayer also results in a much better agreement between calculated and measured intensities than the broken bilayer. Strong multi-layer oscillatory relaxations (about 10%) are found to reach deep into the fifth layer, which can be seen as the structural response to the unusually deep surface state penetration at this surface. The measured relaxations agree well with those from first-principles calculations.

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