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Stability investigation on the non-basal surfaces of topological insulator Bi_2Te_3: a first-principles study NA WANG, Tsinghua Univ, YIYANG SUN, Rensselaer Polytechnic Institute, YUYANG ZHANG, Vanderbilt University, DAMIEN WEST, Rensselaer Polytechnic Institute, WENHUI DUAN, Tsinghua Univ, SHENGBAI ZHANG, Rensselaer Polytechnic Institute — The basal (0001) surface of Bi_2Te_3 is the most stable surface and has been predominantly observed in experiment and studied in great details. The stability of other surfaces has been rarely discussed so far despite the fact that vicinal surfaces are always present at the crystal edges. In this work, we systematically study the thermodynamic stability of the vicinal surfaces of Bi_2Te_3 based on first-principles calculations. In particular, it is found that the $(01\bar{1}5)$ surface has a surface energy of only about two times larger than that of the (0001) surface. Due to the particularly low surface energy, the sidewalls of free-standing Bi_2Te_3 crystals are predicted to be the $(01\bar{1}5)$ surface, which is not perpendicular to the basal (0001) surface. The Wulff construction based on our calculated surface energies is consistent with experiment. However, in the presence of substrates, e.g., in molecular beam epitaxial growth, the shape of a crystal flake is further affected by the interface energy. In this case, the sidewalls could be $(01\bar{1}0)$, $(01\bar{1}\ 10)$ or $(01\bar{1}\bar{4})$ depending on the binding strength between the flake and the substrate.

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