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Geometric effects on surface states in topological insulator Bi_2Te_3 nanowire PARIJAT SENGUPTA, TILLMAN KUBIS, MICHAEL POVOLOTSKYI, GERHARD KLIMECK, Purdue University — Bismuth Telluride (BT) is a 3D topological insulator (TI) with surface states that have energy dispersion linear in momentum and forms a Dirac cone at low energy. In this work we investigate the surface properties of a BT nanowire and demonstrate the existence of TI states. We also show how such states vanish under certain geometric conditions. An atomistic model (sp3d5s* TB) is used to compute the energy dispersion in a BT nanowire. Penetration depth of the surface states is estimated by ratio of Fermi velocity and band-gap. BT possesses a tiny band-gap, which creates small localization of surface states and greater penetration in to the bulk. To offset this large spatial penetration, which is undesirable to avoid a direct coupling between surfaces, we expect that bigger cross-sections of BT nanowires would be needed to obtain stable TI states. Our numerical work validates this prediction. Furthermore, geometry of the nanowire is shown to influence the TI states. Using a combined analytical and numerical approach our results reveal that surface roughness impact electronic structure leading to Rashba type splits along z-direction. Cylindrical and square cross-sections are given as illustrative examples.

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