First-principles study of $X/Bi_2Te_3(0001)$ surface (X=Ag, Ni, Ti)

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We have analyzed the influence of Ag, Ni and Ti on the electronic properties of Bi_2Te_3. The electronic properties of Bi_2Te_3 were studied recently [1-3]. The relaxation of clean $Bi_2Te_3(0001)$ surface and relaxation of silver, nickel and titanium on clean $Bi_2Te_3(0001)$ surface has been studied using *ab-initio* density-functional techniques.

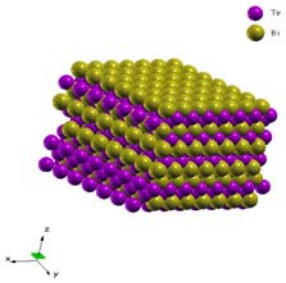

Fig. 1. Crystal structure of clear (0001) bismuth telluride surface.

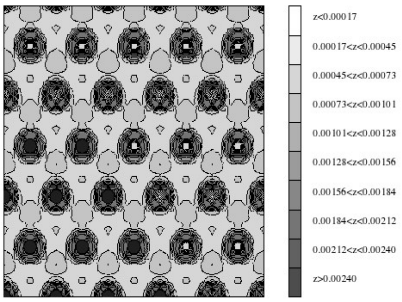

Fig. 2. Simulation of STM image of surface from Fig. 1. (bias voltage +1.0V).

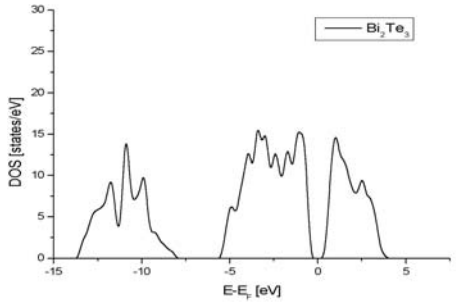

Fig. 3. Total density of states for bismuth telluride slab.

STM images of surface, total density of states and the band structure of bismuth telluride were determined by using the Quantum-Espresso *ab-initio* simulation package based on pseudopotential method [4]. The relaxation was performed on a 12x12x1 k-point mesh, however in the calculations of the density of states the 16x16x1 k-point mesh was used.

[1] S. Katsuki, J. Phys. Soc. Jap. **1** (1969) 26
[2] P. Larson *et al.*, Phys. Rev. B **65** (2002) 085108
[3] P. Larson *et al.*, Phys. Rev. B **61** (2000) 8162
[4] www.pwscf.org or www.quantum-espresso.org

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