Effect of Diameter on Opto-electrical Properties of TiC Nanowires

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Abstract

Calculations of the density of states, dielectric function and optical properties of the nanowires were performed under polarized parallel to the wire axis. In this paper, diameter of TiC nanowire was increased in two directions and electronic properties of the new structure were investigated. Also, the results were compared with measurements of the electronic properties of TiC nanowires. Theoretical calculations were done using density functional theory (DFT) and wien2k code. It was observed in this work that maximum reflectivity coefficient for the nanowire with diameter effect (NDE) of TiC was about 0.391 while, for the nanowire without diameter effect (NWDE) of TiC, it was about 0.36. These results showed that reflectivity for NDE was more than NWDE. Moreover, the maximum absorption coefficient for NDE was around 52.00 while, for NWDE of TiC, it was about 56.07. It was seen that intensity of spectrum for this parameter decreased with increasing diameter of supercell.