Optoelectrical properties of TiC nanowires from density functional theory

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In this paper, diameter of TiC nanowire was increased in two directions and electronic properties of the new structure were investigated. Theoretical calculations were done using density functional theory (DFT) and Wien2k code. The results showed that reflectivity for nanowire by diameter effect (NDE) was more than the nanowire without diameter effect (NWDE). It was also observed that the intensity of spectrum for this parameter decreased with increasing diameter of supercell. Moreover, it was observed that maximum conductivity coefficient for NDE of TiC was about 1.48, while it was about 1.6 for NWDE of TiC. Furthermore, the energy gap was reduced; however, it was still a semiconductor.

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1. Introduction

Recently, nanowires and nanorods of metallic and semiconducting materials have attracted great research interest because of their unique physical properties, which are interesting from the view point of different device applications. Nanowires have two quantum-confined dimensions and one unconfined dimension. Therefore, the electrical conduction behavior of bulk structure [1] is different from that of their nanowires [2].

This issue allows nanowires to be used in applications where electrical conduction, rather than tunneling transport, is required. Changing the dimension of a system usually leads to the creation of new physical properties so that surface structures show a different behavior from the bulk mode. Also, one-dimensional compounds have a very different behavior from two- or three-dimensional ones. Thus, studying nanostructures and changing their diameters have been considerably investigated in recent years.

As mentioned, physical properties of structures depend on size and dimensions. In this paper, effect of diameter variation on the electrical and optical properties of TiC nanowires was investigated. So, for this simulation, the diameter of supercell was changed by about a few angstroms until obtaining optimal parameters. Therefore, physical properties were studied. Change in diameter affects electrical and optical properties of structures. So, to investigate this effect, the cell length was changed in two directions. Also, it was kept along z direction which was growth of nanowire.

2. Computational details

The calculations were obtained from the full potential lineralized augmented plane wave plus local orbital (FLAPW + lo) [3, 4] within density functional theory (DFT) [5-7] using Wien2k code [8-11]. Moreover, for the exchange correlation correction, the generalized gradient approximation (GGA) was applied [12, 13]. An optimized number of k-points were used, while this value was 2000. The convergence parameter RMT Kmax was set to 8. As a convergence criterion, the iteration was stopped when the charge difference was less than 1×10^{-4} between the steps. The number of atoms for NDE and NWDE was respectively 16 (8 carbons and 8 titanium) and 8 (4 carbons and 4 titanium).

In the previous works [14-16], optical properties of Ti and titanium nanochains have been calculated. This paper aimed to investigate the effect of diameter on opto-electrical properties of TiC nanowires.

Fig. 1 shows a view of the nanowire by diameter effect (NDE) and the one without diameter effect (NWDE) supercell. Each of these structures had different electronic properties, which will be introduced below.

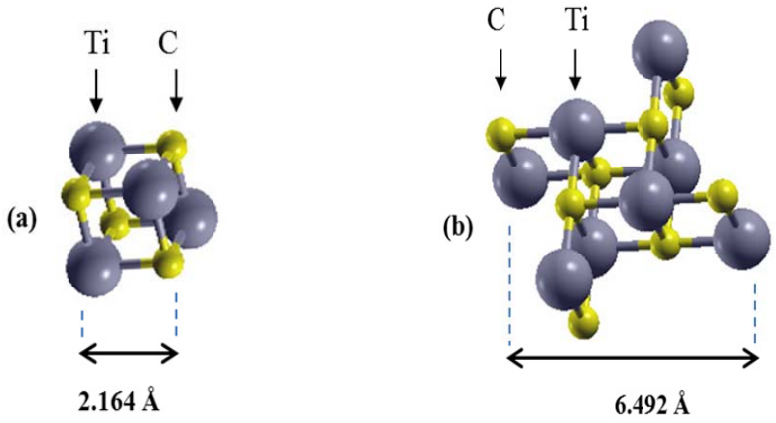

Fig. 1. a) NWDE and b) NDE of titanium carbide.

3. Density of states

Density of states (DOS) was compared for both NDE and NWDE. To show basic trends in electronic energy spectra of carbides, their total and local model densities of states DOS were used (Fig. 2). There were several main peaks in the curve of total DOS of NDE in TiC. The first peaks in the lower energy part of the DOS curve arose from Ti 3s and 3p states, respectively, which were localized and had less contribution to TiC bonding.

Finally, it was observed that intensity of the spectrum for the NDEs was more than NWDEs, which was due to the increasing number of atoms. Also, energy gap was reduced; but, it was still a semiconductor. Width of the band gap was different for various semiconductors [17]. In both figures of DOS, maximum intensity of the spectrum was in 3d orbitals of titanium.

Fig. 3 presents the distribution of difference valence charge density on the (001) plane for NDE and NEDE of TiC. It can be evidently observed that there was a strong interaction between Ti and C atoms, which resulted in the occurrence of energy gap in the DOS curves. Also, electron density was higher for the NWDEs due to the stronger bond between titanium and carbon atoms in this structure.

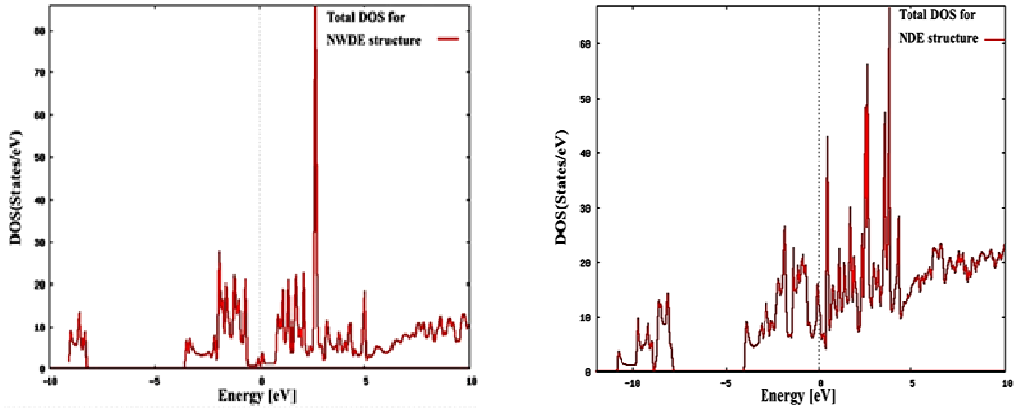

Fig. 2. Calculated total density of states (DOS) for NDE and NWDE in TiC.

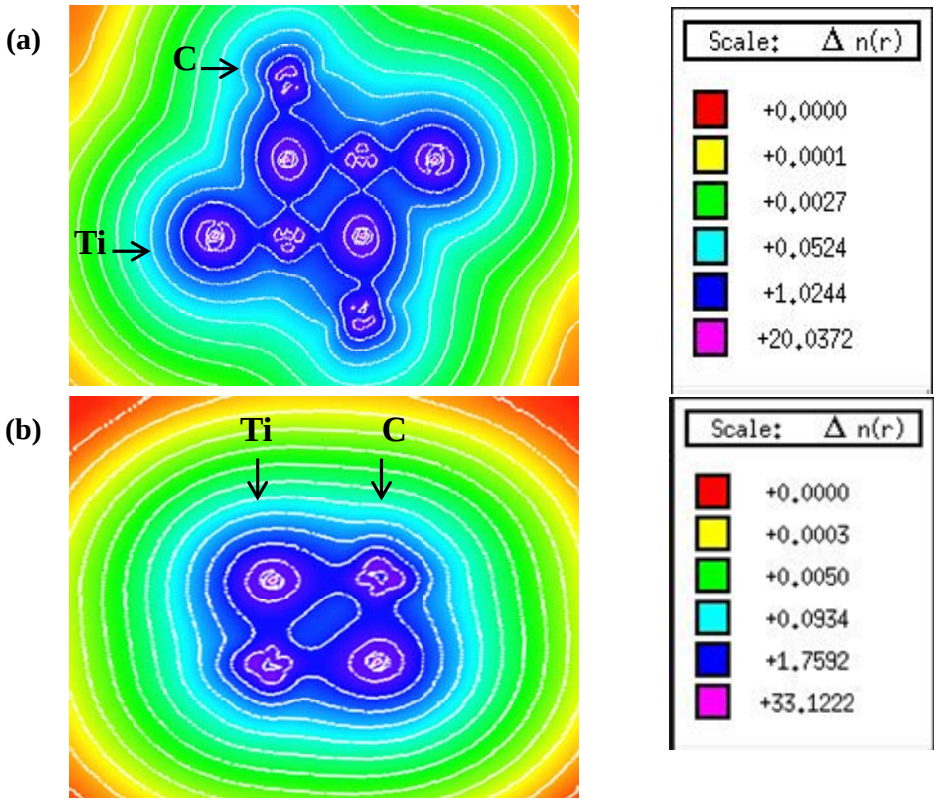

Fig. 3. Distribution of charge density for a) NDE and b) NWDE of TiC.

4. Optical properties

In another step, effect of increasing diameter on optical properties of the nanowires was explained. To investigate optical properties, the dielectric function must be studied [18, 19]. Real and imaginary parts of this function are shown in Fig. 4. Spectrum of the dielectric function with the increasing diameter of supercell moved towards lower energies Also, real ε_{1max} (ω) and imaginary ε_{2max} (ω) parts increased with the increasing diameter of supercell.

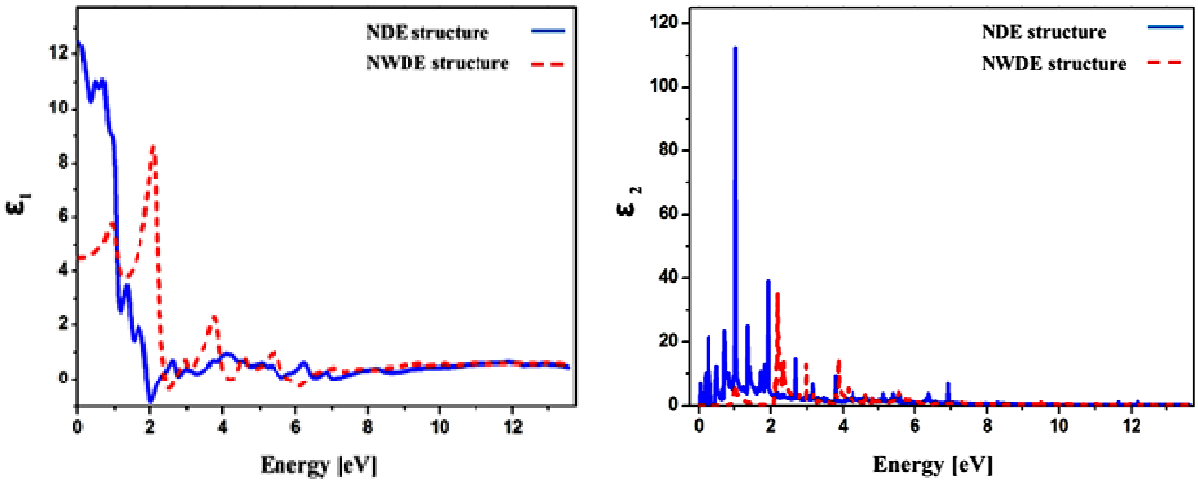

Fig. 4. a) Real and b) Imaginary parts of dielectric function diagram for NDE and NWDE of TiC.

5. Energy loss function and optical conductivity

It is known that the maximum amount of energy loss function is Plasmon peaks. As shown in Fig. 5, the maximum rate of dissipation was related to the structure with larger diameter and intensity of these peaks increased with an increase in the cell length by about 10.8%. Fig. 6 shows optical conductivity for NDE of titanium carbide. It can be observed that maximum conductivity was related to the structure with smaller diameter. With increase in the cell length, displacement of spectrum towards lower energies was observed for this property. The maximum conductivity was 1.48 for NDE with initial value of 6.492 Å and increased for NWDE as 1.6. These results showed that conductivity for NWDE was more than NDE.

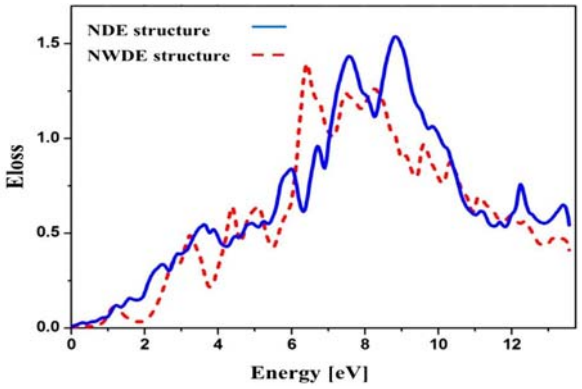

Fig. 5. Energy loss function of TiC nanowires.

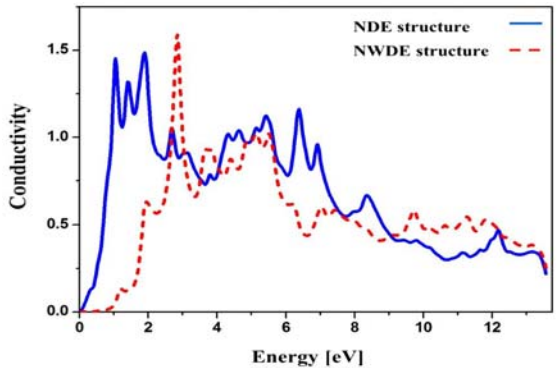

Fig. 6. Optical conductivity of TiC nanowires.

6. Optical absorption and reflectivity coefficients

In Fig. 7, optical reflectivity for the NDEs and NWDEs of titanium carbide nanowire is demonstrated. It can be seen that, by increasing bond length, maximum reflectivity increased by about 8.6%. In addition in Table 1, the maximum and minimum values of optical absorption and reflectivity coefficients were compared for the NWDE and NDE of titanium carbide.

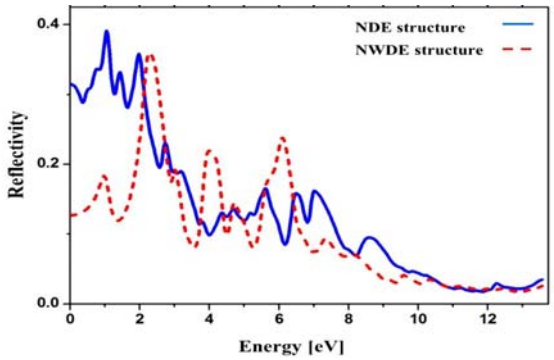

Fig. 7. Optical reflectivity of TiC nanowires.

Table 1. Maximum and minimum of reflectivity, absorption, eloss function, and conductivity coefficients for NWDEs and NDEs of TiC; d, length of supercell

d (Å)	2.164 (NWDE)		6.492 (NDE)
$\mathbf{Reflect_{max}}$	0.36		0.391
$\mathbf{Reflect_{min}}$	0.0175		0.0175
$\mathbf{Absorb_{max}}$	56.07		52.00
$\mathbf{Absorb_{min}}$	0.0027		0.0281
$\mathbf{Eloss_{max}}$	1.39		1.54
$\mathbf{Eloss_{min}}$	0.0042		0.0091
$\mathbf{Conduct_{max}}$	1.6		1.48
$\mathbf{Conduct_{min}}$	0.00007		0.0024

Also, in Fig. 8, optical absorption coefficients for NWDE and NDE structures can be observed. It is seen that the intensity of spectrum for NDEs was less than NWDEs; in other words, absorption coefficient decreased with the increasing diameter of supercell.

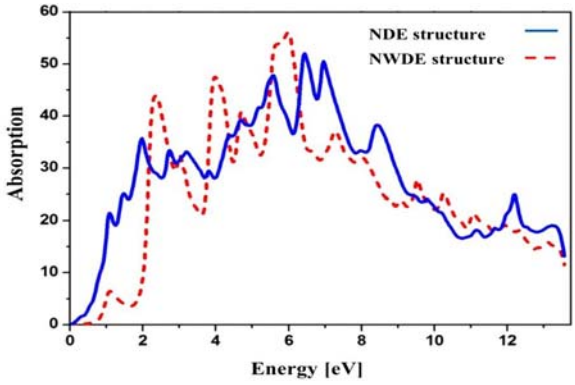

Fig. 8. Absorption coefficient of TiC nanowires.

7. Conclusion

Electronic and some optical properties of semiconductor NDEs of titanium carbide were investigated. So, it was observed that maximum conductivity coefficient for NDE of TiC was about 1.48, while it was about 1.6 for NWDE of TiC. These results showed that optical conductivity for NWDEs was more than NDEs. Moreover, intensity of the spectrum of DOS for the NDE was more than the NWDE, which was due to the increasing number of atoms. Also, the energy gap was reduced. Nevertheless, it was still a semiconductor. In addition, the maximum absorption coefficient for NDE was at around 52.00, while, for NWDE of TiC, it was about 56.07. It was also seen that intensity of spectrum for this parameter decreased with the increasing diameter of supercell. Other optical properties such as eloss function and reflection coefficient of the nanowires were also investigated; both figures were stronger for the NDE of TiC. Further, for the NDE similar to NWDE structure, all the optical properties in the growth axis of nanowire were stronger than the perpendicular one of the wire.

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