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Study of Optical Properties of Titanium Nitride (TiN) Based on DFT Calculation

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ABSTRACT

In this research, the optical properties of TiN have been investigated. These investigations are done by using the linearized augmented plane wave method (LAPW) within density functional theory (DFT) with WIEN2k package. To obtain the optical properties such as real and imaginary parts of dielectric function, refractive index and the extinction coefficient, reflectivity, energy loss function and optical conductivity have been used local spin density approximation (LSDA) and generalized gradient approximation (GGA) with WC function. The aim of this work is to compare difference between two PBE and WC function on optical properties op TiN. Obtained results for lattice parameters are in good agreement with experimental results.

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INTRODUCTION

Transition metal-nitrides have been studied for several decades due to their appealing properties, such as ultra-hardness, high melting point and high Curietemperature. (H.Allmaier, 2009)

Titanium nitride has been known as a material with excellent mechanical properties (high hardness and good resistance to corrosion), low electrical resistance, high thermal and chemical stability and interesting optical properties (colors from golden to dark brown) (B. Rauschenbach, 2000), (T.S.Yeh, 2008), (Nadia Saoula, 2009).

This combination has many applications in industry due to its special characteristics, The examples includes: Increase the useful life of components and tools, Resistance to corrosion, Used in the semiconductor industry as a barrier between the metal conductor and the conductivity of silicon, Protective and decorative coatings, Jewelery making Also, due to the non-toxicity and good compatibility with the human body in medical and dental prostheses (M. Wittmer, 1981), (M. Finetti, 1984), (H.C. Chen, 2003).

TiN has a ***NaCl***-type ***structure***. it's Structural features has been discussed by so many researchers frequently (N. Benzekkour, 2006), (K. Ji Hoon,1999), (S.H. Kim, 2009).

Calculation method:

In this theoretical calculations, the optical properties of crystalline titanium nitride (TiN) have been performed full-potential linearized augmented plane wave (FP-LAPW) method in the farame work of density functional theory (DFT) (E.K.U. Gross and Walter Kohn, 2008) as implemented in the WIEN2k code (P. Blaha, 2001).

All electronic structure calculations in the framework of two types of approximation, generalized gradient (GGA) with the WC function (which is a modified version based on the PBE functional) and local density (LSDA) was performed with the same parameters. The following parameters were chosen for the self-consistency cycle for all computation.

The muffin Tin sphere radius of the compound stood at 2/1100 a.u. and 1/8200 a.u. (in atomic units) for titanium and nitrogen respectively. To separate capacity states from core states, we selected 6D Rydberg energy. We also selected the range of energy conversion from ۰.۰۰۰۱ for all compounds in this work. ۷. There were 256 points in the first Brillouin zone and the Brillouim zone sampling was performed using a 20 × 20 × 20 k-point. The convergence of the basic set is controlled by a cutoff parameter Rm × Km = 7 (R smallest radius Muffin - cut thin and Kmax is the wave vector).

Calculations have been done for TiN crystalline phase and the cubic space group Fcc (Fm-3m) and α= β= γ= 90°. TiN cells have been illustrated in figure 1.

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Journal of Applied Science and Agriculture, 8(5) October 2013, Pages: 652-657

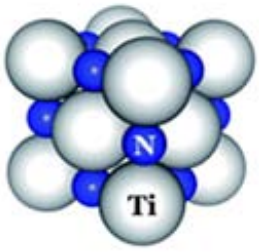


Fig. 1: Illustration of crystalline structure of Titanium nitride.

Results:

Details of the optimization process applied to the lattice constant of TiN have been presented in table 1.

Table 1: The optimized lattice constants and the function of the previous research work.

(A°) Lattice Parametrs		
In this work	Functional (WC)	4.22
	Functional (LSDA)	4.19
Other's Result (p. Haas, F. Tran and P. Blaha, 2009)	Functional (WC)	4.21
	Functional (LSDA)	4.18
Experimental Result	4.26 (C. Stampfl, W. Mannstadt, R. Asahi, and A. J. Freeman, 2001)	
	4.235 (R. W.G. Wyckoff1, 963)	

As seen in table 1, the best correspondence between empirical and theoretical results belongs to WC functional.

Discussions:

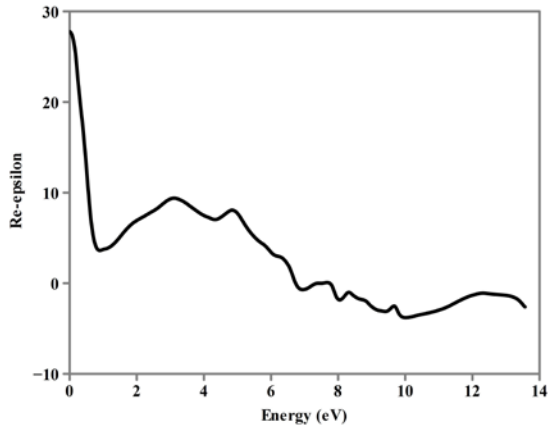
Dielectric function:

To describe the crystal's responses to an electromagnetic field the dielectric function of the material is calculated. The dielectric function has two inter-band and intra-band components. The intra-band component is applied to metals. Dielectric function is a complex function which is shown below:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \quad (1)$$

$\varepsilon_1(\omega)$ changes could be obtained based on Kramers-Kronig transformation when $\varepsilon_2(\omega)$ are available. $\varepsilon_1(\omega)$ roots have physical concepts and in fact are the requirement for volume Plasmons in the material, while the existence of energy loss is the requirement for the existence of these roots. Also, waves are not propagated and processes of absorption and loss do not take place when $\varepsilon_1(\omega)$ is negative.

The real part of TiN dielectric function has been presented in figure 2(a) and the imaginary part of the function has been illustrated in figure 2(b).



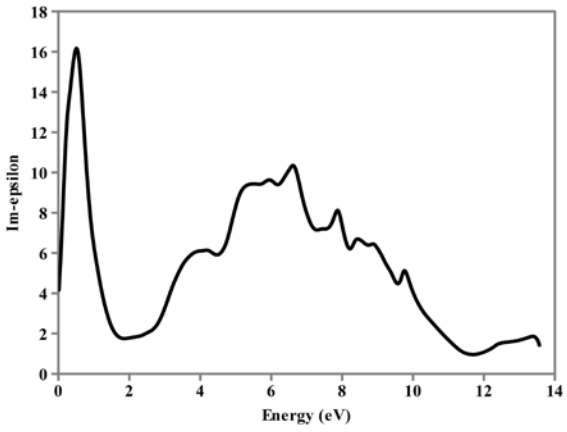


Fig. 2(a): Real part of dielectric function of TiN. **Fig. 2(b):** Imaginary part of dielectric function of TiN.

As can be seen in Figure 2 (a) when energy is zero ε (0) the Static dielectric constant is approximately 27. As seen in figures 2(a) and 2(b), compared the results related to the real and imaginary parts of the functional, It

Journal of Applied Science and Agriculture, 8(5) October 2013, Pages: 652-657

is found that there is complete agreement between the results obtained through the use of LSDA and WC functionals.

Refractive index and extinction coefficient:

When light passes through a medium, some part of it will always be absorbed. This can be conveniently taken into account by defining a complex index of refraction; Refractive index is a complex function which is shown below:

$$n(\omega) = n(\omega) + ik(\omega) \quad (1)$$

Here the real part of the refractive index n (ω) indicates the phase speed, while the imaginary part k (ω) indicates the amount of absorption loss when the electromagnetic wave propagates through the material. Extinction coefficient is for the measurement of the absorption of electromagnetic radiation by matter. If electromagnetic waves can pass through it easily, the material has a low extinction coefficient. The real and imaginary parts of the dielectric function is related to the optical constants of refractive index n (ω) and the extinction coefficient k (ω), the following relations are obtained:

$$k_{ij}(\omega) = \sqrt{\frac{|\varepsilon_{ij}(\omega)| - Re\ \varepsilon_{ij}(\omega)}{2}} \quad (2)$$

Figure 3(a) and 3(b) illustrates acombination of the results of real part of refractive index and have been presented for LSDA and WC functional. According to Figure 3 it can be seen that The maximum peak For the TiN is at zero energy eV and has a refractive index of about 2/5

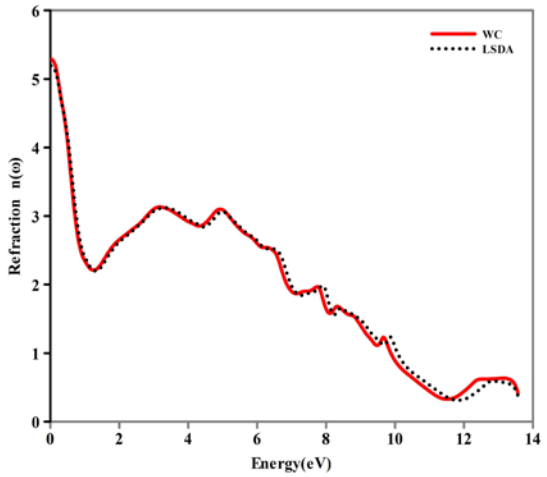


Fig. 3(a): The real part of refractive index of TiN.

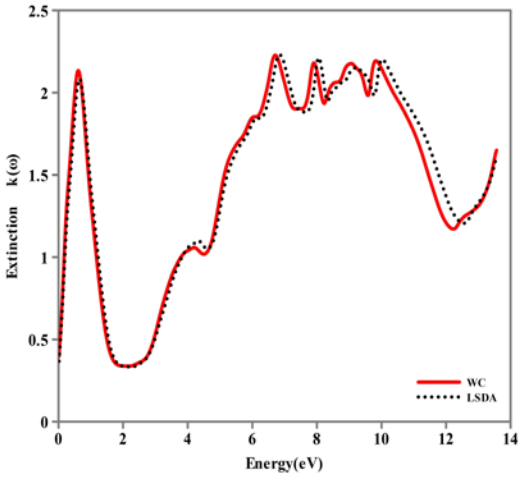


Fig. 3 (b): The extinction coefficient of TiN.

We calculated the refractive index and extinction coefficient and compared the results related.

To each other, finding out that there is little difference between the results obtained through the use of LSDA and WC functionals. With rising energy it can be seen small deflection at LSDA approximation to GGA-WC approximation that the displacement is proportional to the amount of energy.

Electron energy loss function:

Electron energy loss spectroscopy is a powerful way for analyzing populated states above the Fermi level or conducting partial separation. This spectrum involves the mass-stimulation of valence electrons (Plasmons) into the populated states of the conduction band. The most distinctive peak in the electron energy loss function, known as the "Plasmon peak", is indicative of the mass-stimulation of the electron charge density in the crystal.

TiN energy loss graph has been presented in figure 4.

Based on the free election model, the Plasmon energy is obtained through the following relation:

$$E_p = \omega_p = \sqrt{\frac{ne^2}{m_0 \varepsilon_0}} \quad (3)$$

Where, n is free electron density in cell size, m_0 is electron mass and *e* is electric charge unit.

Journal of Applied Science and Agriculture, 8(5) October 2013, Pages: 652-657

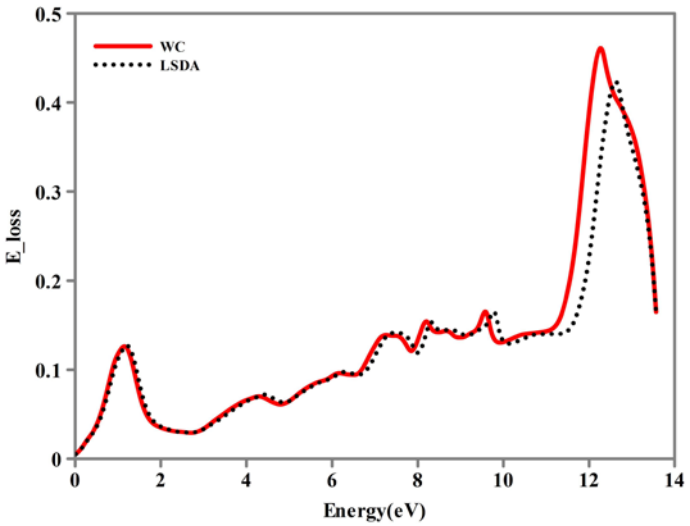


Fig. 4: Energy loss function TiN.

Reflection coefficients:

Reflection coefficient is calculated when a propagated wave is not continuous. It determines the Intensity or range of a reflected wave in relation with an incident wave. Reflection coefficient is closely related to transfer coefficient. Optical reflectivity can be calculated by using the following equation:

$$R_{ij}(\omega) = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \quad (4)$$

N is the characteristic of the real part of the refraction index and k is the imaginary part of the refraction index (extinction coefficient). The reflection coefficient of the TiN have been presented for LSDA and WC functionals in figures 5.

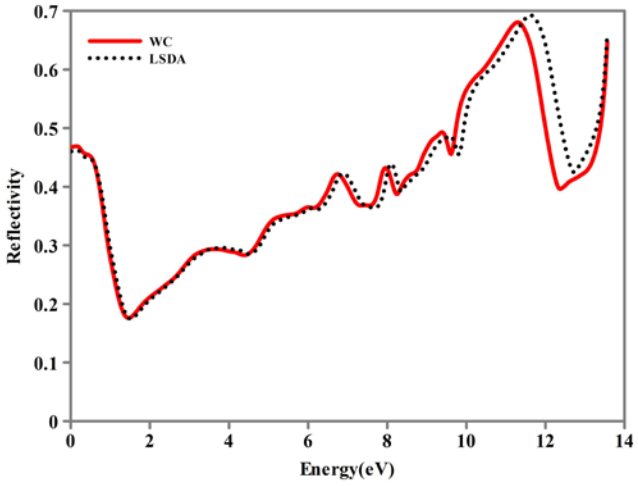


Fig. 5: Reflection coefficient of TiN.

Az seen in Figure 5, maximum amount of reflection for this combined Have been seen in energy range 10 to 12 Electron Volt by applying both approximation.

Optical conductivity:

Relevance between optical conductivity σ (ω) Inter-band of frequency dependent and the imaginary part of the dielectric function is as follows:

$$\sigma(\omega) = \left(\frac{\omega}{4\pi}\right)\varepsilon_2(\omega) \quad (5)$$

Journal of Applied Science and Agriculture, 8(5) October 2013, Pages: 652-657

Conductivity function is a complex function and calculated from the following equation:

$$\sigma(\omega) = \sigma_1(\omega) + i\sigma_2(\omega) \quad (6)$$

σ_1 (ω) is real part conductivity and σ_2 (ω) is the imaginary part of conductivity. Real part of the optical conductivity in terms of energy for the TiN is shown in Finger 6(a).

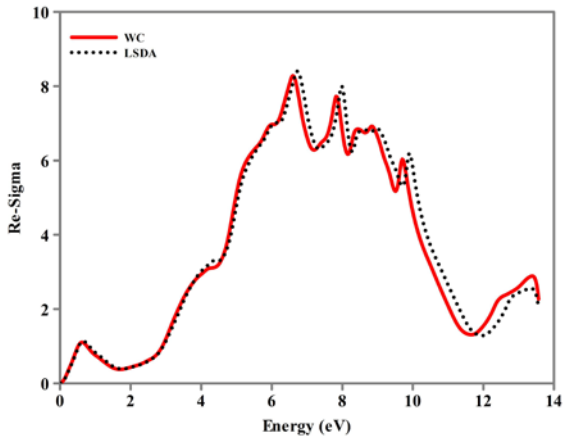


Fig. 6 (a): Real part of conductivity of TiN.

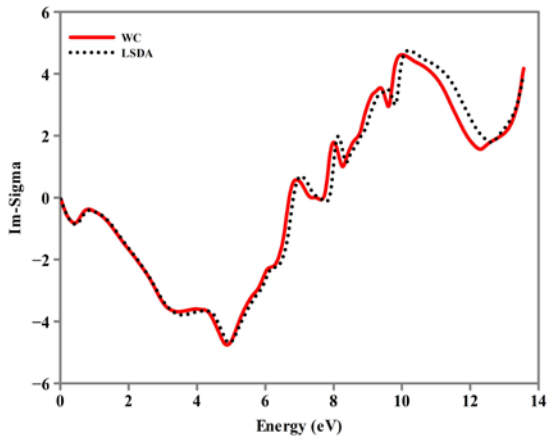


Fig. 6 (b): Imaginary part of conductivity of TiN.

The Imaginary part of the optical conductivity in terms of energy for the TiN is shown in Figure 6(b).

Conclusion:

The current study examined the optical properties of TiN with LSDA and WC functionals through the use of WEIN2k software program and compared the results with each other. We calculated the dielectric function, Electron energy loss function, reflection coefficient, optical conductivity, refractive index and extinction coefficient and compared the results related to the LSDA and WC functionals, finding out that there is little difference between the results obtained through the use of LSDA and WC functionals.

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