JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. **5** No 4, 04051(3pp) (2013)

ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том **5** № 4, 04051(3cc) (2013)

Optical Properties of MgF_2 / MgF_2 / Glass and MgF_2 / TiO_2 / Glass

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(Received 09 June 2013; revised manuscript received 08 July 2013; published online 31 January 2014)

MgF_2 thin films by thickness of 93 nm were deposited on MgF_2 / glass and TiO_2 / glass thin layers by resistance evaporation method under ultra-high vacuum (UHV) conditions, rotating pre layer for sample one and normal deposition for second one. Optical properties were measured via spectrophotometer in spectral range of 300-1100 nm wave length. The optical constants such as, real part of refractive index (n), imaginary part of refractive index (k), real and imaginary parts of dielectric function ε_1, ε_2 respectively and absorption coefficient (α), were obtained from Kramers-Kronig analysis of reflectivity curves. Band-gap energy was also estimated for these films.

Keywords: Multilayer semiconductors, Magnesium fluoride, Titanium dioxide, Kramers-Kronig.

PACS numbers: 78.20.Ci, 78.67.Pt

1. INTRODUCTION

Thin films producing technologies are developing rapidly and nowadays Nano techniques are using in producing them. Producing diodes and transistors was the first stage of using thin films. Most of modern and complex optical, electrical and electronic devices are covered by thin films.

Thin films mechanical properties are much dependent on microstructure and chemical composition, and so it depends on deposition technology. Conditions of thin films before deposition, deposition conditions and coatings are important [1, 2].

It is clear that the use of magnesium fluoride as a support for different catalytic materials, transition metal oxides like MoO_3 [3], V_2O_5 [4], WO_3 [5] and binary systems such as CuO and Cr_2O_3 [6, 7] more over for metallic catalysts like ruthenium ones [8, 9] is appealing. MgF_2 is a nonconductor with a wide band gap and has good thermal stability and considerable hardness.

Magnesium fluoride (MgF_2) is an optical material which stands cost-competitive methods transparent in a broad band of photon energies [10]. MgF_2 and LiF_2 are two materials with property of transmit ion in the vacuum ultraviolet range and applications in optical windows, lenses, prisms. The MgF_2 crystal is used in the electrolysis of aluminum ore and anti-reflective coatings [11], for which the surface structure and quality are important.

TiO_2 films under ultraviolet light act as antibacterial, deodorizing and self-cleaning (Matsubara et al 1995; Negishi et al. 1995; Kikushi et al. 1997). Conversely, the band-gap energy of TiO_2 is ~ 32 eV, so, UV illumination is essential to photo activate this semiconductor which is a weakness of it.

A number of techniques used to prepare films based on TiO_2 like sputtering, spray pyrolysis (Yanagi et al. 1997), sol-gel processing (Yoko et al. 1991) and chemical vapour deposition (CVD) (Lee et al. 1994; Schvisky et al. 2000).

For those applications these processes needs the and expensive devices for film deposition Titanium dioxide (TiO_2) has widely been studied as a good form material for solar cell, water splitting, and Photo catalysts [12-16]. These days attempts to find a material for improving performance, impregnation of guest elements in transition of metal oxides and surface revision of oxides is under performance [13, 17-23]. Enache et al. [19] used TiO_2 as a support for Au / Pd catalyst, and applied in oxidation of alcohols with remarkable results. Kim et al. [22] made a double (undoped TiO_2 and Cr-doped TiO_2) layer solar cell, and in comparison to TiO_2 single layer they got an improvement in efficiency.

In this paper we calculate optical properties of multilayers semiconductors such as MgF_2 / MgF_2 / glass and MgF_2 / TiO_2 / glass by Kramers-Kronig method.

2. EXPERIMENTAL DETAILS

Magnesium fluoride and Titanium dioxide thin films were deposited on glass substrates ($18 \times 18 \times 1$ mm cut from microscope slide) by resistive evaporation from Molybdenum and Tungsten boats for MgF_2 and TiO_2 respectively at room temperature and high vacuum conditions. The purity of Magnesium fluoride powder was 96 % and purity of TiO_2 powder was 98%. An ETS 160 (Vacuum Evaporation System) coating plant with a base pressure of $\sim 10^{-6}$ mbar was used. Prior to deposition, all glass substrates were ultrasonically cleaned in heated acetone first and then in ethanol. The substrate holder was a disk of 36.5 cm in diameter with adjustable height up to 50 cm and also adjustable holders for placing any kind of substrates. The distance between the center of the evaporation boat and the center of the substrate was 40 cm. Thickness of layers were determined by quartz crystal microbalance technique ($d = 90$ nm for MgF_2 and $d = 71$ nm for TiO_2 layers). Other deposition conditions such as deposition rate, vacuum pressure, and substrate temperature was same in all tests. Second step of experiments were as follow: for sample one, we used rotating MgF_2 / glass as substrate and we coat MgF_2 on

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substrate that tends to heterogeneous MgF_2 / MgF_2 / glass layer. For sample two, MgF_2 powder with normal deposition angle coated on TiO_2 / glass substrate and tends to four phase MgF_2 / TiO_2 / glass thin layer. Transmittance of the films was measured by using VIS spectrophotometer (Hitachi U-3310) instrument. The spect of layers were in the range of 300-1100 nm wave length (VIS), and for using Kramers-Kronig relations [24], we extrapolated of reflectivity curves with bulk standard samples [25].The optical properties such as n, k, ε_1, ε_2, α and Band-gap energy were obtained. There was a good agreement between them. Table 1 shows details of layers produced in this work.

Table 1 – Detail of layers produced

Sample	Multilayers	Vacuum presure (torr)	Thick-ness (nm)	Deposi-tion rate (A˚/S)
One	MgF_2 / MgF_2 / glass	~ 10^{-6}	93 and 93	0.7 and 0.7
two	MgF_2 / TiO_2 / glass	~ 10^{-6}	93 and 72	0.7 and 0.2

3. RESULTS AND DISCUSSION

Positions (a) and (b) in figure 1are showing transmittance and reflectance curves of layers in visible light range (300-1100 nm) respectively. As it can be seen reflectance and transmittance are different for layers.

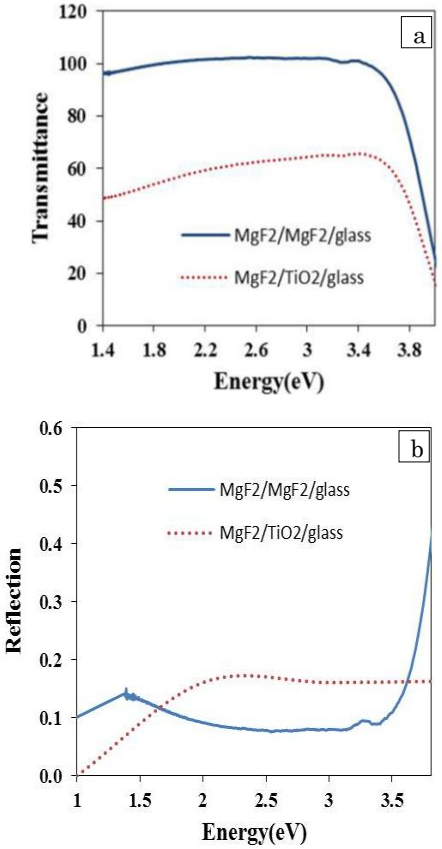


Fig. 1 – Transmittance and Reflectance curves of MgF_2 / MgF_2 / glass and MgF_2 / TiO_2 / glass: (a) Transmittance curve, and (b) Reflectance curve

The real and imaginary parts of reflective indices are shown in figures 2a and 2 b respectively. Real part of reflective index for sample one is a wide peek begin from 1.4 eV and ends 3.4 eV. Real part of refractive index for sample two, begins from a minimum at 1.4 eV and reach to a maximum at 3.8 eV. By changing material of last layer n, completely changes.

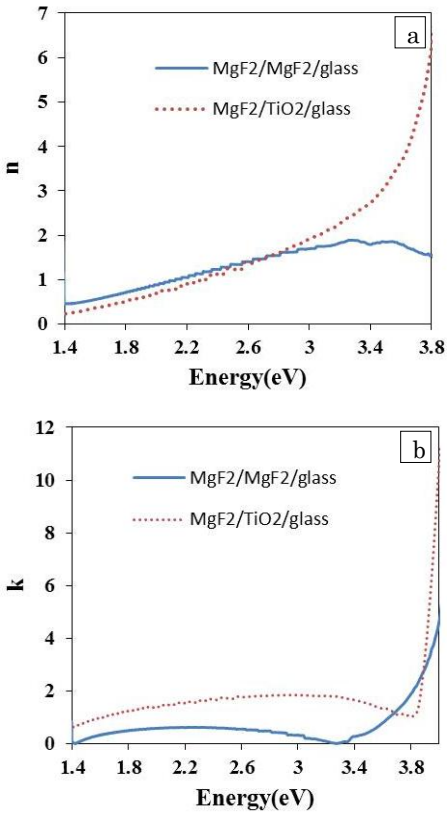
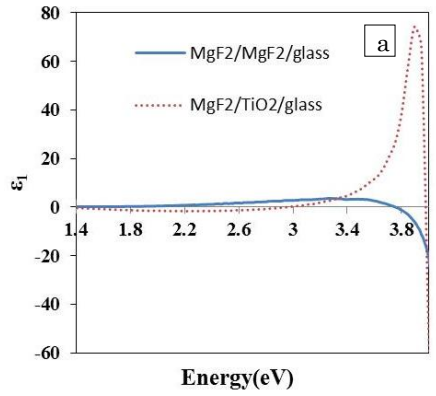


Fig. 2 – Real and Imaginary parts of reflective indices: (a) Real part, n, and (b) Imaginary part, k

Imaginary parts of refractive indices have same trend for both samples (one and two). There is a minimum at 3.3 eV for sample one and this minimum shifts to 3.8 eV for sample two.

Figures 3a and 3b show real and imaginary parts of dielectric constants respectively ε_1 and ε_2 for samples are completely different. In general second sample shows higher dielectric property.



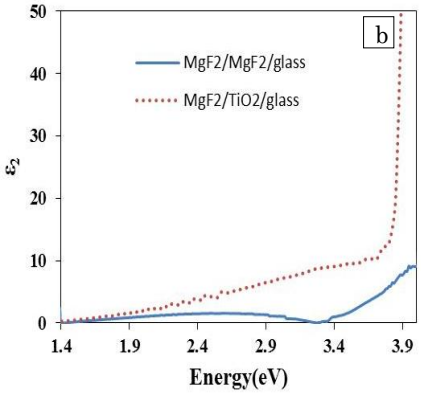


Fig. 3 – Real and Imaginary parts of dielectric constant: (a) Real part, ε_1, and (b) Imaginary part, ε_2

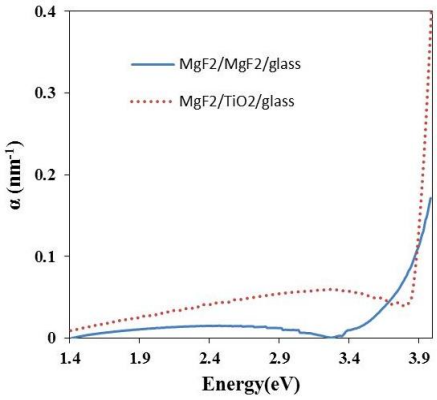


Fig. 4 – Absorption coefficient of MgF_2 / MgF_2 / glass and MgF_2 / TiO_2 / glass thin layers

Figure 4 shows absorption coefficient for both samples (one and two). Sample two in general shows higher absorption coefficient. That is because of formation more void on sample one by rotating substrate and of course TiO_2 had an ideal deposition angle that tends to less voids on layer.

Figure 5 shows band gap values for sample one and two, the value of band gap is 3.8 eV for sample one and 3.9 eV for sample two, that is in agreement with dielectric constants and other optical properties.

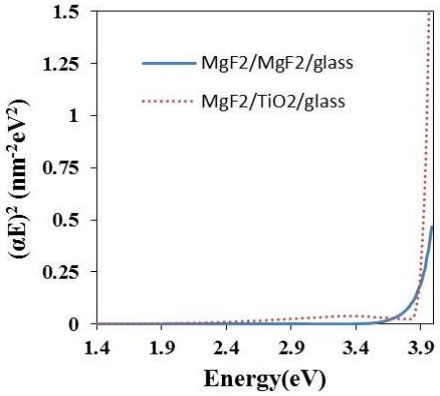


Fig. 5 – Band Gap of MgF_2 / MgF_2 / glass and MgF_2 / TiO_2 / glass thin layers

4. CONCLUSION

MgF_2 / MgF_2 / glass and MgF_2 / TiO_2 / glass multi layers were produced in this work at room temperature and HV conditions.

Reflectivity and transmittance of layers are completely different.

By using Kramers-Kronig relations on reflectivity curves optical parameters calculated MgF_2 / TiO_2 / glass layer in general showed higher dielectric property.

That is because of gettering property of Ti atoms. Band gap is about 3.9 eV for this layer.

For MgF_2 / MgF_2 glass band gap is about 3.8 eV that is much more less than a bulk MgF_2 (10.8 eV) almost insulator, so by Nano metric deposition we can produce semiconductors of MgF_2.

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