

PHYSICAL PROPERTIES OF ZnTe NANOCRYSTALS by ELLIPSOMETRY SPECTROSCOPIC

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Introduction

Recently the researches are focused on the elaboration and structural analysis of ZnTe nanocrystals (ZnTe-nc). The control of depth profile in the oxide layers can be made by controlling the implantation energy. However, high energy and dose of ion implantation can induce disorders and defects in the oxide [1]. In this work, these defects are taken into account in the modeling the data of variable angle ellipsometry. The Bruggeman effective medium approximation (EMA) combined with Critical Points (CPs) model [2] have been used to determine the values of layers thickness and optical properties of ZnTe-nc, and volume fractions of nanocrystals in silica. This model gives the optical gap value and all optical transitions of the ZnTe-nc.

Experimental and modeling details

Sample used in this study are 250 nm thick SiO₂ implanted with ZnTe and deposited on the Si substrate. Te⁺ and Zn⁺ are implanted using dose of 2.9.10¹⁶ ions/cm². Firstly, Zn⁺ is implanted at 115 keV and then Te⁺ at 180 keV. The temperature of the final annealing after implantation was 700° during 15 mn. Their respective energies for Zn⁺ and Te⁺ (115 and 180 keV) have been chosen to produce 5 at.% to 10 at.% maximum concentration for each species. The previous studies by X-ray diffraction and high resolution TEM show the formation of single-crystalline ZnTe precipitates (mainly cubic phase) [ref1]. Fig.1 shows the TEM image of the ZnTe-nc embedded in the SiO₂ matrix. The nanocrystals in this sample are organized

into a single band near to the surface with the radius ranging between 5 to 27 nm.

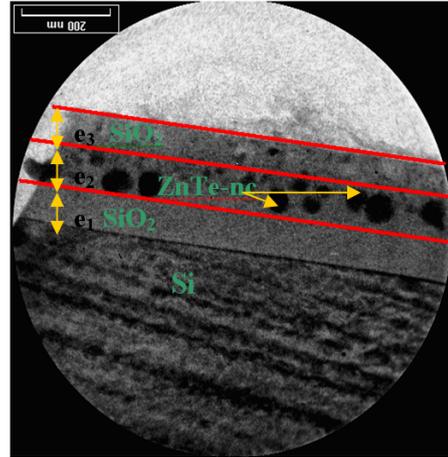


Fig.1 TEM images of the sample implanted with Zn (at 115 keV) and Te (at 180 keV) ions at dose 2.9.10¹⁶ ions/cm², the sample is annealed at 700°C during 15mn.

SE analysis are performed in air at room temperature at angles of incidence of 55°, 60° and 65° over the spectral range of 1.4 to 5 eV using rotating polarizer ellipsometer. According to the TEM image, the physical model is regarded as three sublayer system (Si/SiO₂ + nc-ZnTe/SiO₂). In the first step, the modeling of ellipsometric data is done by considering the optical properties of perfect SiO₂ matrix without defects. The calculated spectra for all angles of incidence show a disagreement with the experimental data. Different methods and strategies are tested to reduce this disagreement. The most realist model is found by considering the defects induced by implantation in oxide. The breaking of chemical bonds in host matrix is the principal effect of ionic implantation. The defects of the silica related to the breaking of these bonds are essentially the deficiencies or the excess of oxygen. The

major optically active defects in silica are the B₂ center with absorption line around 5 eV and the E' center with absorption line around 5.8 eV. Other defects and their characteristics related to the excess of oxygen with a peak positions of absorption bonds near to 2, 4.4 and 4.8 eV have been observed. Although most of them are located in the ultraviolet, the transitions linked to these defects could have the direct consequences on the visible spectrum. The modeling of such defects is not obvious. We made the choice of modeling the oxide defects by adding an oscillator to the silica dielectric function. The new dielectric functions of SiO₂ with defects are given in Fig. 2.

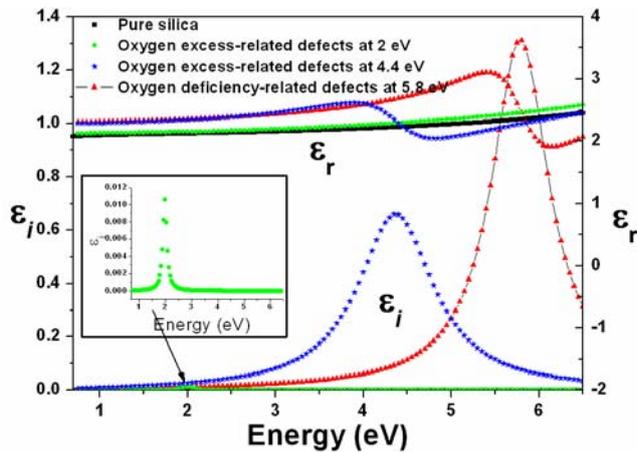


Fig.2 calculated dielectric function of SiO₂ matrix by considering defects attributed to oxygen excess.

In this case, a good agreement is found between experimental data and calculated spectra by considering 25% of the silica in the top layer as damaged by E' center defects. The second sublayer is considered as a mixture between ZnTe-nc and silica having 25% of defect with an absorption peak at 4.4 eV. Finally, the first sublayer is containing only the silica, damaged at 10% by silica defects characterized by a peak of absorption at 2 eV. The SiO₂ sublayer with embedded ZnTe-nc is considered as an effective medium according to the Bruggeman effective medium approximation (EMA). The complex dielectric function of ZnTe-nc (ϵ_{nc}) is

determined using the dispersion model based on Critical Points (CPs) formalism. The details formulas of this optical dispersion model are given in Ref. [2]. This model can yields not only the information about the dielectric function, but also the band gap and other optical transitions that can be occur in the considered spectral range.

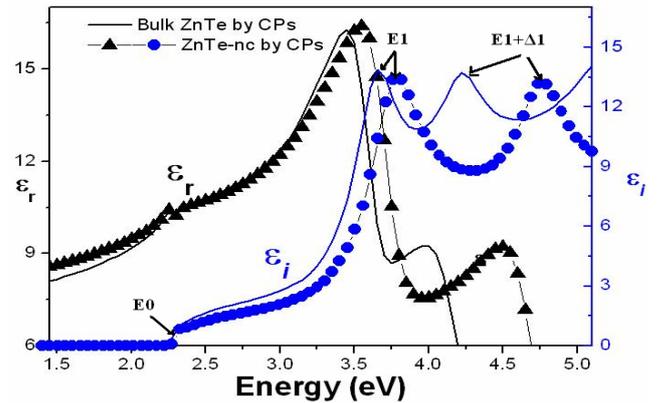


Fig. 3 Dielectric function of ZnTe nanocrystals in comparison with bulk ZnTe [2]. E_0 is direct optical gap, E_1 , $E_1 + \Delta_1$ represent the optical transitions.

Conclusion

We have investigated by spectroscopic ellipsometry the dielectric function of ZnTe nanocrystals (ZnTe-nc) over the spectral range of 1.45–5 eV. The size of nanocrystals has an influence on the optical properties in comparison with bulk ones. This influence is clearly observed on the distinct structures E_0 , $E_0 + \Delta_0$, E_1 , and $E_1 + \Delta_1$ associated with the direct optical gap and spin orbit splitting. The high dose implantation leads to increase the density of defects in silica. These defects are located at 2.7, 4.4 and 5.8 eV.

References

- [1] A. En Naciri, M. Mansour, L. Johann, J. J. Grob, and H. Rinnert. *J. chem. Phys.* **129** (2008) 184701-184708
- [2] K. Sato and S. Adachi *J. Appl. Phys.* **73** (1993) 926-931