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The Effect of Changing Pb Molar Concentration on Some Optical CTP properties of TiO3

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Abstract
Titanium oxides are extensively used in many optoelectronic applications. This encourages to dope TiO2 with Pb to see how the optical properties change. The results obtained indicated that the absorbance, absorption coefficient, extinction coefficient increases upon increasing the Pb molar concentration. However increasing the Pb concentration decreases the transmittance .The reflection coefficient attains maximum values in the range of 250 to 330 nm.
Keywords: Titanium oxide, Lead, absorption coefficient, transmission, reflection, extinction

1.Introduction
Thin films were nowadays one of the most important widely used techniques in electronics and telecommunications.

[1]. The optical and the electric properties of thin films are the important parameters which are adjusted and modified to satisfy the desired requirement . The material interaction with electromagnetic variation spans the wide range of frequencies from X-rays, ultraviolet visible, infrared, down to radio waves [2]. The materials can classified according to their electrical properties to conductor, semiconductors, insulators and superconductors [3].The electric permittivity and magnic permeability reflect the ability of the medium to allow electric and magnetic fields to pentrate [4, 5]. optical properties and the electrical properties of matter are important in solar cells [6,7].Solar cells are nowadays widely used in solving the energy problem [8,9].The silicon solar cells are now the widely used and available source of energy free from pollution .Unfortunately the silicon solar cells are very expensive and have low efficiency. This encourages researchers to search for new solar cells types. The most promising alternative is the so called nano solar cells. Nano solar cells are based on the so called nano science [10] . Nano science is concerned with describing he behaviour of nano materials.Nano materials are aggregates of a large number of small tiny particles having dimensions ranging from 1 to about 300 nano meter (nm).

Naon is the Greek word (meaning dwarf) refers to a reduction of size, or time, by 10^{-9}, which is one thousand times smaller than a micron. One nanometer (*nm*) is one billionth of a meter and it is also equivalent to ten Angstroms. Nanoscience is a new discipline concerned with the unique properties associated with nanomaterials, which are assemblies of atoms or molecules on a nanoscale. Nanoscience is actually the study of objects/particles and its phenomena at a very small scale, ranging roughly from 1 to 300 nm [12].Nanomaterials physical properties can be easily controlled, since they are described by quantum lows. This encourages to do a lot of work to improve the physical properties of thin films like titanate films doped with lead. One of these work was done by Hassan Chaib to study the electrical and optical properties of lead titanate (PbTiO3) at room temperature. The properties are theoretically investigated by using a microscopic model based on the orbital approximation in correlation with the dipole-dipole interaction. Using the microscopic quantum model based on theorbital approximation and the dipole-dipole interaction due to the local electric field acting on the constituent ions, of PbTiO3 at room temperature[13], the findings shows that the experimental data of the spontaneous polarization and refractive indices are successfully explained by considering the nonlinearity and anisotropy of the first-, second- and third-order electronic polarizabilities of the constituent ions, particularly that of the O2−z-ions. The local electric field points along the 3-direction, sponteneous polarizability is found to measure ~ 0:7078C=m 2, while no and ne are 2.7031 and 2.6678. Another different theoretical approach for studying the spontaneous polarization and refractive indices of PbTiO3 at room temperature was also developed [14]. The microscopic model takes into account the anisotropy in the first-, second-, and third-order electronic polarizabilities of all constituent ions, their ionic shifts as well as the crystalline deformations. The model was previously tested for determination of bulk properties of mono-domain tetragonal perovskites like BaTiO3and KNbO3, i.e. their ferroelectricity and optical anisotropy as well as their linear electrooptical coefficients. [15]. Furthermore the same model was successfully applied for modelling electrical and optical properties of LiNbO3 single crystals and ferroelectric domain walls in BaTiO3 [16] Based on those experiences which agree excellently well with the corresponding experimental data, we initiate here the application of this model to PbTiO3.

The study of Maryam Lanki [16] aimed to decrease the crystallization temperature of the tetragonal perovskite PbTiO3 nanopowders below the PbTiO3 Curie temperature. The calcination temperature was selected based on the thermal analysis of the PbTiO3gels, came out at 680°C. However, reconsidering the thermal properties of the PbTiO3 gel revealed the possibility of the formation of single tetragonal perovskite phase at lower temperatures. The results obtained indicate that well crystalline pure phase PbTiO3 nanopowders have been synthesized after calcination of the PbTiO3 gel at 460°C, which is quite to the Curie temperature of the PbTiO3nanoparticles[17]. To improve crystallization of the samples prepared at 460°C, the effect of the heat treatment parameters and Pb content on gel crystallization and the Pb-partitioning phenomenon were investigated on the nano scale. The researchers have obtained single phase crystallization of lead titanate nanopowders by the sol-gel method at 460°C which is a much lower temperature than the 650-700°C range, as reported by others [18]. Crystallization at 460°C decreases Pb evaporation efficiently during the heat treatment , which can minimize release of toxic Pb compounds in the environment and can protect the stoichiometric ratio of Pb/Ti. XRD results on the calcinated nanopowders indicated that the complete crystallization of the amorphous PbTiO3 into the PbTiO3 perovskite is possible only after optimizing the heat treatment condition and investigating the effect of Pb concentration . TEM results showed that well crystalline PbTiO3 nanoparticles with a uniform morphology

can be produced at 460°C whereas formation of such nanoparticles have already been reported above 650°C .

Massaud Mostafa Lank [19] studied Lead titanate (PbTiO3; PT) powders properties prepared by a sol –Gel technique. PT powders were heated at different calcination temperatures, ranging from 500 to 1000 ºC, for 2 h at a heating/cooling rate of 5 ºC/min. The findings showed that well crystalline pure phase PbTiO3 nanopowders have been synthesized after calcination of the PbTiO3 gel at 1000 ºC. The second phases such as PbO, and TiO2 were detected in the powders calcined below 1000 ºC. The electrical properties were determined for deferent annealing time. PbTiO3 nanoparticles were prepared by Sol-Gel method . The research out comes showed that PbTiO3 was successfully synthesized as nanoparticles at 1000 °C calcinations temperature for 2 hours. TEM results indicated that the average grain size of pure PT powder is about 12.49 nm. The SEM findings indicated the presence of wall domains at 180° .The energy gap assumed the value equal to 2.6 eV. Dramatical change in the curie temperature (635 °C) was observed and the maximum dielectric reached high value about (312) .
The work of Jair Baltazar [20], Lead titanate ceramics modified by xenotime (Xm) with nominal composition (Pb, Xm)TiO3, Xm10 or 15 mol %, were prepared by oxide mixture technique. Xenotime is a natural mineral consisting of a mixture of rare earth oxides. The results obtained indicate a higher density and free of cracks ceramic body , compared to pure PbTiO3 prepared by the same techniques . The structural characteristics and Curie temperature are nearly the same as those of pure PbTiO3. The hysteresis loop measured at room temperature showed a hard ferroelectric material with coercive field of 10.7 kV/cm and a remanent polarization of 0.2 µC/cm2 . Lead titanate ceramics modified with 10 and 15 mol% of a natural mixture of rare earth oxide of xenotime were prepared by conventional technique . The obtained samples were found to be dense and free of cracks ceramic bodies [21]. PXT compositions show low relative dielectric permittivity and high Curie temperatures, compared to others based PbTiO3 ceramics. These features are important to produce piezoelectric devices to operate at high frequencies and high temperatures. The dielectric permittivity and Curie temperature of PXT ceramics showed a very low sensibility of these compositions to different xenotime contents, confirmed by similar properties of PXT10 and PXT15 compositions [22].

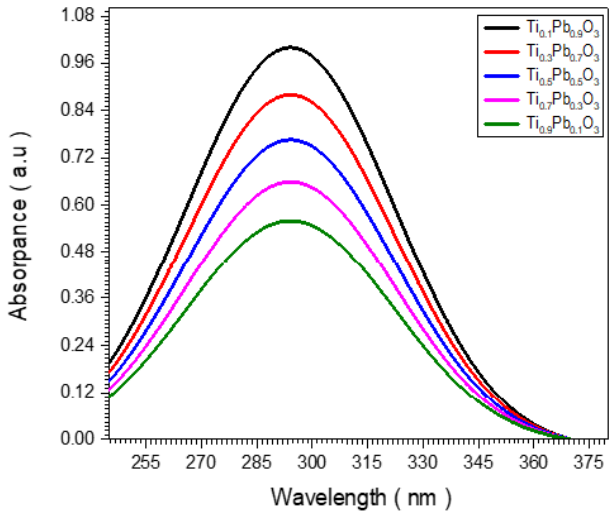
The work done by M. F. M. Taib [23] studied the physical properties of cubic (Pm3m, 221 space group) perovskite prototypes PbTiO3(PTO), SnTiO3(STO) and SnZrO3(SZO). Their physical properties were investigated using the density functional theory as implemented in CASTEP computer code. The lattice parameters of PbTiO3(as the reference compound) were calculated. The theoretical findings of the functional (GGA-PBEsol) were in agreement with the experimental results with typical error of approximately 0.6% underestimate . The density of state studies indicated hybridizations among anion O 2p, cation Pb 6s/Sn 5s and the Ti 3d/Zr 4d states of PTO, STO, and SZO. An indirect band gaps were obtained for both PTO and STO at the X-G point. A direct band gap was attained for SZO at the X-X point along the high-symmetry direction in the Brillouin zone. The born effective charge values of PTO, STO, and SZO were attributed to the responses of the bond charges to the displacement caused by the strong covalency between the cation orbital and O 2p (strong covalency A-O and B-O bonding). The findings showed that anion O 2p, cation Pb 6s/Sn 5s, and Ti 3d/ Zr 4d states are essential for the instability of perovskite oxide. Comparative results from the PTO, STO, and SZO prototypes indicated that the theoretical and experimental values were in good agreement. The properties of the cubic PTO, STO, and SZO prototypes were studied via the first-principles calculation using GGA-PBEsol functional

technique [26]. The results obtained indicate that different properties are comparable with previously reported theoretical and experimental studies. All compounds are mechanically stable, and the electronic results show the hybridizations of Pb-O and Ti-O in PTO, Sn-O and Ti-O in STO, and Sn-O and Zr-O in SZO. The BEC results show the covalencies of A-O and B-O exist in Sn-based compounds. Hence, this property is very important for the instability of the perovskite structure [24]

Sergio de Lazaro [25] studied structural and electronic properties of the bulk and relaxed surfaces (TiO2and PbO terminated) of cubic PbTiO3 using periodic quantum-mechanical calculations based density functional theory. The results obtained indicate that the difference in surface energies is small and relaxations effects are most prominent for Ti and Pb surface atoms [28]. The electronic structure shows a splitting of the lowest conduction bands for the TiO2 terminated surface and of the highest valence bands for the PbO terminated slab. The indirect band gap assumed the values : 3.18, 2.99 and 3.03 eV for bulk, TiO2 and PbO terminations, respectively . The structural and electronic properties of the bulk and the two possible (0 0 1) surface terminations of cubic PbTiO3 have been studied by employing first-principles calculations based on B3LYP . The findings showed that The bulk equilibriumgeometry, equation of state parameters and the optical band gap are in agreement with experimental results . The relaxed optimal positions are most prominent for Ti and Pb atoms at the 1st layers. In both terminations, the surface dipole points toward the bulk, whereas the subsurface dipole points toward the vacuumregions; the magnitude of dipole moment decreases from the surface to the central layer. This and the fact that our slab is symmetric causes that this moment disappears and the slab is paraelectric. The optical band gap values are 3.18, 2.99 and 3.03 eV for bulk, TiO2 and PbO terminations, respectively .

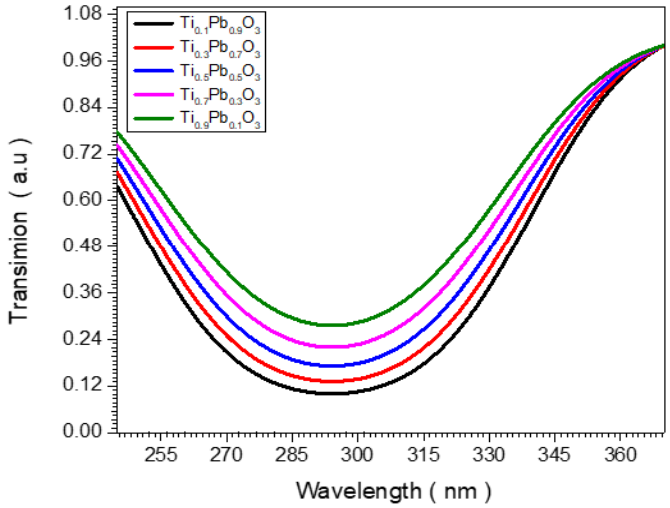
The aim of this work is to study the behavior of Titanium oxide doped with lead. This work is exhibited in section 2.Section 2 and 3 are devoted for discussion and conclusion.

2.*Optical Results of* Titanium Oxide doped by Lead Oxide*($Ti_x Pb_{1-x} O_3$) samples and discussion*



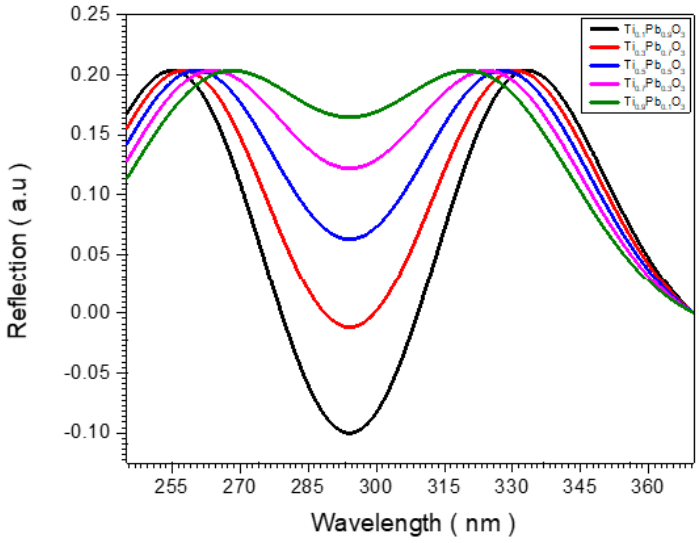
Fig(1) relation between absorbance and wavelengths of ($Ti_x Pb_{1-x} O_3$) samples

Absorbance spectra for Titanium Oxide doping by Lead Oxide by the form ($Ni_xPb_{1-x}O_3$) samples were studied using UV-VS min 1240 spectrophotometer. It shows maximum increase of the a absorption at wavelengths 290 nm responding photon energy 4.28 eV . The effects of increase molar concentration of Pb indicated that the absorbance increases upon increasing Pb concentration .



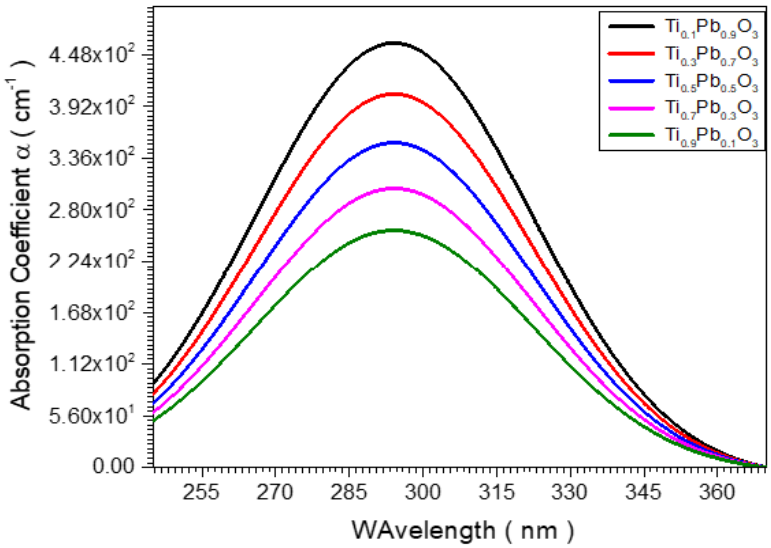
Fig(2)relation between transmission and wavelengths of ($Ti_xPb_{1-x}O_3$) samples

The transmission spectra for Titanium Oxide doped by Lead Oxide in the form ($Ni_xPb_{1-x}O_3$) were studied also using UV-VS min 1240 spectrophotometer . The findings showed minimum decrease of the a transmission at wavelengths 290 nm associated with the observed maximum absorption. Upon increasing molar concentration of Pb the transmission decreased .



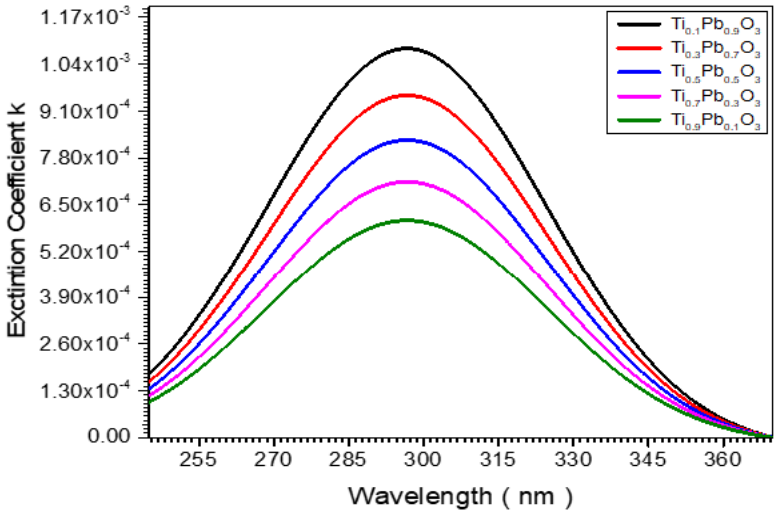
Fig(3) relation between reflection and wavelengths of ($Ti_xPb_{1-x}O_3$) samples

The optical reflectance(R) spectra in the range of (245 - 380) nm indicated that the maximum reflection observed is in the range (250 to 330) nm for all samples , where it decreases beyond 330 nm.



Fig(4) relation between absorption coefficient and wavelengthsof ($Ti_x Pb_{1-x} O_3$) samples

Absorption coefficient (α):The absorption coefficient (α) of the five prepared samples shows that for ($Ti_xPb_{1-x} O_3$) ,$\alpha = 0.459x10^3$ cm^{-1} and for ($Ti_{0.9}Pb_{0.1} O_2$) is equal to $0.257x10^3$ cm^{-1} .This means that the transition must correspond to a indirect electronic transition, and the properties of this state is important since it is responsible for electrical conduction .The absorption coefficient (α) for Titanum Oxide doped by Lead increases when Pb concentration increased .



Fig(5) relation between extinction coefficient and wavelengthsof ($Ti_x Pb_{1-x} O_3$) samples

For the extinction efficient it is observed that the spectrum shape of (K) is the same as the shape of (α). The Extinction coefficient (K) depends on the samples molar concentration. The value of (K) at 290 nm for ($Ti_{0.1}Pb_{0.9} O_3$) is equal $1.08x10^{-3}$ while for the other sample ($Ti_{0.9}Pb_{0.1} O_3$) at the same wavelength is equal to $6.05 x10^{-4}$ .The results shows that the extinction coefficient was increased when the Pb concentration was increased .

Conclusion

Doping TiO2 with Pb change some optical properties . The results obtained indicated that the absorbance, absorption coefficient, extinction coefficient increases upon increasing the Pb molar concentration. However increasing the Pb concentration decreases the transmittance . The reflection coefficient attains maximum values in the range of 250 to 330 nm.

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