

Remoción de Cr^{6+} de lixiviados de tiraderos de basura empleando arcillas modificadas o activadas

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Los residuos sólidos depositados en los rellenos sanitarios a cielo abierto generan los lixiviados, con la consecuente biodegradación molecular de la materia orgánica y la presencia de metales pesados como plomo, cromo, cadmio, hierro, etc., los cuales originan la afectación directa del subsuelo y de los mantos freáticos. Si se considera que los metales pesados son carcinógenos, teratológicos y tóxicos a la salud humana, hay razones de peso para implementar tratamientos que eliminen estos contaminantes. Por ello, los estudios de procesos que lleven a la disminución, eliminación o encapsulamiento del Cr^{6+} son de particular importancia, dadas sus características adversas a la salud.^{1,2}

El uso de arcillas como agente adsorbente de cromo,³ como fotocatalizador o como soporte,^{4,5} como decolorante,⁶ en la eliminación de pesticidas,⁷ o bien como aditivo en la industria cosmética⁸ y recientemente en el estudio de liberación de drogas,⁹ se ha documentado ampliamente. Dada la complejidad de su composición química, su aplicación depende principalmente del contenido de los diferentes tipos de arcillas para un material en particular. Usualmente, es difícil separar cada constituyente y, debido a ello, es más común que una vez caracterizado el material, se busque un uso para éste.

Las arcillas naturales se clasifican con respecto a su forma como minerales arcillosos en placas (filosilicatos), arcillas minerales fibrosas y arcillas amorfas.¹⁰ Asimismo, es normal encontrar que una arcilla natural contenga cantidades significativas de feldespatos (aluminosilicatos). Estas estructuras, en general, se caracterizan por formar cadenas de SiO_2 (feldespatos), mientras que en las arcillas las unidades que las conforman son del tipo $\text{Si}_2\text{O}_5^{2-}$. Este es un dato importante a considerar, pues la “avidez de carga” que presentan las arcillas, aunada a la debilidad de los enlaces interlaminares, hacen proclives estos materiales a un intercambio iónico en sus espacios tetraedrales u octaédrales. Una razón más para im-

plementar el uso extensivo de las arcillas sería, principalmente, por sus valores de área superficial, los cuales oscilan entre 80 y 300 m^2/g .

En el presente trabajo se muestran los resultados de la aplicación de una arcilla compuesta principalmente por los elementos Si, Mg, Mn, Fe, K, Ca, asociados en las fases montmorillonita, haloisita y ortoclasa, la cual se modificó o activó para determinar su capacidad de adsorción de Cr^{6+} contenida en un lixiviado de tiraderos de basura de la ciudad de Morelia. La aplicación de este caso de estudio puede extrapolarse a la limpieza de tiraderos de otras partes del país donde haya escurrimientos similares y de ahí la importancia del presente trabajo.

EXPERIMENTAL

La arcilla utilizada en todas las pruebas provino de la Mina de Agua Blanca, municipio de Ciudad de Hidalgo, Michoacán. A partir de resultados de investigaciones preliminares se determinó la granulometría adecuada como malla 14-30 serie Tyler.^{11,12} En los experimentos exploratorios se manejó un volumen constante de lixiviado de 50 mL, variando el peso de arcilla. Inicialmente, se dispuso de una arcilla constituida por montmorillonita, haloisita y ortoclasa (feldespato), con la composición Mg 0.36, Al 4.18, Si 27.36, K 1.15, Ca 0.64, Mn 0.19, Fe 1.44, O 64.68 (expresados como % atómico). Los datos sobre la determinación de su estructura inicial y composición se resumen en las secciones subsecuentes.

Proceso de activación de la arcilla

Este se realizó mediante el procedimiento establecido por Amirtharajah.¹³ La arcilla triturada se mezcló con una solución a 3.5% de ácido sulfúrico para formar una mezcla espesa; la proporción aproximada de la solución fue 35% del peso total de la arcilla. Posteriormente se trató la mezcla con vapor a temperatura de 93 a 99°C durante 5 a 6 h. La mayor parte

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Research Article

Assessment of Functionals for First-Principle Studies of the Structural and Electronic Properties of δ -Bi₂O₃

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Fully relativistic full-potential density functional calculations with an all-electron linearized augmented plane waves plus local orbitals method were carried out to perform a comparative study on the structural and electronic properties of the cubic oxide δ -Bi₂O₃ phase, which is considered as one of the most promising materials in a variety of applications including fuel cells, sensors, and catalysts. Three different density functionals were used in our calculations, LDA, the GGA scheme in the parametrization of Perdew, Burke, and Ernzerhof (PBE96), and the hybrid scheme of Perdew-Wang B3PW91. The examined properties include lattice parameter, band structure and density of states, and charge density profiles. For this modification the three functionals reveal the characteristics of a metal and the existence of minigaps at high symmetry points of the band structure when spin-orbit coupling is taken into account. Density of states exhibits hybridization of Bi 6s and O 2p orbitals and the calculated charge density profiles exhibit the ionic character in the chemical bonding of this compound. The B3PW91 hybrid functional provided a better agreement with the experimental result for the lattice parameter, revealing the importance of Hartree-Fock exchange in this compound.

1. Introduction

The VI-bismuth compounds Bi₂O₃, Bi₂S₃, and Bi₂Te₃ comprise a family of technological semiconductors [1] employed in diverse areas of industry. Bi₂O₃ has been used as an effective cocatalyst for oxidation of ammonia since the beginning of the last century; also it has been used as the precursor for the production of Bi₂MoO₆, a catalyst popularly used in the selective oxidation of propylene into acrolein [2]. Galván et al. [3] showed that, using the same compound in CO to CO₂ conversion, a significant improvement in the oxidation process could be obtained, while it is likely to be used as a catalyst in catalytic converters to clean the exhaust discharge. Moreover, metal oxides, bismuth oxides, and rare-earth oxides form the basis for some of the ceramic high T_c -superconductors [4].

Bismuth oxide is a polymorphic material that crystallizes in five modifications [5]. δ -Bi₂O₃ is formed from heating monoclinic α -Bi₂O₃ at 730°C and it is stable up to the melting point of 824°C. Tetragonal (β -Bi₂O₃) and body-centered cubic (γ -Bi₂O₃) modifications have been obtained below 650°C as metastable phases [6]. The hydrothermal method was used to obtain ϵ -Bi₂O₃ phase [7]. It is currently accepted that the cubic oxide δ -Bi₂O₃ is one of the most promising materials which can be used as solid electrolyte [8] in high technology equipment such as fuel cells, sensors, and membrane devices which utilize the unusual high oxide ion conductivity of this compound, a conductivity which exceeds that of stabilized zirconia [9, 10]. Several structural models for δ -Bi₂O₃ have been proposed [8, 11–13]. According to a model by Sillen [12], six possible oxygen sites of the fluorite unit cell are occupied and two others are empty and ordered

The influence of Ce doping on the structural and optoelectronic properties of RF-sputtered ZnO films

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Abstract Using X-ray diffraction, UV-Visible spectroscopy, XPS and photoluminescence (PL) measurements, the structural, optical and electronic properties of ZnO and Ce-doped ZnO thin films were investigated; the films were deposited on glass substrates by RF reactive-magnetron sputtering and post-annealed at 300 °C in an oxygen atmosphere. Under similar deposition conditions, both films crystallized into hexagonal wurtzite lattice structures. The pure ZnO film exhibited a c-axis preferential orientation, whereas the Ce-doped exhibited an a-axis preferential orientation. The films display uniform textured surfaces with columnar-like microstructures. The UV-Vis spectra showed high transparencies of 90 % on average for both films. Band gaps of $E_g = 3.23$ eV and $E_g = 3.27$ eV for pure and Ce-doped film, respectively, were measured. The doped film spectrum was shifted to the blue as a result of the Burstein-Moss effect. The XPS spectra show that the VB edge of the doped film shifts toward lower binding energy, at ~ 1.3 eV below E_F , while the VB edge of the pure film is located at ~ 2.0 eV below E_F . Additionally, Ce^{3+} and Ce^{4+} ions coexist in the ZnO matrix in fractions of ~ 70 and ~ 30 %, respectively. The PL spectra show that both types of ions induce extra electron states that allow multiple emission peaks in the blue-green region.

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A new correlation for the prediction of refractive index and liquid densities of 1-alcohols

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ABSTRACT

This paper presents a new correlation for the refractive index of 1-alcohols. The correlation relies upon a linear behavior with temperature from (293 to 353) K. This correlation uses the carbon number as a variable, and the universal constants result from curve fits of 117 experimental refractive index measurements for 1-alcohols from methanol to 1-decanol. The new equation correlates the refractive index within an average absolute percentage deviation of 0.05%. The correlation for the density also uses the temperature, the carbon number and the refractive index as variables. The new density equation correlates the density of 1-alcohols from (159 to 373) K within an average absolute percentage deviation of 0.08%. The extrapolative ability of both equations agrees with the data within the experimental error.

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1. Introduction

Refractive index is a parameter related to the behavior of light as it crosses a medium. From a microscopic point of view, the refractive index depends upon the electric and magnetic characteristics of the medium, and the temperature and the wave length of the emitted light [1]. The refractive index can indicate the purity of a substance or quantify the amount of a component in a binary mixture. Ortega [2] measured the refractive index of pure 1-alcohols from methanol to 1-decanol at temperatures from (293 to 353) K. He used a straight line to represent the temperature functionality of the refractive index. Several authors [3,4] have tried to calculate the refractive index of mixtures using different mixing rules. To the best of our knowledge, no correlation exists for the pure 1-alcohols refractive indices. This work presents a generalized correlation for the refractive index of 1-alcohols as a function of the carbon number and the temperature.

Development of generalized correlations for the prediction of densities is important for design of unit operations equipment, and to determine flow through pipes, heat exchangers or mass transfer equipment [5].

Many researchers have developed different correlations for the densities of homologous series [6,7]. Generalized correlations for the density of 1-alcohols at atmospheric pressure do not exist, but some attempts exist to provide generalized correlations for the density of 1-alcohols at high pressure. Assael et al. [8] correlated the liquid densities for methanol through 1-dodecanol using individual polynomials of temperature. Later, Saleh et al. [9] proposed an isothermal equation for the molar volume of pure 1-alcohols as a linear function of the number of CH₂ groups. Their equation predicts the density from ethanol to higher carbon number alcohols. Nasrifar and Moshfeghian [10] developed an equation to calculate the liquid densities of pure components and their mixtures using as variables the critical properties and the dipole moments of the pure components. In the literature, relationships exist between the refractive index and the liquid density such as the Lorentz–Lorentz [11,12], Dale–Gladstone [13], Eykman [14], Oster [15], Arago–Biot [16] and Newton [17] equations. This work uses this concept to develop a generalized correlation for the calculation of the liquid densities of 1-alcohols. No generalized correlations for the liquid densities of 1-alcohols appear in the literature. The new correlation uses the number of carbon atoms and the temperature as independent variables.

In this work, it became obvious that the Eykman [14] relationship successfully correlates refractive indices with the liquid densities for 1-alcohols to form a generalized correlation.

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Investigation of the annealing effects on the structural and optoelectronic properties of RF-sputtered ZnO films studied by the Drude–Lorentz model

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Abstract Zinc oxide films were deposited on glass substrates by RF reactive magnetron sputtering and post-annealed in vacuum at 100, 200, and 300 °C. Structural and optical properties of films were obtained using X-ray diffraction and UV–visible spectroscopy. Optical parameters were extracted from transmittance curves using the single-oscillator Drude–Lorentz model. The evolution of the optical and structural properties of films with the annealing process was investigated. The films crystallized into the hexagonal wurtzite lattice structure, with preferential growth along the *c*-axis [0002]. The results indicate that the crystalline quality of films improved with annealing, whereas transparency was reduced from 90 to 80 % at 300 °C. With post-annealing, the absorption edge shifted to the red, while the optical band gap decreased from $E_g = 3.28$ to $E_g = 3.26$ eV because of the Burstein–Moss effect. Calculated values of plasma frequency, ω_p , fall within the IR range and decrease with temperature, from $\omega_p = 5.56 \times 10^{14}$ rad/s (2950 cm^{-1}) to $\omega_p = 1.1 \times 10^{14}$ rad/s (587 cm^{-1}).

1 Introduction

Zinc oxide (ZnO) is a binary transparent conducting oxide (TCO) with properties of great interest due to their basic scientific research and potential technological applications [1–6]. ZnO has a wurtzite crystalline structure (lattice spacing $a_0 = 3.24 \text{ \AA}$ and $c_0 = 5.20 \text{ \AA}$). ZnO also possesses a wide ordinary optical band gap (E_g) of ~ 3.3 eV, which makes it transparent in the UV–Vis–NIR region, and a large exciton binding energy (60 meV), which enhances the luminescence efficiency of light emission [1, 7, 8]. This material has garnered much commercial and scientific interest compared with other TCO films, such as indium tin oxide [9]. The numerous advantages of ZnO include the tuning of its physical properties, its low cost, its abundance in the earth, its non-toxicity, and its compatibility with large-scale processes and relative easy fabrication [5, 9–11]. Several techniques have been used to grow ZnO films, such as pulsed laser deposition [3], DC reactive magnetron sputtering [4, 5], atomic layer deposition [6], electron beam evaporation [12], sol–gel [13], and spray pyrolysis [14]. In this context, reactive radio-frequency (RF) magnetron sputtering is an attractive alternative method for growing ZnO films because of the more accurate thickness control and a higher uniformity compared with other thin-film deposition techniques [15, 16]. The properties of the ZnO films deposited by RF magnetron sputtering depend on the deposition parameters involved in the growth process, such as the RF power, sputtering gas pressure, gas flow rate, and temperature. By adjusting these processing parameters, ZnO films with properties that are compatible with optical devices may be obtained [8, 15, 16]. In regard to experimental parameters, post-annealing is a process widely used to improve the crystallinity and to reduce surface

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Advantages of Hydrothermal Synthesis to Produce Tunable TiO_2 Nanomicro Sized Photocatalysts and Their Effect in Lignin Degradation

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Studies on photocatalytic degradation of lignin are scarce, even though it is an effective method for treatment of industrial effluents. In the present work, an advanced oxidation process (AOPs), leading to the photodegradation of lignin aqueous solutions, is proposed by using microstructured (T-MT) and nanostructured (T-NT) titanium dioxide compounds. Hydrothermal synthesis, in accordance with an experimental factorial design considering time of synthesis, NaOH concentration and synthesis temperature, was used to produce tunable TiO_2 photocatalysts for further study of its effects on the degradation of lignin. Photocatalytic reactions were conducted in a micro reactor batch system under UV irradiation. The catalysts were analyzed by means of X-ray diffraction (XRD), scanning electron microscopy (SEM), surface area and porosity analyzer (BET), energy-dispersive X-ray spectroscopy (EDS) and UV-Vis diffuse reflectance spectroscopy. In order to optimize the yield reaction, an experimental factorial design was performed. According to our results, nanostructured TiO_2 consisting in different structural features and light absorption properties were produced using this method. It is shown that T-MT and T-NT compounds exhibit a wide range of values, for the kinetic parameters, in photoinduced degradation of methylene blue (MB) and lignin.

Keywords: Nanostructured titania; titania nanotubes; lignin degradation; hydrothermal; photocatalysis

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