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Síntesis coloidal (pH:8) de *CdSe* nanoestructurado y caracterización estructural por STM
Colloidal synthesis (pH:8) of nanostructured *CdSe* and structural characterization by STM

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Resumen

El estudio y creación de nuevos materiales semiconductores nanoestructurados son de gran importancia en el desarrollo de la ciencia, en particular el *Seleniuro de Cadmio* (*CdSe*) es uno de ellos. En este trabajo, se reportan los resultados de la síntesis coloidal del *CdSe* nanoestructurado para $pH: 8$. Las muestras fueron analizadas con el Microscopio de Tunelamiento (STM), del cual se concluyo que el material es un semiconductor electronegativo y, usando la Transformada de Fourier (FFT), se identificaron dos fases cristalinas: una cúbica con Factor de Empaquetamiento Atómico (FEA) equivalente al 69.12%, y una hexagonal con un FEA de 41.4%, además, fue posible identificar los parámetros de red de cada estructura, entre propiedades físicas del material. A partir de estos datos, se presenta una completa discusión y análisis de los resultados, tanto de laboratorio como con en el espacio de Fourier.

Palabras Clave: CdSe, FFT, Microscopio STM, pH.

Abstract

The study and creation of new nanostructured semiconductor materials are great importance in the science advances, in particular, one of them is *Cadmium Selenide* (*CdSe*). This work reports the results of the colloidal synthesis of the nanostructured *CdSe* at $pH: 8$. The samples were analyzed with scanning tunneling microscopy (STM), from which it was concluded that the material is an electronegative semiconductor and using FFT, two phases were identified: a cubic with an atomic packing factor (APF) equivalent to 69.12%, and hexagonal with an APF of 41.4%, it was also possible to identify the lattice parameters of each structure, among other physical parameters of the material. From these data, a complete discussion and analysis of the results is presented both in the laboratory and in Fourier space.

Keywords: CdSe, FFT, STM microscope, pH.

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1. Introduction

To know the physical characteristics of a material, different techniques are used, such as XRD, IR, atomic force microscopy and tunneling, among others. In this work the tunneling microscope (STM) was used to obtain information at the nanometer level of the *CdSe* semiconductor, since this material presents a direct gap type that can range from 1.4 to $3.8\ eV$ and shows two crystalline structures, being a material to which different applications can be given, according to its nature.

Some of the important characteristics to know about *CdSe* using the STM are its crystalline structure, which with the help of the FFT can be verified in the micrographs obtained, revealing some agglomerations of atoms in specific regions [11-13].

2. System Volume

The structure, crystal lattice and type of bond depend on the properties and characteristics of cadmium (*Cd*) and selenium (*Se*). Due to its electronic configuration, the

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distribution of the electrons in each element is identified and the structure of the compound is defined by the ionic bond between them, defining the electronic cloud. This bond allows us to identify that *Cd* yields electrons to *Se*, this process is favored since its conduction band is $1.7eV$ at room temperature [14-16].

Because every crystalline system is defined by an atomic volume, which depends on the number of atoms within each cell of the system under study, is very important know the atomic number in each cell. This case, for *CdSe* its volume was determined from equation 1:

$$N_{atom} = n_I + \frac{n_f}{2} + \frac{n_v}{6} \quad (1)$$

where N_{atom} = atoms number, n_I = number of atoms inside the cell, n_f = number of atoms on the faces and n_v = number of atoms at the apex (vertex).

We used $n_I = 1,\ n_f = 0,\ n_v = 12$ and from (1), the number of atoms per cell is $N_{atom} = 3$. This data only refers to the number of atoms in a cell, so it is repeated in the next parallel cell, it is considered twice as many atoms contained in a volume formed by both, i.e. $N_{atom} = 6$.

For the volume (eq. 2) contained within the structure of the hexagonal prism we have:

$$V_c = \frac{3\sqrt{3}}{2}a^2c \quad (2)$$

the values $a,\ c$; that are used into the (2), they were obtained with the help of the STM software; where the length between each spatial lattice is defined by the interatomic distance of the *CdSe*, with $y \approx 2.29$ Å y $x \approx 2.55$ Å. These data determine a hexagonal perimeter of $P \approx 1.38\ nm$.

With the perimeter and area $A_{Hexagon} \approx 4.96\times10^{-21} m^2$, the total volume of the system has an value of $V_{TT} \approx 1.28\times10^{-30} m^3$ [17-19] and this way the Atomic Packing Factor (APF) can be calculated. Due to *CdSe* has a hexagonal structure, its APF is determined using the equation (3):

$$APF \approx \frac{N_{atom} \bullet V_{atom}}{V_T} \quad (3)$$

where N_{atom} = number of atoms inside the cell, V_{atom} = atomic volume and V_T = total volume of the crystal (known parameter).

To determine the atomic volume of its structure, the atom is considered as a spherical particle, therefore the spatial shape formed by the periodicity of the hexagons centered on the bases is considered, where each base is a unit cell. This is obtained by the volume equation of a sphere; and since the average atomic radius is given by the atomic radium between selenium (115 pm) and the cadmium (155 pm), we have to $r_p = 1.35$ Å, so, the atomic volume of the system under study is $V_{atom} \approx 1.03\times10^{-29} m^3$.

Now then, considering (2), (3) and the value of the total volume of the system already mentioned, the result for the hexagonal structure is $APF \approx 0.4140$, or $APF \approx 41.40\%$.

Using equation (1) and because the *Cd* structure has an atom located at each vertex, indicating that $n_I = 0,\ n_f = 0,\ n_v = 8$. So, the total number of atoms in this arrangement is $N_{atom} = 1$.

Repeating the procedure performed to obtain the volume of the hexagonal prism, and knowing the measurements in $x \approx 2.55$ Å and $y \approx 2.29$ Å, the total volume for the cubic arrangement is $V_T \approx 1.48\times10^{-29} m^3$ and from (2) and (3); the atomic packing factor for the cube is $APF \approx 0.6912$, or $APF \approx 69.12\%$ [17-19].

3. Analysis and Results

The *CdSe* samples were grown by colloidal synthesis at a pH: 8 and were analyzed with the STM (nanosurf easyscan 2.0), by parameters: voltage of $50\ mV$, scanning on the surface in a range of 128 – 256 ppl (points per line), at a time of 0.2 spp (seconds per points).

3.1. *Micrographs*

In the figure 1, it shows a STM micrograph of the *CdSe* nanostructured, in which it is observed that the surface it looks like a periodic lattice, particular characteristic of a crystalline material. Its also observed the 3D representation of the *CdSe*; the following information was also obtained; the signal peaks vary between a maximum value of $17.61\ pAmp$ and a minimum of $-\ 19.06\ pAmp$ and $z = 36.67\ pAmp$.

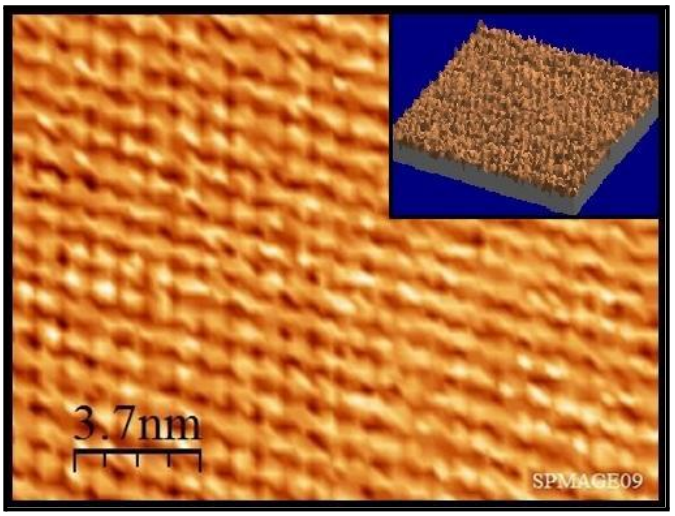

Figure 1. STM micrograph of *CdSe*, it show 3D spatial representation too (upper right).

In order to obtain the physical information of the material, the micrograph obtained was visualized with the microscope software and moreover to zooming on different regions, how shown on figures 2 and 3 in a randomly taken area on the micrograph. On the figure 2, the lattice green marked, represents the hexagonal arrangement shape on an area of the micrograph and each blue dot represents the position of an atom and the separation between them which is approximately $0.45\,nm$ and $APF = 41.4\%$ [24]. Also, zooms were also made in other regions of the material on study, as can be seen in figure 3.

As can be seen in figure 3, there is also a cubic-shaped crystalline arrangement in the study material, which leads us to conclude that the material has or presents both phases: cubic and hexagonal; due to the nature of *Selenium and Cadmium*, which is in accordance with the specialized literature [20-23].

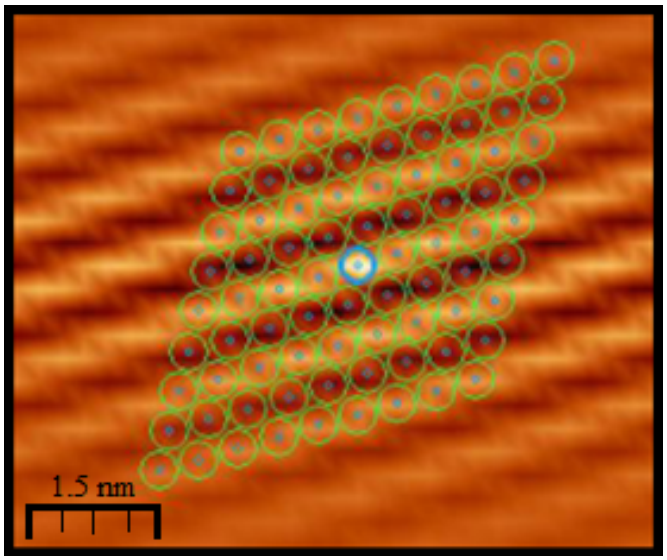

Figure 2. Region of the micrograph where shown overlapping lattice typical of a hexagonal arrangement.

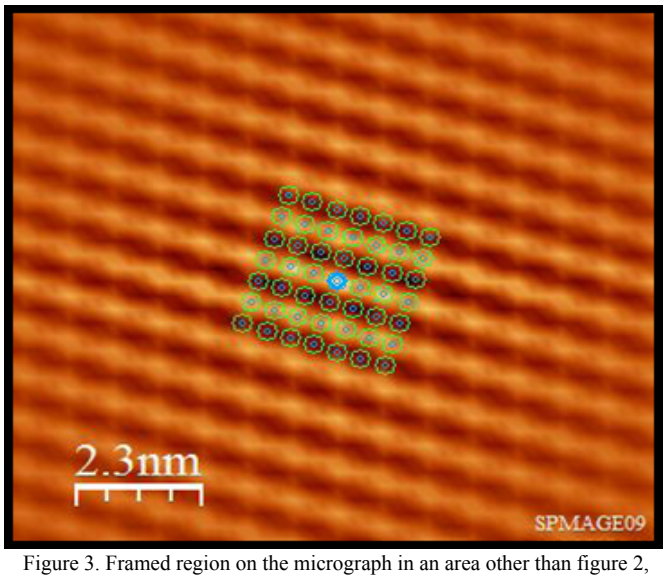

Figure 3. Framed region on the micrograph in an area other than figure 2, where a cubic arrangement is observed.

For this particular case, it was found that the distance between each lattice point of the cubic cell is approximately $0.575\,nm$ and the occupied atomic volume is only 69.12%, as mentioned [24].

3.2. FFT and Miller indices of the CdSe

The Fast Fourier Transform (FFT) method was used to analyze the micrograph and find the scattering centers, which in turn identifies the distribution and defines the crystal lattice of the system. When defining the lattices, the position or superposition of the planes that define the structure of the material is determined. The Fourier spectra of the arrangement on figure 1, is shown in the figure 4.

Due to the periodicity observed in the micrograph of figure 1, its deduced that it is a crystalline material, as confirmed by the FFT spectra (fig. 4) in which the corresponding peaks (fig. 5B) are observed to the typical and characteristic dispersing centers of a system with high regularity. The distance between scattering centers in the reciprocal space shows us that they have the same magnitude, which leads to being able to calculate the lattice parameter of the physical system: $\alpha = 4.13$ Å.

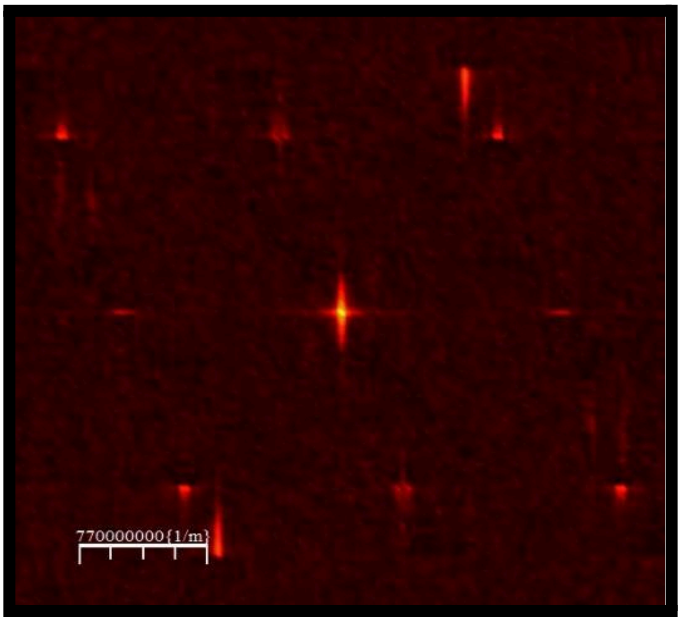

Figure 4. FFT spectra showing the scattering centers.

In figure 5, the connection of the scattering points and the crystal structure given by them is shown:

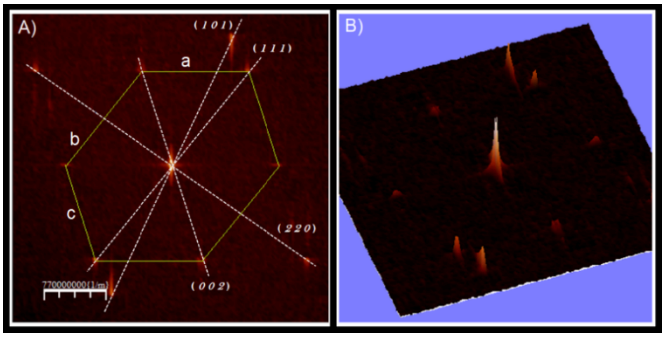

Figure 5. A) FFT spectra where the Miller indices and the "bond" of the scattering centers in 2D, B) 3D image of the FFT spectrum *CdSe*.

From the previous figure, the scattering centers (fig. 5A) given by the FFT of the CdSe sample can be observed, forming a hexagon with: **a**= 7.66 Å, **b**= 6.71 Å y **c** = 8.03 Å, Miller indices are also indicated; which were identified based on the specialized literature on semiconductor materials [25 – 29]: (1 0 1) and (0 0 2) correspond to the Wurtzite type [30,31], while (2 2 0) and (1 1 1) to the Zinc-Blende type [32]. In fig. 5B, the three-dimensional Fourier spectra is shown where the relative magnitude of the scattering intensity of each point is more clearly appreciated.

The figure 6 shows the original micrograph of the *CdSe* (fig. 6a) obtained with the help of the STM, which when obtaining its FFT (fig. 6b), projects the points where the scattering centers are identified; and thus, the structure of the material is defined, which shows the periodicity of the cells (fig. 6c) in the material and their distribution. Finally (fig. 6d) an adjustment of this is obtained, thus defining the dispersing centers that determine the planes that make up the material and their relationship with its structure shown in figure 5; defined by a, b, c.

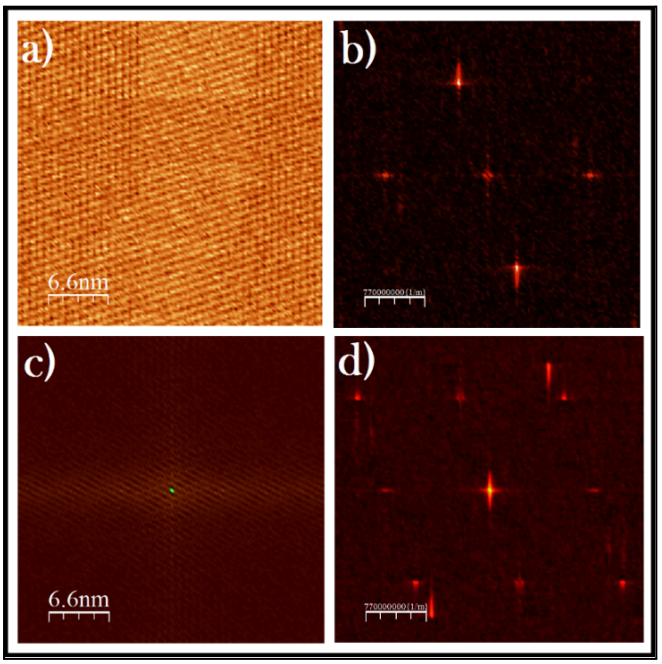

Figure 6. The image shows: a) the micrograph of the *CdSe*, b) the first corresponding FFT, c) the Fourier grid and d) the FFT of the Fourier grid.

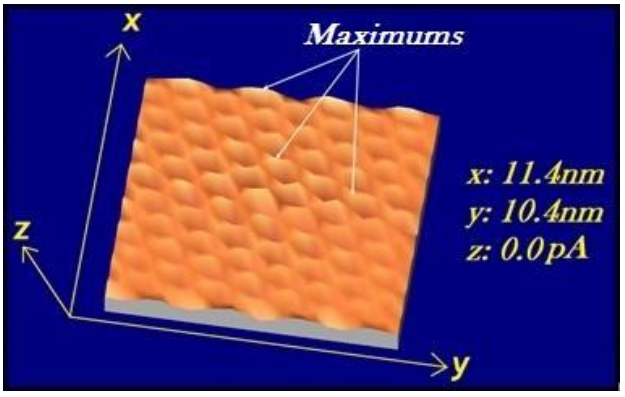

Figure 7. Representation of the lattice Fourier in 3D, where pointed are the maximums.

In the figure 7 shows the spatial structure of the Fourier lattice in 3D, in which the maxima representing the spatial lattices corresponding to the *CdSe* representing a hexagonal arrangement can be seen.

3.3. Electronegativity of physical system

One of the important aspects of every physical system to be analyzed with this characterization technique is the electronegativity given by the type of bond between elements that make it up [33]. For the specific case of *CdSe*, this was determined from the micrograph shown in figure 1, for this it was necessary to obtain the profile that relates current intensity with voltage, as can be seen in figure 8. In the figure, it can be verified that the value of the parameters established for the intensity (*I*) and the potential (*V*) in the operation of the microscope will have to vary to achieve the adequate voltage, with which the tunneling effect will be carried out.

If we carefully observe the curve profile in figure 8, it can be deduced that the lower the value of the intensity (*I*) applied to the conductive tip of the STM; the higher the voltage (*V*) that must be applied to the tip.

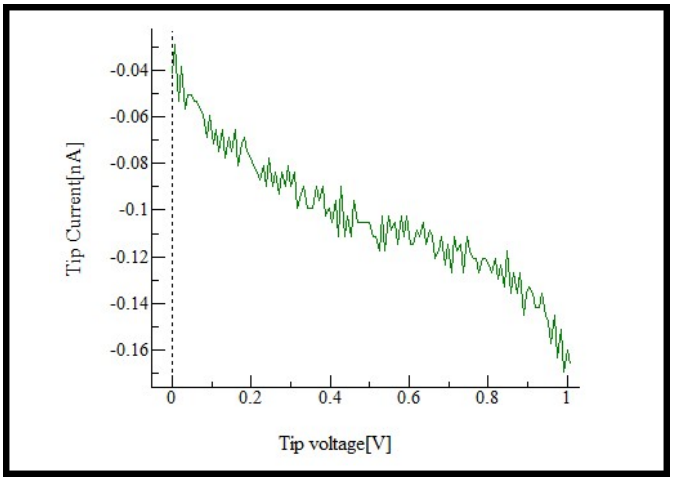

Figure 8. Current intensity profile with respect to the potential applied in the STM conductive tip.

Corroborating in this way and according to specialized literature [33] that the ionic bond type is mainly electronegative due to the presence of *Cadmium*.

4. Conclusions

The study of this material (*CdSe*) allowed the cubic and hexagonal type phases to be found.

The APF for each phase of the system under study was determined, for the hexagonal structure it 41.40% and for the cubic structure 69.12%.

The crystallographic directions were identified and we obtained the Miller indices that define the crystal structures of the *Zinc-Blende* and Wurtzite type.

The electrical potential used to study the material as a function of the current intensity, denotes that it is a material with electronegative semiconductor properties.

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To the academic group of Radiation Interaction with Matter, Faculty of Sciences, UAEMéx.

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