UDC 538.913

INVESTIGATION OF THE ATOMIC DYNAMICS OF CdSe THIN LAYERS BY RAMAN SPECTROSCOPY

N.M. Abdullayev[1], L.N. Ibrahimova[2], M.E. Aliyev[3], Y.I. Aliyev[4,5]

[1]Institute of Physics, Ministry of Science and Education of Azerbaijan, Baku, AZ-1143, Azerbaijan
[2]Institute of Natural Resources, Nakhchivan, AZ-7000, Azerbaijan
[3]Nakhchivan State University, Nakhchivan, AZ-7012, Azerbaijan
[4]Azerbaijan State Pedagogical University, Baku, AZ-1000, Azerbaijan
[5]Western Caspian University, Baku, AZ-1001, Azerbaijan
e-mail: yusifafshar@gmail.com

Received 06.01.2024
Accepted 28.02.2024

Abstract: *This study is focused on investigating the atomic dynamics and vibrational properties of thin layers of cadmium selenide with thickness ranging from 200–500 nm. The studies were carried out using Raman spectroscopy at room temperature. Raman spectra were obtained in the frequency range ν = 100-800 cm^{-1}. Two vibration modes were observed within the specified frequency range. It has been established that these vibration modes correspond to vibrations of Cd–Se covalent bonds. The frequency of these vibrational modes was observed to increase as the thickness of CdSe thin films increased, which was attributed to the formation of a thickness-dependent phase.*
Keywords: *CdSe thin layer, atomic dynamics, lattice vibrations, Raman spectroscopy.*
DOI: 10.32737/2221-8688-2024-2-231-236

Introduction

Studying the atomic dynamics of semiconductor materials allows for the research of a variety of processes that occur within them. Therefore, extensive research is being conducted to study the atomic dynamics and lattice vibrations of these materials. Phase transitions in crystals can lead to changes in the elementary lattice, as is known. The oscillation frequencies of the lattice cell are also changing during this time. The study of atomic dynamics is crucial when examining phase transitions that are affected by temperature and pressure [1-5].

The atomic dynamics of solid states allows for the formation of various physical properties, such as ferroelectricity, ferromagnetism, and superconductivity, which are influenced by lattice vibrations. It is known that at low temperatures thermal vibrations of the lattice begin to fade. Therefore, the magnetic properties of materials manifest themselves predominantly at low temperatures. These processes can be experimentally studied by using Raman and infrared spectroscopy [6-8].

Recently, a number of materials have been studied in the form of thin films, and the physical and chemical properties of these films are becoming increasingly interesting. Devices that use thin layers have a lower volume. Special technologies are used to produce thin layers of materials with metallic and semiconductor properties [9-12]. Observing the physical properties of these materials in thin layers increases the possibilities of their application. One of the most studied semiconductor materials is the CdSe compound. These crystals are widely used as the active medium in semiconductor lasers, displays, detectors, photoresistors, and LEDs [13-15]. Maintaining the properties of the material at small sizes is a major challenge in producing thin films. Therefore, Studying the structure and vibration properties of the resulting layers is necessary. Several properties of CdSe thin films have been studied [16, 17]. However, the atomic dynamics of these layers has not been studied.

In this work, thin films of CdSe were obtained by chemical deposition and their atomic dynamics were studied. The studies were carried out using Raman spectroscopy at room temperature.

Experimental part

The research studied the atomic dynamics of thin layers of cadmium selenide with a thickness h = 200 – 500 nm. Thin layers of CdSe were obtained in laboratory conditions by chemical deposition. The solution used for obtain thin layers was prepared as follow: 0.5 M cadmium chloride ($CdCl_2$ × $2.5H_2O$), 13.4 M (25%) sodium hydroxide (NH_3OH), 7.4 M triethanolamine ($C_6H_{15}NO_3$), 0.2 M sodium selenosulfate (Na_2SSeO_3). The chemical precipitation process was carried out in a laboratory beaker with a capacity of 60 ml at room temperature and normal conditions using a specially developed technology.

Na_2SeSO_3 (sodium selenosulfate) was obtained by reacting 6 grams of Se powder with 10 grams of Na_2SO_3 (sodium sulfite) in a solution of 100 ml of distilled water for 7 hours at a temperature of 90 ºC. After completion of the chemical reaction, the solution was cooled to room temperature and insoluble selenium particles were removed from the solution through a filter. After completion of this process, a clear solution of sodium selenosulfate was obtained. When using sodium selenosulfate as a selenium component in the production of CdSe, the best results can be obtained at a solution pH of 9. A thin layer of CdSe with a crystalline structure can be obtained only at a pH of 9 so that the pH of the solution in the above mixture is equal to 9. To measure the pH of the solution, an Aquilon pH-410 pH meter was used.

Thin layers of CdSe were obtained on glass substrates. To obtain a thin layer, glass substrates were immersed in a chemical solution. Amorphous glass substrates (38 × 26 × 1 mm) were kept in a chromium solution for several hours, washed with distilled water and air-dried before being introduced into the solution. Glass coasters are placed vertically in a glass with a solution. The chemical deposition process was carried out at room temperature and normal conditions for 48 hours. This process was carried out simply, no rotation was used. During the process of obtaining thin layers, a white precipitate formed at the bottom of the glass. After three to four hours, this precipitate and the clear solution in the beaker first became dark yellow and then red, which corresponds to cadmium selenide. After this process, the glass base was removed from the glass, washed with distilled water and dried. As a result, thin layers of CdSe were obtained on the surface. The thickness of the resulting layers was determined by the gravimetric method. It was determined that the thickness of these layers is h = 200, 400 and 500 nm.

A structural and phase analysis of the resulting thin layers was carried out by X-ray diffraction technique on a D8 Advance (Bruker) diffractometer (Parameters: 40 kV, 40 mA, CuKα radiation, λ = 1.5406 Å). The analysis of the obtained spectra revealed that thin layers of CdSe were discovered on glass substrates.

The atomic dynamics and vibrational properties of thin layers CdSe obtained on glass substrates have been studied. The vibrational properties of the samples were studied by the Raman spectroscopy. The experiments were carried out on the Nanofinder 30 Raman spectrometer at room temperature. Nd:YAG laser with a wavelength λ = 532 nm and a maximum power of 10 mW was used as an excitation source. The obtained spectra were analyzed by the Gaussian function.

Results and discussion

The phase analysis of thin films of cadmium selenide obtained by chemical deposition was studied by X-ray diffraction at room temperature. The X-ray spectra of the resulting layers with thicknesses *h* = 200, 400 and 500 nm are presented in **Fig. 1**.

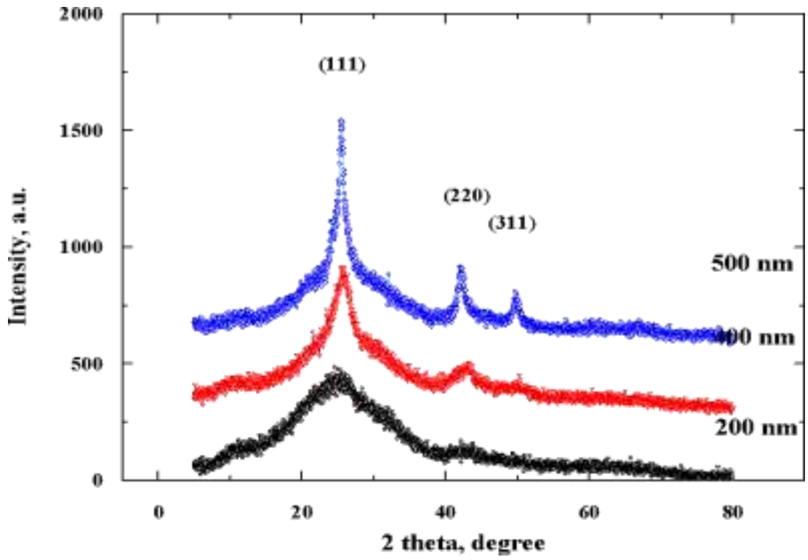

Fig. 1. X-ray diffraction spectra of CdSe thin layers.

It is clear from the X-ray spectroscopy that a phase corresponding to CdSe crystals has formed in the thin layers with a thickness of *h* = 200–500 nm. Three diffraction maxima corresponding to this structure were observed [18]. The results of the analysis showed that that these diffraction maxima correspond to (111), (220), and (311) Miller indices. The CdSe thin films crystallize in a hexagonal structure.

To study the atomic dynamics of the system, the vibrational properties of thin layers were studied by means of Raman spectroscopy. The spectra obtained at room temperature and under normal conditions are presented in **Fig. 2**. Two active modes of Raman scattering were observed in the frequency range ν = 100-800 cm^{-1}. The spectra indicate that the frequencies of vibration modes shift towards higher frequencies as the thickness of thin layers increases. It is known that the composition of these layers remains constant. The change in frequencies of dance modes occurs in connection with the process of phase formation.

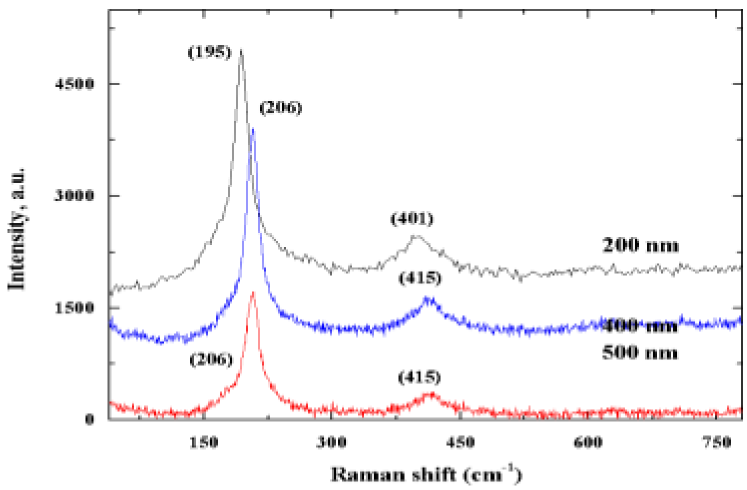

Fig. 2. Raman spectra of thin layers CdSe.

Thus, as the bond lengths of the same chemical elements decrease, the frequency of vibrations increases. Therefore, in studies carried out at high pressures, an increase in the vibration frequency is observed as the crystal lattice is destroyed [19

]. With increasing thickness in thin CdSe films, due to the phase formation process, the atoms are packed more densely and therefore the frequencies of the Raman modes increase. From the spectra shown in **Fig. 2**, it is clear that there are significant differences in the Raman frequencies of the 400 nm thick layers compared to the 200 nm thick layers. But compared to layers 400 nm thick, there are no significant differences in the Raman frequencies of layers 500 nm thick. From this it can beseen that the phase formation process has been completed in layers 400 nm thick.

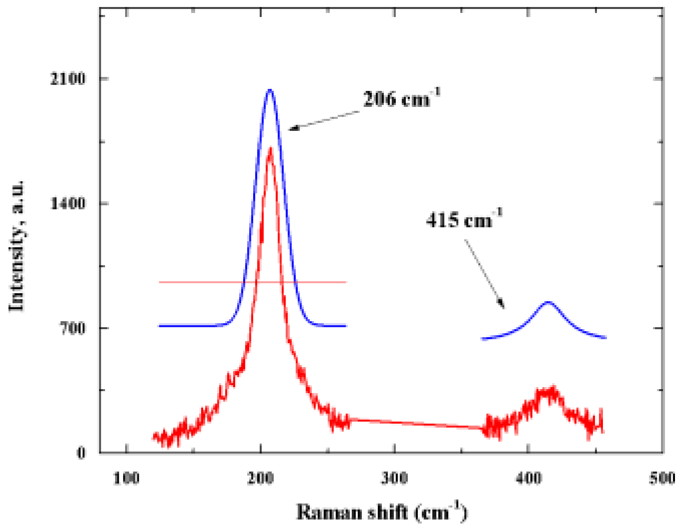

Fig. 3. Frequencies of Raman modes of thin layers CdSe with a thickness of h = 500 nm.

The Raman modes obtained in CdSe thin films were interpolated by a Gaussian function and the frequencies of the Raman modes were determined. The interpolation process was carried out for layers obtained with a thickness of h = 500 nm. From **Fig. 3** it can be seen that the vibration frequencies correspond to $\nu 1$ = 206 cm^{-1} and $\nu 2$ = 415 cm^{-1}, respectively. These frequencies correspond to the frequencies observed for the CdSe compound in previous studies [20].

Conclusions

In this work, thin layers of CdSe were obtained by chemical deposition and their atomic dynamics were studied. Two different vibration modes were observed in the Raman spectra of thin layers of cadmium selenide with thicknesses h = 200, 400, and 500 nm. As a result of interpolation of the spectra with the Gaussian function, it was established that the vibration modes corresponding to the frequencies $\nu 1$ = 206 cm^{-1} and $\nu 2$ = 415 cm^{-1} belong to vibrations of Cd–Se covalent bonds. The process of phase formation in thin films of cadmium selenide based on dance modes has been studied and it has been established that it is CdSe layers that are formed in layers with a thickness of$h$ = 400 nm.

References

1. Kozlenko D.P., Dang N.T., Kichanov S.E., Lukin E.V., Pashayev A.M., Mammadov A.I., Jabarov S.H., Dubrovinsky L.S., Liermann H.-P., Morgenroth W., Mehdiyeva R.Z., Smotrakov V.G., Savenko B.N. Competing magnetic and structural states in

multiferroic YMn2O5 at high pressure // *Physical Review B*, 2015, vol. 92, pp.134409.
2. Azimova S.R. Structural and vıbratıonal propertıes of $Bi_2(Sb_2)Se_3(Te_3)$ bınary semıconductors // *Advanced Physical Research*, 2021, vol.3, pp.46-51.
3. Aliyev Y.I., Ilyasli T.M., Dashdemirov A.O., Allazov M.R., Trukhanov A.V., Asadov Y.G., Jabarov S.H., Dang N.T. The structural and vibrational properties of Ni-doped chalcopyrite $CuFeS_2$ // *Journal of Ovonic Research*, 2018, vol.14, pp.165-169.
4. Mammadov F.M. FeS- $FeGa_2S_4$- $FeGaInS_4$ system // *Chemical Problems*, 2020, vol.18, No. 2, pp.214-221.
5. Ayyubova G.Sh. Vibrational properties of indium doped barium hexaferrite at low temperature // *Advanced Physical Research*, 2020, vol.2, pp.108-112.
6. Aliyev Y.I., Asadov F.G., Ilyasli T.M., Dashdemirov A.O., Huseynov R.E., Jabarov S.H. Vibrational properties of $YbAs_2S_4$ and $YbAs_2Se_4$ compounds: by infrared spectroscopy // *Ferroelectrics*, 2020, vol. 599, pp.78-82.
7. Trukhanov A.V., Dang N.T., Trukhanov S.V., Jabarov S.H., Kazakevich I.S., Mammadov A.I., Mekhdiyeva R.Z., Turchenko V.A., Huseynov R.E. Crystal structure, magnetic properties, and raman spectra of solid solutions $BaFe_{12-x}Al_xO_{19}$ // *Physics of the Solid State*, 2016, vol.58, pp. 992-996.
8. Niftiyev N.N., F.M.Mammadov. Dielectric properties of layered $FeGaInS_4$ single crystals in an alternating electric field // *Semiconductors*. 2016, vol. 50, no. 9, pp. 1203–1207.
9. Mursakulov N.N., Abdulzade N.N., Jabarov S.H., Sabzalieva Ch.E. Investıgatıon of $CuIn_{1-x}Ga_xSe_2$ thın fılms for solar cells obtaıned by the magnetron sputterıng method from two magnetrons shıfted to each other // *New Materials, Compounds and Applications*, 2022, vol. 6, pp. 140-147.
10. Ahmadova Kh.N., Jabarov S.H. Obtaining of Al nanosized thin layers and their structural properties // *Arabian Journal for Science and Engineering*, 2023, vol. 48, pp. 8083-8088.
11. Majidzade V.A., Jafarova S.F., Javadova S.P., Aliyev A.Sh., Tagiyev D.B. The latest progress on synthesis and investigation of Sb2S3-based thın films // *Chemical Problems*, 2023, vol. 21, No. 2, pp. 99-122.
12. Zeynalova A.O., Javadova S.P., Majidzade V.A., Aliyev A.Sh. Electrochemical synthesis of iron monoselenide thin films // *Chemical Problems*, 2021, vol. 19, no. 4, pp. 262-271
13. Wageh S. Raman and photoluminescence study of CdSe nanoparticles capped with a bifunctional molecule // *Physica E: Low Dimensional Systems and Nanostructures*, 2007, vol. 39, pp. 8-14.
14. Potyrailo R.A., Leach A.M. Selective gas nanosensors with multisize CdSe nanocrystal/polymer composite films and dynamic pattern recognition // *Applied Physics Letters*, 2006, vol. 88, pp. 134110.
15. Dai X., Zhang Z., Jin Y., Niu Y., Cao H., Liang X., Chen L., Wang J., Peng X. Solution- processed, highperformance light-emitting diodes based on quantum dots // *Nature*, 2014, vol. 515, pp. 96.
16. Huseynaliyev M.H., Ibrahimova L.N. Optıcal propertıes of CdSe thın fılms produced by the cbd method from four-component and three-component solutıons // *International Journal on "Technical and Physical Problems of Engineering" (IJTPE)*, 2023, vol. 55, pp. 318-321.
17. Huseynaliyev M.H., Qarayev A.M., Abdullayev N.M., Ibrahimova L.N. Optical properties of CdSe thin films obtained by chemical bath deposition (CBD) at room temperature. *The 17th International Conference on "Technical and Physical Problems of Engineering"*, 18-19 October 2021, Istanbul, Turkey, pp.83-85.
18. Singh A., Kunwar A., Rath M.C. L-cysteine capped CdSe quantum dots syntesized by photochemical route // *Journal of Nanoscience and Nanotechnology*, 2017, vol.17, pp.1-8.
19. Jabarov S.H., Dang N.T., Kichanov S.E., Kozlenko D.P., Dubrovinsky L.S., Park J.-G., Lee S., Mammadov A.I., Mehdiyeva R.Z., Savenko B.N., Nghia N.X., Khiem L.H., Lieu N.T.T., Thao L.T.P. Crystal structure and vibrational spectra of

hexagonal manganites YMnO3 and LuMnO3 under high pressure // *Materials Research Express*, 2019, vol. 6, pp. 086110.
20. Baranov A.V., Rakovich Yu.P., Donegan J.F., Perova T.S., Moore R.A., Talapin D.V., Rogach A.L., Masumoto Y., Nabiev I. Effect of ZnS shell thickness on the phonon spectra in CdSe quantum dots // *Physical Review B*, 2003, vol. 68, pp. 165306.

CdSe NAZİK TƏBƏQƏLƏRİNİN ATOM DİNAMİKASININ RAMAN SPEKTROSKOPİYASI İLƏ TƏDQİQİ

N.M. Abdullayev[1], L.N. İbrahimova[2], M.E. Əliyev[3], Y.İ. Alıyev[4,5]

[1]*AR ETN Fizika İnstitutu*
[2] *AR ETN Təbii Ehtiyatlar İnstitutu*
[3]*Naxçıvan Dövlət Universiteti*
[4]*Azərbaycan Dövlət Pedaqoji Universiteti*
[5]*Qərbi Kaspi Universiteti*

Xülasə: İşdə h = 200 - 500 nm qalınlıqlı kadmium selenid nazik təbəqələrinin atom dinamikası və rəqs xassələri tədqiq edilmişdir. Tədqiqatlar otaq temperaturunda Raman spektroskopiyası metodu ilə yerinə yetirilmişdir. Raman spektrləri ν = 100-800 cm^{-1} tezlik intervalında alınmışdır. Göstərilən tezlik intervalında 2 rəqs modası müşahidə edilmişdir. Bu rəqs modalarının Cd – Se kovalent rabitələrinin rəqslərinə uyğun gəldiyi müəyyən edilmişdir. CdSe-in nazik təbəqələrinin qalınlığı artdıqca bu rəqs modalarının tezliyinin artması müşahidə edilmişdir ki, bu da qalınlıqdan asılı olaraq fazanın formalaşması ilə izah edilir.
Açar sözlər: CdSe nazik təbəqəsi, atom dinamikası, qəfəs rəqsləri, Raman spektroskopiyası.

ИЗУЧЕНИЕ АТОМНОЙ ДИНАМИКИ ТОНКИХ ПЛЕНОК CdSe МЕТОДОМ РАМАНОВСКОЙ СПЕКТРОСКОПИИ

Н.М. Абдуллаев[1], Л.Н. Ибрагимова[2], М.Е. Алиев[3], Ю.И. Алиев[4,5]

[1]*Институт физики МНО АР*
[2]*Институт природных ресурсов МНО АР*
[3]*Нахичеванский государственный университет*
[4]*Азербайджанский государственный педагогический университет*
[5]*Западно-каспийский университет*

Аннотация: В работе изучена атомная динамика и вибрационные свойства тонких пленок селенида кадмия толщиной h = 200-500 нм. Исследования проводились методом рамановской спектроскопии при комнатной температуре. Спектры комбинационного рассеяния были получены в диапазоне частот ν = 100-800 $см^{-1}$. В указанном частотном интервале наблюдались две моды колебаний. Установлено, что эти моды колебаний соответствуют колебаниям ковалентных связей Cd – Se. Наблюдалось увеличение частоты этих мод колебаний по мере увеличения толщины тонких пленок CdSe, что объяснялось образованием фазы, зависящей от толщины.
Ключевые слова: тонкая пленка CdSe, атомная динамика, колебания решетки, рамановская спектроскопия.