DOI: 10.53992/njns.v10i4.285 NUST Journal of Natural Sciences, Vol. 10, Issue 4, 2025

Research Article

Optical properties analysis of tungsten diselenide nanosheet for optoelectronic applications

Arbab Tahir[1], Abdul Rehman[2]*, Awais Shahid Minhas[3]

[1]Department of Physics, International Islamic University, Islamabad, 44000, Pakistan
[2]HITEC, School and College for Girls, HIT Taxila.
[3]Department of Basic Sciences and Humanities, University of Engineering and Technology, 47050, Taxila, Pakistan

***Corresponding author's email:** abdul.rehman@hitec.edu.pk

Abstract

Two-dimensional transition metal dichalcogenides (TMDCs) have attracted a lot of interest in optoelectronic applications because of their special optical and electrical characteristics. Tungsten diselenide (WSe_2) is unique among them because of its powerful photoluminescence, high charge carrier mobility, and adjustable bandgap. The synthesis and characterization of WSe_2 nanosheets made using a hydrothermal process are investigated in this work. Diffuse reflectance spectroscopy (DRS), and X-ray diffraction (XRD) were used to examine the optical and structural characteristics. According to the findings, the WSe_2 nanosheets have a bandgap of about 1.87 eV, which qualifies them as possible options for high-efficiency solar cells and photodetectors.

Keywords: Transition Metal Dichalcogenide, Tungsten Diselenide, Hydrothermal.

Article History: **Received:** 16 Feb 2025, **Revised:** 8 Dec 2025, **Accepted**: 9 Dec 2025, **Published:** 22 Dec 2025.

Introduction

With the development of nanotechnology, 2D materials have emerged as promising candidates for next-generation optoelectronic devices [1]. 2D materials are the crystalline materials in which atoms contain layered arrangement with having strong covalent bonds with each layer and between layers is Weak Vander Waals forces which make it useful for different applications [2]. The appropriate band gaps for 2D arranged semiconductors are between 1 to 2eV. Two-dimensional layered semiconductors are very flexible, translucent, and photoluminescent single layers that are only three atoms thick. These special qualities make these 2D materials promising in a number of applications, including solar cells, chemical and biological sensors, electron devices, optoelectronics, catalysts, and energy storage devices. The controlled development of 2D materials' thickness, size, and crystallinity is essential. Graphene, Transition Metal Dichalcogenide TMDCs, nanosheets, thin film are the examples of 2D materials. Graphene is a poor semiconductor device material. It is also a very good conductor of electricity

[3]. Graphene has a zero bandgap. which is not suitable for optoelectronic application fabrication of good quality of graphene is expensive and complex process because toxic chemicals are being used at high temperature, so we are looking for alternate materials like TMDCs [4]. Transition-metal dichalco-genides (TMDCs) are representative 2D semiconductors with tunable band gaps and good mobility of electrons. TMDCs consists of an individual atom thick layer with MX2 structure, in which M is a transition metal (Re, W, Mo, Nb, etc) and X is a chalcogen atom (Se, Te, S, etc).This type of material gives semiconductor, and it depends on the combinations of both transition metal and chalcogen atoms [5]. Additionally, the band structures of many TMDCs vary noticeably as the number of layers decreases from the bulk crystal, giving the TMDCs a special sensitivity to thickness [6]. Band structure engineering allows for the tuning of 2D TMCDs' diverse features, such as values of bandgap that match the solar spectrum [7, 8], suppress defects [9], or altering the number and type of free carriers [10] for p-n junctions and field-effect transistors (FETs), which are crucial components for optoelectronics and integrated electronics. Additionally, these materials are great choices for their application since they can tolerate high strain levels without deteriorating. TMDCs have a strong potential for integration into several electronic device applications based on two-dimensional materials since there are numerous material combinations accessible in this class of compounds. Similar to graphene and h-BN, TMDCs compounds exhibit a number of thickness-dependent characteristics, such as changes in band gap behaviour from direct to indirect with thinning from multi to few-layer films for a number of dichalcogenide compounds, such as MoS2 and WS2 [11]. Tungsten selenide having the formula WSe2, it is an inorganic compound [12]. WSe2 is hexagonal crystalline structure. Each selenium atom is covalently connected to three tungsten atoms in a pyramidal geometry, whereas each tungsten atom forms a trigonal prismatic organization sphere with six selenium ligands by covalent bonds. The distance between the selenium atoms in tungsten selenium is 0.334 nm, while the bond length of the tungsten–selenium link is 0.2526 nm [13]. It is a well-studied example of layered material. [14, 15] studied the van der Waals interactions between the layers WSe2. WSe2 is a very stable semiconductor in the group-VI transition metal dichalcogenides. With a band gap that varies from an indirect gap of 1.2 eV in the bulk to a direct gap of around 1.6 eV in the monolayer [16]. It was reported that the different morphologies of synthesized rod-like tungsten disulfide (WS2) nanostructures [17, 18]. To create superior WSe2 films on a quartz substrate, a hydrothermal approach was devised [19]. A modified hydrothermal method has been developed and employed for synthesis of few layers Tungsten disulfide-nanosheets (WS2-NS) [20] Tungsten selenide (WSe2) film was successfully deposited on FTO substrate by brush plating technique. A two-dimensional semiconductor, WS2 has attracted great attention due to its rich physical properties and potential applications [21].

Experimental details

Materials

The complete details of chemicals used for the synthesis of the tungsten diselenide nanosheet are stated below in Table 1.

Table 1: list of chemicals used for the synthesis of WSe2 nanosheets.

S/No	Compounds	Chemical Formula	Moler Mass	Purity (%)
1	Selenium	SE	78.96	>99%
2	Tungstic acid	H2WO4	249.9	>99%
3	Sodium borohydride	NaBH4	37.83	>99%
4	DMF	C3H7NO	73.09	>98%

Hydrothermal synthesis of tungsten diselenide nanosheet

Tungsten diselenide Nanosheets were synthesized by using the hydrothermal method. 2.82gram solution of tungstic acid having molarity 0.12M, 1.51grame of selenium having molarity 0.24M and 1.14 grams of sodium borohydride was added into the beaker of 80ml with the DMF. Stirring the solution continuously up to 1.30 hours without heat during constants stirring until the color of the solution changed from greenish-yellow to black then the reaction was transferred to autoclave in the furnace for 2 hours at 200 degree centrifugate. After the completed the reaction, autoclave was naturally cooled down up to 12 hours mixture was washed with distilled water and centrifuged several time the product was dried at 100 degree centrifugate for 3 hours at the last grading the same procedure was followed with different concentration as shown in Figure 1.

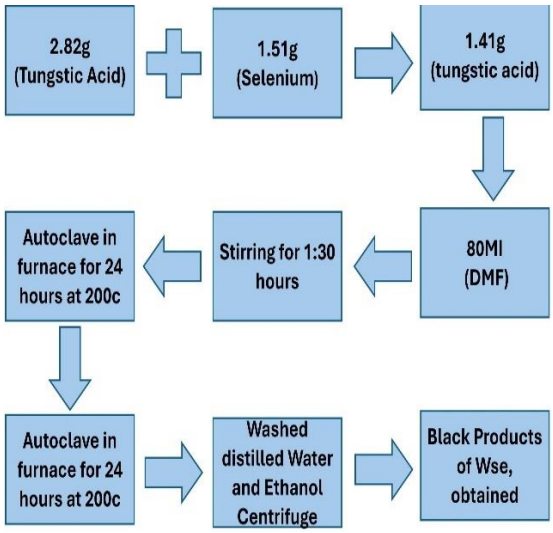

Figure 1: Synthetic representation of Wse_2.

Results and Discussion

X-ray diffraction analysis

X-ray diffraction characterization techniques have been used to investigate the phase identification and crystalline structure of materials synthesized by Hydrothermal method. This technique is used to calculate the average crystallite size of the sample. To examine, the tungsten diselenide nanosheet crystal structure (unit cell, lattice constant, and unit cell volume, etc.) XRD data of all the samples. The XRD spectrum of Tungsten Selenide (WSe2) nanosheet is shown in Figure 2, These samples were synthesized at different concentrations viz 0.01, 0.02 and 0.05 which are labelled respectively. The XRD patterns of these samples show similarity in the peak position and intensity distribution as can be seen All the peaks might be indexed to Hexagonal structure (JCPDC File No. 00-038-1388) the sample synthesized at low in the diffraction peaks were observed at 13.624, 27.463, 31.410 and 37.805 which corresponds to (002), (004), (100), and (102) planes respectively for Tungsten Selenide (WSe2) nanosheet.

$$D = \frac{0.9\,\lambda}{\beta\,\cos\theta}$$

Where ‘D’ is the crystallite dimension ‘λ’ wavelength of incident CuK_α radiation beam, and ‘β’ is the calibrated as full width at half maximum (FWHM) ‘θ’ the Bragg’s angle. Table 2 provides the crystallite size values derived from these diffraction results, while Figure 2 illustrates the XRD patterns of WSe_2 samples 1–4.

Table 2: Crystallite size of WSe_2 samples 1- 4.

Sample No	2θ	FWHM (rad)	Crystallite size (nm)	Miller indices (hkl)
1	13.6	0.0052	24.3	002
	27.4	0.003	21.4	004
	31.4	0.0027	20.3	100
	37.8	0.0036	27.6	103

Sample No	2θ	FWHM (rad)	Crystallite size (nm)	Miller indices (hkl)
2	14.5	0.0056	26.6	002
	28.3	0.0036	22.9	004
	34.3	0.0026	31.8	100
	38.4	0.0035	38.4	103
3	13.6	0.0056	24.8	002
	27.4	0.0076	29.5	004
	31.4	0.0065	30.7	100
	34.1	0.0035	18.7	101
	37.8	0.0086	34.9	102
	39.2	0.0076	16.8	103
	42.1	0.0097	22.7	006
4	14.4	0.0058	23.9	002
	23.5	0.0087	31.98	004
	33.3	0.0045	29.9	100
	34.6	0.0079	17.9	101
	36.1	0.0085	40.8	102
	39.2	0.0069	15.7	103
	43.3	0.0089	23.8	006

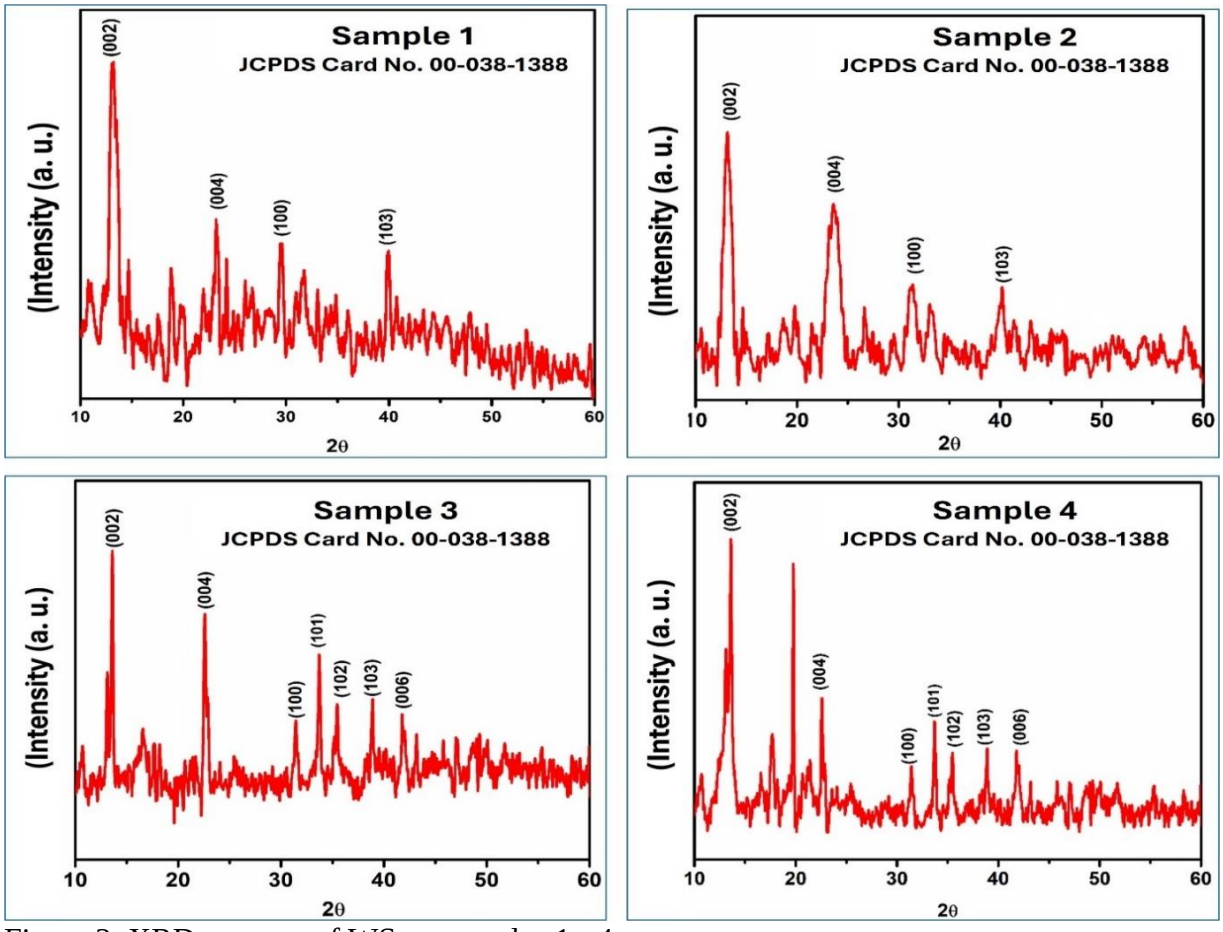

Figure 2: XRD patterns of WSe_2 samples 1 - 4.

Diffuse reflectance spectroscopy (DRS)

Diffuse reflectance spectroscopy is in optical techniques use for finding the band gap of material. The optical band gap of powder samples is calculated by using kubelka-munk function. First of all, the percentage reflected date is converted into the kubelka-munk function, and the graph is plotted between kubelka-munkl and energy.

$$\propto hv = (E - hv)^n$$

The value of 'n' shows the transition from allowed energy states which deepened on the material. The diffuse reflectance spectroscopy (DRS) results used to estimate the optical band gap of WSe_2 samples 1–4 are shown in Figure 3.

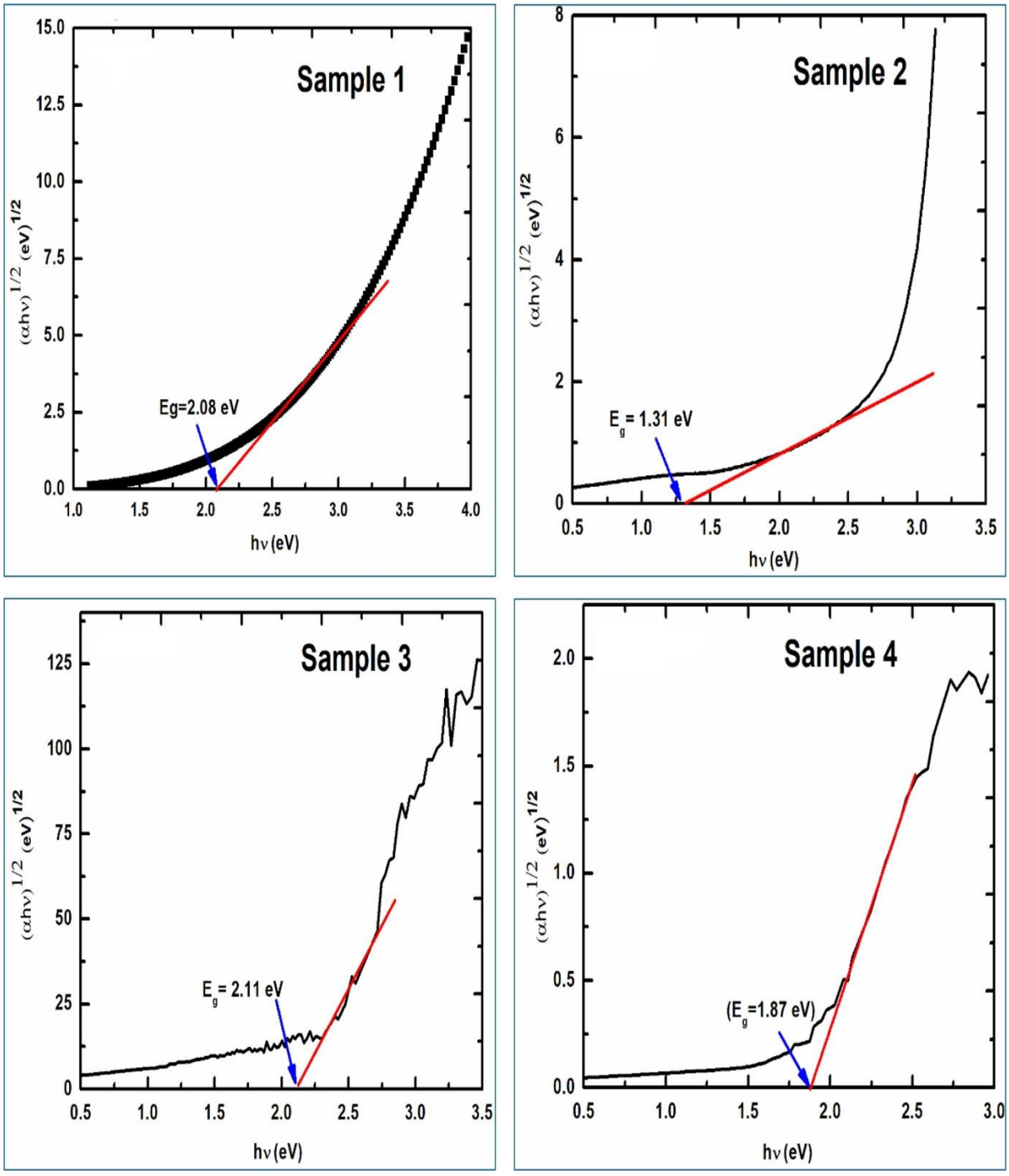

Figure 3: Diffuse reflectance spectroscopy (DRS) of WSe_2 samples 1- 4.

Conclusion

TMDCs materials such as WSe2 is p-type 2D material. WSe2 showed great interests for electronic engineering for device design. WSe2 was successfully synthesized by a hydrothermal method. DMF was used to dissolve selenium powder and tungstic acid, and sodium borohydride was used as a reducing agent. Direct Band gap of WSe2 is 1.87 eV which is calculated by using diffuse reflectance spectroscopy (DRS) which show that is promising for optoelectronic applications. XRD patterns show that WSe2 is a hexagonal structrure. Crystallite size for WSe2 was calculated by using Scherrer equation at different temperature.

References

1. Cheng Z, Cao R, Wei K, Yao Y, Liu X, Kang J, Dong J, Shi Z, Zhang H, Zhang X. 2D materials enabled next-generation integrated optoelectronics: from fabrication to applications. Advanced Science. 2021 Jun;8(11): 2003834.
2. Novoselov KS, Mishchenko A, Carvalho A, Castro Neto AH. 2D materials and van der Waals heterostructures. *Science*. 2016;353 (6298):aac9439.
3. Das S, Pandey D, Thomas J, Roy T. The role of graphene and other 2D materials in solar photovoltaics. *Advanced Materials*. 2019;31(1):1802722.
4. Dutta T, Yadav N, Wu Y, Cheng GJ, Liang X, Ramakrishna S, Sbai A, Gupta R, Mondal A, Hongyu Z, Yadav A. Electronic properties of 2D materials and their junctions. Nano Materials Science. 2024 Feb 1;6(1):1-23.
5. Zhao M, Huang YH, Ma F, Hu TW, Xu KW, Chu PK. Electronic states in hybrid boron nitride and graphene structures. *Journal of Applied Physics*. 2013;114(6).
6. Liu Z, Song L, Zhao S, Huang J, Ma L, Zhang J, Lou J, Ajayan PM. Direct growth of graphene/hexagonal boron nitride stacked layers. Nano letters. 2011 May 11;11(5):2032-2037.
7. Watanabe MO, Itoh S, Mizushima K, Sasaki T. Bonding characterization of BC2N thin films. *Applied Physics Letters*. 1996;68(21):2962-2964.
8. Kawaguchi M, Kawashima T, Nakajima T. Syntheses and structures of new graphite-like materials of composition BCN(H) and BC3N(H). *Chemistry of Materials*. 1996;8(6): 1197-1201.
9. Song L, Ci L, Lu H, Sorokin PB, Jin C, Ni J, Kvashnin AG, Kvashnin DG, Lou J, Yakobson BI, Ajayan PM. Large scale growth and characterization of atomic hexagonal boron nitride layers. Nano letters. 2010 Aug 11;10(8):3209-3215.
10. Han GH, Rodríguez-Manzo JA, Lee CW, Kybert NJ, Lerner MB, Qi ZJ, Dattoli EN, Rappe AM, Drndic M, Johnson AC. Continuous growth of hexagonal graphene and boron nitride in-plane heterostructures by atmospheric pressure chemical vapor deposition. Acs Nano. 2013 Nov 26;7(11):10129-11138.
11. Zhao W, Ghorannevis Z, Chu L, Toh M, Kloc C, Tan PH, Eda G. Evolution of electronic structure in atomically thin sheets of WS2 and WSe2. *ACS Nano*. 2013;7(1):791-797.
12. Schutte WJ, De Boer JL, Jellinek F. Crystal structures of tungsten disulfide and diselenide. *Journal of Solid State Chemistry*. 1987;70(2):207-209.
13. Voß D, Krüger P, Mazur A, Pollmann J. Atomic and electronic structure of WSe2 from ab initio theory: bulk crystal and thin film systems. *Physical Review B*. 1999;60(20):14311.
14. Fominski Y, Nevolin VN, Romanov RI, Titov VI, Scharff W. Tribological properties of pulsed laser deposited WSex(Ni)/DLC coatings. *Tribology Letters*. 2004;17:289-294.
15. Makarov D, Pallesche R, Maret M, Ulbrich TC, Schatz G, Albrecht M.

Growth of Pt thin films on WSe2. *Surface Science*. 2007;601(9):2032-2037.
16. Fang H, Chuang S, Chang TC, Takei K, Takahashi T, Javey A. High-performance single layered WSe2 p-FETs with chemically doped contacts. *Nano Letters*. 2012;12(7):3788-3792.
17. Cao S, Liu T, Hussain S, Zeng W, Peng X, Pan F. Hydrothermal synthesis of variety low-dimensional WS2 nano-structures. *Materials Letters*. 2014;129: 205-208.
18. Wen R, Wei A, Tao L, Luo D, Liu J, Yang Y, Xiao Z, Liu Z, Zhao Y. Hydrothermal synthesis of WSe2 films and their application in high-performance photodetectors. *Applied Physics A*. 2018;124:1-8.
19. Zhang DQ, Jia YX, Chai JX, Xu ZX, Zhao ZL, Cao MS. Preparation of WS2 nanosheets by one-step hydrothermal method. In: *2017 International Conference on Manufacturing Engineering and Intelligent Materials (ICMEIM 2017)*. Atlantis Press. 2017:433-436.
20. Packiaseeli SA, Rajendran V, Vijayalakshmi R. Structural, optical and morphological study of tungsten selenide thin films. *Nanosystems: Physics, Chemistry, Mathematics*. 2016;7(4):703.
21. Lan F, Yang R, Xu Y, Qian S, Zhang S, Cheng H, Zhang Y. Synthesis of large-scale single-crystalline monolayer WS2 using a semi-sealed method. *Nanomaterials*. 2018;8(2):100.