

## Optical and electric transport properties of undoped and niobium doped tungsten diselenide

Jhih-Jhong Jheng<sup>1</sup>, Der-Yuh Lin<sup>1</sup>, Tsung-Shine Ko<sup>1</sup>, Hung. Pin. Hsu<sup>2</sup>, Yu Ye<sup>3</sup>

<sup>1</sup> Department of Electronic Engineering, National Changhua University of Education, No.2, Shi-Da Road, Changhua City, Changhua County 500, Taiwan

Phone: +886-4-723-2105-8337 E-mail: dylin@cc.ncue.edu.tw

<sup>2</sup> Department of Electronic Engineering, Ming Chi University of Technology, 84, Gungjuan Road, New Taipei City 243, Taiwan

<sup>3</sup> School of Physics, Peking University, No.5, Summer Palace Road, Haidian District, Beijing 100871, China

### Abstract

**Nb-doped and undoped WSe<sub>2</sub> layered crystals were grown by chemical vapor transport (CVT) method using iodine as the transport agent [1]. The indirect band gap and excitonic transition energies have been determined to be 1.2, 1.61, and 2.08 eV at 300 K, respectively, by piezoreflectance spectroscopies (PzR) and photoconductivity (PC) measurements. We have performed temperature dependent I-V characteristic measurements at different temperatures to determine the resistivity and Schottky barrier height for these two samples. Due to the doping of niobium, the resistivity has been decreased from to, and the Schottky barrier height decreased from 310 to 93 meV. Furthermore, we also studied the optical response at different bias voltages, light intensity and on/off frequency of the pumping laser. The niobium doping can effectively enhance the responsivity over 70 times but also a little bit increase in the rise and fall times.**

### 1. Introduction

WSe<sub>2</sub> is a layered semiconductor and belongs to the family of transition-metal dichalcogenides (TMDCs) [1]. The compound adopts a hexagonal crystalline structure similar to molybdenum disulfide. Every tungsten atom is covalently bonded to six selenium ligands in a trigonal prismatic coordination sphere while each selenium is bonded to three tungsten atoms in a pyramidal geometry. It is crystallized in a lattice with strong covalent bonds within a unit layer and weak interactions, usually of the van der Waals type, between different layers. WSe<sub>2</sub> is a p type semiconductor with a high intrinsic hole mobility of up to 500 cm<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup> and high photo responsivity up to 7 A/W and low photo response times in the order of 10 microseconds monolayer devices. In this study, we have grown undoped and Nb-doped WSe<sub>2</sub> crystals by CVT method and checked they are all p type semiconductors with field effect mobility of 26.75 and 1.86 cm<sup>2</sup>/Vs, respectively, from I<sub>D</sub>-V<sub>GS</sub> data. We studied the electrical and optical properties of undoped and Nb-doped WSe<sub>2</sub> crystals by PzR, PC and I-V measurements at different temperatures between 20 and 300 K. In order to understand the doping effect on the optical response, we set up a versatile automatic

measurement system to measure the photo responsivity at different bias voltages, light intensity and on/off frequency of the pumping laser.

### 2. Results and discussions

Figure 1 shows the PzR spectra [2] of the undoped and Nb-doped WSe<sub>2</sub> crystals measured at different temperatures between 20 and 300 K. In the spectra two main resonance features are observed and assigned to be A and B features, respectively. Comparing the transition energies of undoped with that of Nb-doped WSe<sub>2</sub>, we found the two direct transitions, which are located at 1.61 and 2.08 eV at 300 K for A and B features, respectively, do not have obvious change. This result demonstrated that the band structure, which corresponds to the lattice structure, does not have significant distortion due to the doping of niobium atoms.

We carried out the temperature-dependent I-V measurements at different temperatures to determine the conductivity and Schottky barrier height  $\Phi_B$ . The results are shown in figure 2. In order to investigate the Schottky barrier height, it is common to use Arrhenius plot, i.e.,  $\ln(I_{ds}/T^{3/2})$  against  $1000/T$  for various  $V_{ds}$ . By fitting the data to each  $V_{ds}$ , we obtained the slopes using  $S = -\frac{q}{1000k_B}(\Phi_B - \frac{V_{ds}}{n})$ . Then by plotting the slopes as a function of  $V_{ds}$ , the SBH could be extracted from the y-intercept  $S_0 = -\frac{q\Phi_B}{1000k_B}$ . The calculated results of the SBH for undoped and Nb doped WSe<sub>2</sub> are 310 and 93 meV, respectively [3].

Figure 3 presents the responsivity, which are extracted from PC measurements at frequency of 9 Hz, of undoped and Nb doped WSe<sub>2</sub> [4]. In this figure, we can find that the indirect energy gap is 1.2 eV, where the energy gap of the exciton A is at 1.61 eV and the one of exciton B at 2.08 eV. It is worth to note that the responsivity of Nb doped WSe<sub>2</sub> is about ten times of undoped one at low light intensity level. Figure 4 indicated the frequency dependence of normalized responsivity, which is excited by a 652 nm wavelength laser operating at various frequencies between dc and 10 kHz. It is obvious that the frequency response can be separated into two regions and characterized by one short time constant and one long time constant. For undoped one, a half of the photo response is contributed by

short time constant (24  $\mu$ s) response and the other half comes from long time constant response (8 ms). For Nb-doped one, short time constant (26  $\mu$ s) part is 35 % and long time constant (4 ms) part is 65 %.

Figure 5 shows the result of photoresponsivity using  $R_\lambda = \Delta I_\lambda / (P_\lambda S)$ , where  $\Delta I_\lambda$  is the photocurrent,  $P_\lambda$  is the power density and  $S$  is the area of the incident light. We found that the maximum photoresponsivities of Nb-doped and undoped are 1.075 A/W and 17.7 mA/W at 652 nm under 1.58 mW/cm<sup>2</sup> photo-illumination [5]. Furthermore, we used a 652 nm laser the photon energy of which is larger than the energy band gap to understand the effect of the sample's operating voltage on the photoresponsivity. The photocurrent values of niobium doped and undoped samples at different voltages were measured. The results shown in Fig. 6 indicated that the responsivity of undoped WSe<sub>2</sub> increases with the bias voltage up to 250 V. And for the Nb doped sample the responsivity increases very fast as the bias voltage increases up to 25 V. We believe that could contribute from avalanche effect.

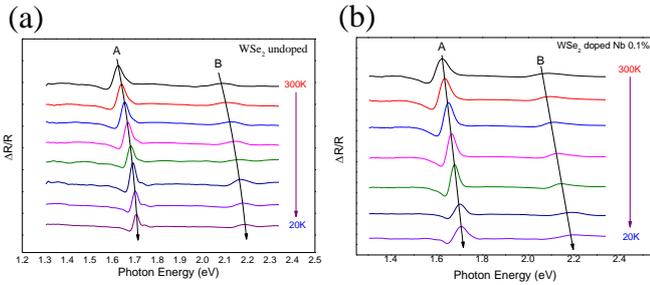


Fig.1 Piezoreflectance (PzR) spectra of (a) undoped WSe<sub>2</sub> and (b) Nb-doped WSe<sub>2</sub> at different temperatures.

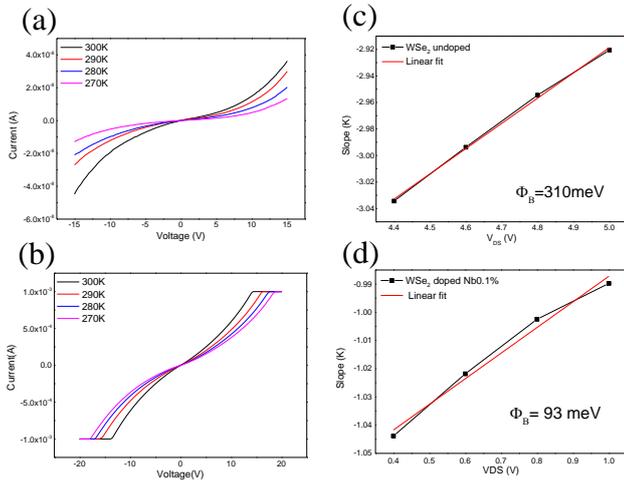


Fig.2 (a) and (b) shows the I-V curves for undoped and Nb doped WSe<sub>2</sub>. (c) and (d) are the Schottky barrier height calculations corresponding to (a) and (b), respectively.

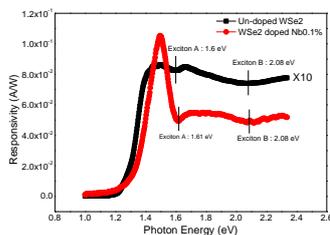


Fig. 3 PC spectra for WSe<sub>2</sub> undoped and WSe<sub>2</sub> doped Niobium at frequency of 9 Hz.

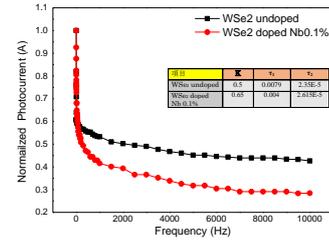


Fig. 4 Frequency response of photoconductivity and time constant fitting for WSe<sub>2</sub> undoped and WSe<sub>2</sub> doped Niobium.

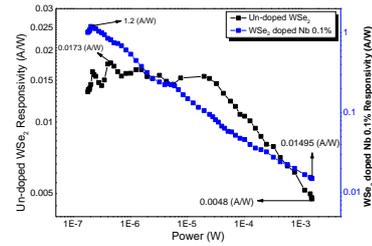


Fig. 5 Photoresponsivity of undoped and Niobium doped WSe<sub>2</sub>, the maximum photoresponsivities of undoped and Nb-doped are 1.075 A/W and 17.7 mA/W.

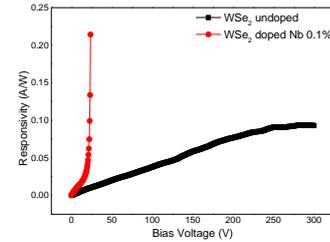


Fig. 6 Bias voltage-dependent of undoped and Niobium doped WSe<sub>2</sub>.

### 3. Conclusions

We have grown undoped and niobium doped WSe<sub>2</sub> crystals by CVT method and performed a series of optical and electrical studies by using IV, PzR, PC and Photoresponsivity measurements. In this study we found that the responsivity of the Nb doped WSe<sub>2</sub> has been increased about Seventy times compared with the undoped WSe<sub>2</sub>, the resistivity and the Schottky barrier height are also significantly reduced. So we can obtain higher efficiency for doped WSe<sub>2</sub> under the identical apply Voltage.

### References

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