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Electrical and optical properties of Ni-doped and undoped MoS_2

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Abstract

Ni-doped and undoped MoS_2 layer crystals were grown by chemical vapor transport (CVT) method with iodine as the transport agent. Hall measurements were carried out to consider the effect of Ni dopants on MoS_2, which indicate that the Ni-doped MoS_2 sample has a higher carrier concentration and lower mobility than the undoped MoS_2 sample. According to electron spectroscopy for chemical analysis (ESCA) measurements, the results confirm that the Ni dopants actually exist in the Ni-doped MoS_2 samples. The optical properties for whole samples were also analyzed by temperature dependent optical reflectance (R) and absorption measurements. In addition, two direct band edge transitions of excitons at 1.9 and 2.1 eV are observed for samples by R. Furthermore, Ni dopants introduce an addition deep level existing at 1.2 eV indicated in contrast to undoped MoS_2 using photocurrent (PC) measurements.

1. Introduction

MoS_2 is a layered semiconductor and belongs to the family of transition-metal dichalcogenides (TMDCs) [1]. MoS_2 forms a layered structure consisting of two hexagonal plans of sulfur atoms and an intermediate hexagonal plan of molybdenum atoms, trigonal prismatically coordinated to the sulfur atoms. It is crystallized in a lattice with strong covalent bonds within a layer and weak interactions, usually of the van der Waals type, between the individual layers. Owing to the unique optical and electrical properties, the layered semiconductors have attracted considerable interest in basic studies and applications. Moreover, MoS_2 is more properly to apply to some opto-electronic and electronic devices. For the optoelectronic devices which follow the mechanism of electron-hole transition principle, such as light emitting diodes, solar cell and optical detectors, the efficiency of direct band gap materials is better than indirect ones. The existence of band gap makes the device much easier to being switch which is an essential characteristic of transistors [2]. Furthermore, the optical properties of whole samples were studied by reflectance R and absorption spectra at different temperatures between 20 and 300 K. Hall measurements were performed to study the carrier concentrations and mobilities. PC measurements were also carried out to observe the effect of Ni dopants on opto-electronic behavior.

2. Results and discussions

The optical microscope images of undoped and Ni-doped MoS_2 are presented in Fig. 1. It can be observed that the samples have layered structure with flat surface. Their carrier concentrations and mobilities are measured at room temperature and listed in Table 1. Ni-doped MoS_2 has a higher carrier concentration and lower mobility than the undoped MoS_2. The lower mobility of the Ni-doped MoS_2 sample reflects the fact that the Ni dopants introduce more lattice imperfections and impurities. The marked differences in Hall results between the samples in terms of concentration and mobility prove that the Ni atoms were doped effectively into MoS_2 samples. Fig. 2 shows the reflection spectra of the Ni-doped and undoped MoS_2 samples at 300 K, which indicate two main resonance features located about the range at 1.83 and 2.02 eV and are assigned to be A and B features, respectively. The photon energy values of features A and B are a little lower than that observed in the absorption peaks and PL peaks of atomically thin MoS_2 samples [3]. These two features arise from direct band gap transitions between the maxima of split valance bands and the minimum of the conduction band. The temperature-dependent R results from 20 to 300K can be used to analyze the characteristics of MoS_2. In the photo energy below 1.7 eV, multi-layer interference signals are observed for the Ni-doped MoS_2 sample. An unclear feature observed around 1.39 eV is indicated as x. Figure 3 is the ESCA spectrum of Ni-dope MoS_2 sample, which shows that the sample contains the Mo, S and Ni elements and the atomic ratio of the elements is summarized in the table 2. The calculated atomic ratio of Mo to S element is a little different from the stoichiometric value [4]. Also, it can be seen that a small quantity of Ni has been incorporated in to the sample. We conducted PC measurement without additional DC bias, which measures the current generating from MoS_2 samples. According to the experimental results, for the undoped MoS_2 sample, there is a transiting exciton signal at about 1.4 eV. For Ni-doped MoS_2 sample, an obvious feature in the photo energy range between 1.4 and 2.6 eV. In additions, there is an extra signal occurs at 1.2 eV indicated by I, which indicates a doping level [5]. It is worth to note that the photocurrent has been enhanced up to several tens of times and the response wavelength has also been extended. This result indicates that the doping is a good way to improve their applications in solar cells and photo detectors. Figure 5 shows the temperature dependence of absorption spectra from 20 to 300 K. An obvious absorption edge

starting around 1.8 eV has been found that is marked by S. In Fig 6 the fit excitonic transitions A and B are indicated by solid squares and hollow triangles, respectively. Their temperature dependences are fit to Varshni equation and the empirical expression proposed by O'Donnel and Chen.

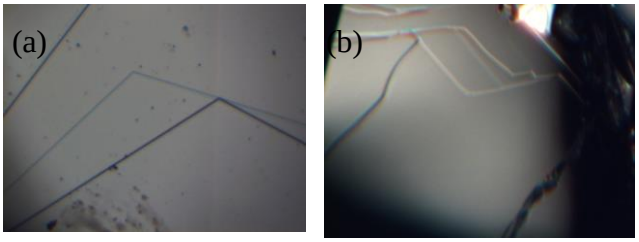

Fig. 1 Optical microscope (OM) of (a) Ni-doped MoS_2 and (b) undoped MoS_2.

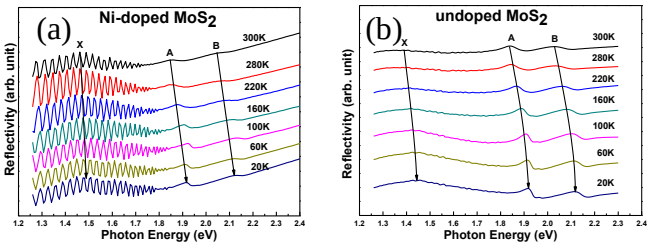

Fig. 2 Reflection sprctra of (a) Ni-doped MoS_2 and (b) undoped MoS_2 at different temperatures.

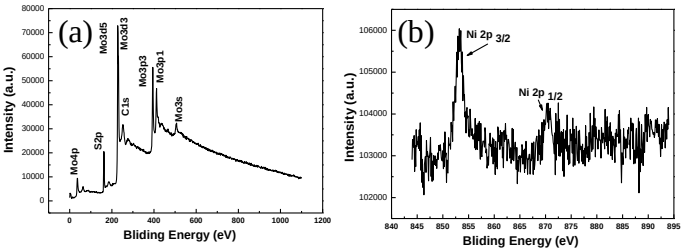

Fig. 3 ESCA spectra of Ni-doped MoS_2 (a) full spectrum and (b) high-resolution of Ni spectrum.

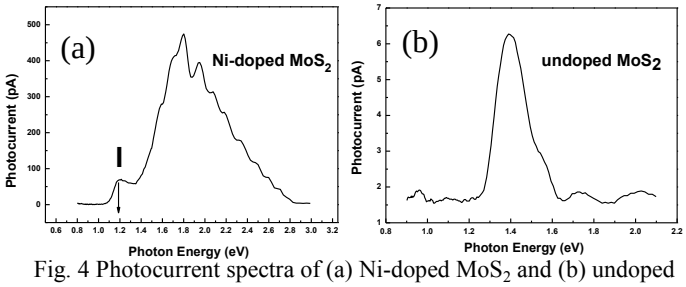

Fig. 4 Photocurrent spectra of (a) Ni-doped MoS_2 and (b) undoped MoS_2.

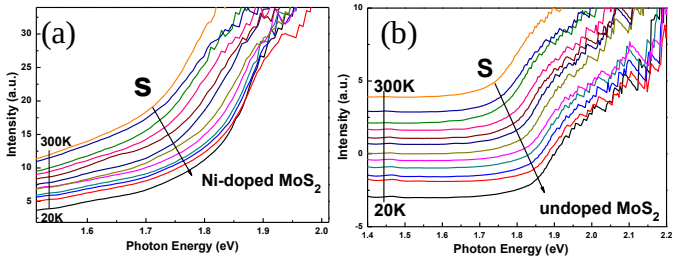

Fig. 5 Absorption spectra of (a) Ni-doped MoS_2 and (b) undoped MoS_2.

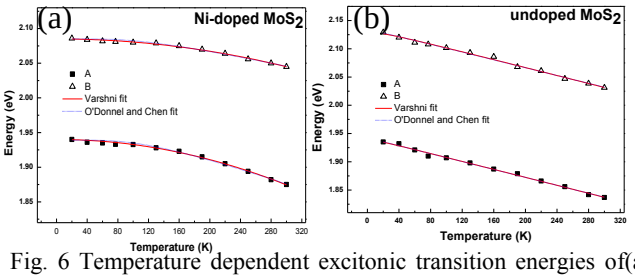

Fig. 6 Temperature dependent excitonic transition energies of(a) Ni-doped MoS_2 and (b) undoped MoS_2.

Table 1 Hall measurement of MoS_2 and Ni-doped MoS_2 at room Temperature.

Sample	MoS_2	MoS_2:Ni
Type	n	n
Resistance(Ω)	6733	283188
Carrier density(cm^-2)	1.102E13	1.183E13
Mobility(cm^2 / V * s)	78.5089	1.86593

Table 2 Atomic ratio of Ni-doped MoS_2 and MoS_2.

Material	S(S2p) (%)	Mo(Mo3d) (%)	Ni (%)
MoS_2:Ni	61.8	37.9	0.2
MoS_2[4]	67.2	32.7	0

3. Conclusions

In this study, we investigated the effect of Ni dopants on the electrical and opto-electronic properties of MoS_2 using Hall, R, absorption and PC measurements. Tow direct transitions and one indirect transition were observed successfully via R and absorption measurements. From the results of Hall measurements, we found that both of them are n-type semiconductors and a higher carrier density and lower carrier mobility is induced by the Ni dopants. PC results indicate Ni dopants introduce an addition deep level existing at 1.2 eV and the photocurrent is enhanced significantly and the response range is broadened. These results provide a guideline of electronic properties and applications for the Ni-doped and undoped MoS_2.

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