

# Palladium Doped WSe<sub>2</sub> for Gas Sensing Applications

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## Summary:

In the concurrent research era, doping transition metal dichalcogenides (TMDCs) with noble metals has drawn significant attention to enhance gas sensing performance. In this regard, we report for the first time a highly sensitive palladium doped WSe<sub>2</sub> (Pd-WSe<sub>2</sub>) sensor for trace level detection of NO<sub>2</sub> gas at room temperature. The Pd-WSe<sub>2</sub> was synthesized by the combination of aerosol assisted chemical vapor deposition (AACVD) and hydrogen free simple atmospheric pressure chemical vapor deposition (APCVD) methods. Morphological and compositional analysis have revealed good yield for adsorbing the target gas. The sensor exhibited remarkable response towards 800 ppb NO<sub>2</sub> at room temperature even in the presence of humidity without applying any external stimuli. This finding will surely have high impact towards ongoing TMDCs based gas sensor research as well as environmental sustainability.

**Keywords:** APCVD, gas sensor, NO<sub>2</sub>, TMDCs, nanomaterials

## Background, Motivation and Objective

The explicit detection of NO<sub>2</sub>, a greenhouse gas emitted from the vehicular exhaust and industrial pollution, has become one of the prime concerns in order to ensure public health safety as well as environmental conservation. In this regard, Metal Oxide (MOX) based gas sensors have been widely used but they suffer from long recovery time, poor selectivity and high operational temperature. Alternatively, some low dimensional materials e.g. carbon nanotube, black phosphorous, conductive polymer, graphene have been explored, however they are affected by humidity, deterioration and complex manufacturing process. Researchers have found 2D semiconducting TMDCs as potential substitutes because of their unprecedented physical, chemical and electronic properties. In particular, WSe<sub>2</sub> exhibiting p-type semiconductive behavior has large surface area, tunable electronic properties and excellent chemical stability [1]. Nevertheless, pristine WSe<sub>2</sub> often exhibits limited sensitivity and slow responses at room temperature. Doping with noble metal like Pd is a possible solution to address this limitation. Pd atoms acts as catalytic sites facilitating charge transfers between NO<sub>2</sub> molecules and enhancing overall gas sensing performance [2]. In this study, Pd doped WSe<sub>2</sub> sensor has outperformed for the trace level detection of NO<sub>2</sub> at room temperature under stimulus-free conditions.

## Materials and Methods

The sensing film was deposited on SiO<sub>2</sub>/Si substrate in two steps. First, Pd-WO<sub>3</sub> was deposited using AACVD technique. In this aspect, 25 mg tungsten hexacarbonyl and 5 mg palladium acetate were dissolved in 9 ml acetone and

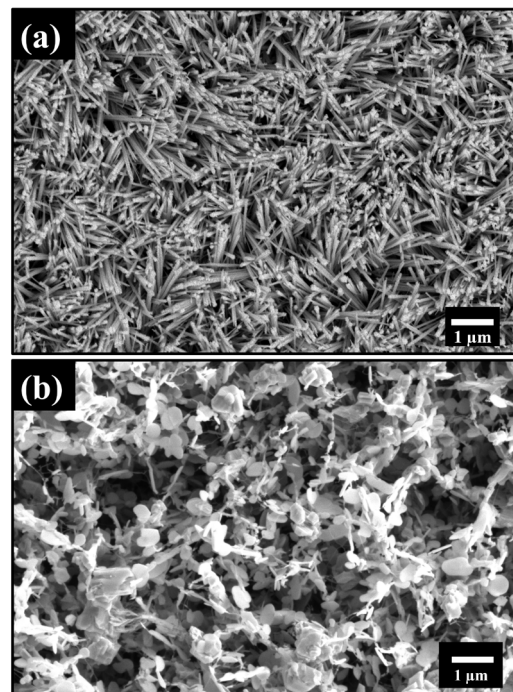
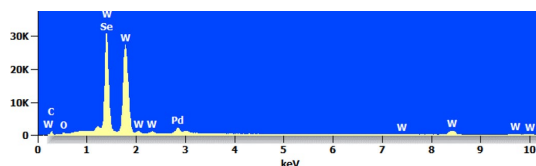
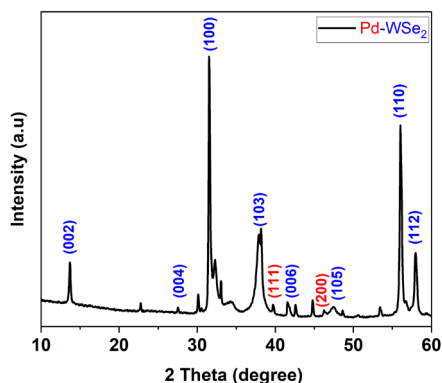


Fig. 1. FESEM images of (a) Pd-WO<sub>3</sub> and (b) Pd-WSe<sub>2</sub>.

Fig. 2. EDX analysis of Pd-WSe<sub>2</sub>.Fig. 3. XRD diffractogram of as-grown Pd-WSe<sub>2</sub>.

5 ml methanol respectively. These two solutions were then mixed in a glass flask, sonicated for 20 minutes and placed in an ultrasonic humidifier to create aerosol. Nitrogen (0.5 L/min) was used to carry this aerosol to the substrate placed inside the hot wall reactor. The deposition temperature was maintained 350°C. Then the as grown Pd-WO<sub>3</sub> was selenized with hydrogen free simple APCVD method using argon as a carrier gas and Se powder as precursor.

## Results

The morphology illustrated in Fig. 1(a) indicates the as-grown Pd doped WO<sub>3</sub> nano needles. These nano needles were converted to edge enriched nano sheets of Pd-WSe<sub>2</sub> as shown in Fig. 1(b) having distinct porosity which is effective for trapping the target gas molecules. Fig. 2 shows the EDX analysis indicating a strong presence of W, Se and Pd with minimal impurities. The XRD pattern exhibited in Fig. 3 reveals the intense peaks at 13.6°, 27.5°, 31.4°, 37.8°, 41.7°, 47.4°, 55.9° and 57.9° corresponding to the (002), (004), (100), (103), (006), (105), (110) and (112) crystal planes (marked blue) of 2H-WSe<sub>2</sub>. Two distinct peaks at 39.7° and 46.2° ascribe to the (111) and (200) crystal planes (marked red) of Pd, respectively.

For gas sensing measurements, first the Pd-WSe<sub>2</sub> sensor was tested towards 800 ppb NO<sub>2</sub> at room temperature. A decrease of the resistance was observed when the sensor was exposed to the oxidizing gas NO<sub>2</sub>, indicating p-type semiconducting behaviour. In Fig. 4(a) the sensor exhibited a 26% response having complete recovery to the baseline. The sensor took 3

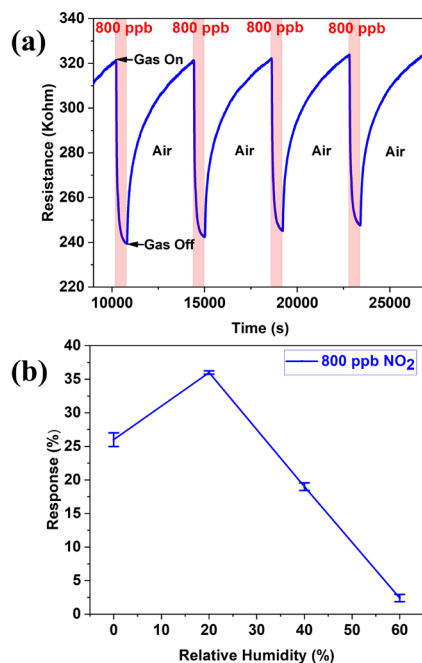


Fig. 4. (a) Pd-WSe<sub>2</sub> sensor resistance dynamic towards 800 ppb NO<sub>2</sub> at room temperature, and (b) its response in different relative humidity levels.

minutes to reach its 90% of the response. Meanwhile, the recovery time was found around 40 minutes which is noteworthy for room temperature gas sensing. Moreover, the sensor showed excellent cyclic repeatability over the long tenure.

The sensor was also tested under the presence of different relative humidity (RH) levels in room temperature to verify its feasibility in real world applications. For 800 ppb NO<sub>2</sub> exposure, the sensor responses 36%, 19% and 2.4% were recorded for 20%, 40% and 60% RH respectively. From these results we can conclude that, the sensor provided with its optimal performance while it was under 20% RH.

## Conclusions

In this work, we have proposed a highly sensitive Pd doped WSe<sub>2</sub> gas sensor for detecting trace levels of NO<sub>2</sub> at room temperature without any external influence. Thus, our sensor holds great potential for next-generation IoT compatible gas sensing applications.

## References

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