Optical and electrical properties of the MoSe$_2$/graphene heterostructures

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Abstract. Optical and electrical properties of MoSe$_2$ monolayer transferred to graphene/SiC substrate are studied by scanning probe microscopy and photoluminescence spectroscopy. By Kelvin probe microscopy it was measured a work function of the MoSe$_2$ monolayer (4.3 eV) and it was revealed the n-type of doping. With the increasing of MoSe$_2$ layers quantity the work function also increases which leads to the reducing of the Schottky barrier height between the SPM probe and the layers. Monolayer graphene quenches photoluminescence of the MoSe$_2$ monolayer while the bilayer graphene does not perturb the photoluminescence.

1. Introduction

Van-der-Waals (vdW) materials are promising for designing electronic and optoelectronic devices with improved characteristics[1]. From monolayers of these materials a layered heterostructures can be formed. The most studied vdW material is a graphene[2]. However narrow bandgap of the graphene impedes its using in optoelectronic devices in a visible range. Transition metal dichalcogenides (TMD) are another vdW materials which have a wider band gap suitable for visible optoelectronics and polaritonics[3]. Concept of the vdW heterostructures is in formation of multilayer sandwiches from monolayers of conducting (graphene), semiconducting (TMD) and dielectric (h-BN) materials. Due to the 2D nature of the vdW materials their electronic properties are extremely sensitive to the interface and surface configuration of the heterostructure. The aim of our work was to study optical and electrical properties of the vDW heterostructure formed by MoSe$_2$ monolayer and a graphene/SiC substrate.

2. Samples and methods

2.1. Samples

MoSe$_2$ layers were exfoliated from bulk sample using a scotch tape and then transferred to the graphene/SiC substrate. This substrate was covered by high-quality monolayer graphene (MLG) with randomly distributed bilayer (BLG) islands (10% of the area). Graphene film was obtained using a method of the thermal decomposition of a 6H-SiC surface[4]. Note that this method allows to form wafer-scale graphene with the quality exceeding the quality of the CVD grown graphene[5]. Moreover, SiC substrate is a semi-insulating and a transparent in a visible range.

2.2. Methods
Study of the electrical properties of the MoSe\(_2\)/graphene heterostructure was based on scanning probe microscopy (SPM) methods. These methods include Kelvin probe microscopy (KPM) and conductive atomic force microscopy (C-AFM)[6]. By the KPM method[7] it was measured a surface potential distribution of the heterostructure providing the values of work function of MoSe\(_2\) and graphene layers. The C-AFM method allows to measure I-V curves in regions with different number of MoSe\(_2\) layers on graphene. The study was performed using a Ntegra Aura (NT-MDT) scanning probe microscope in ambient conditions. During the measurements a surface of the graphene was grounded.

Optical properties were studied by measuring of microphotoluminescence (PL) spectra. The experiments were carried out at room temperature (300 K) using Horiba Jobin Yvon T64000 and LabRAM HR spectrometers equipped with a Linkam THMS600 temperature-controlled microscope stage. The measurements were performed with continuous-wave (cw) excitation using the 532 nm laser line of a Nd: YAG laser. We used a Mitutoyo 100× NIR (NA=0.90) long working-distance objective lens to focus the incident beam into a spot of ~0.7 μm diameter.

3. Results and discussion

Figure 1 (a) shows a surface potential distribution measured in the area with the transferred MoSe\(_2\) layers. With the measured surface potential, a surface topography map was simultaneously obtained (not shown here). From the topography it was defined a quantity of the MoSe\(_2\) layers in the area. A local number of layers is labeled in figure 1 (a), in assuming that thickness of monolayer is of 0.7 nm.

Surface potential distribution in figure 1 (a) is non-uniform. The value of the surface potential correlates with the number of MoSe\(_2\) layers. To estimate a work function of the MoSe\(_2\) it was analyzed a surface potential of the graphene substrate. It is known that the work functions of the graphene monolayer and bilayer on SiC are of 4.55 and 4.44 eV, respectively[8]. Fortunately, during the transfer the MoSe\(_2\) layer covered graphene with monolayer (MLG) and bilayer (BLG) regions. The BLG regions can be find in figure 1(a) as diagonal stripes with higher surface potential. Since the surface potential it is a difference between work function of the probe and the studied surface, the work function of the 1ML MoSe\(_2\) was defined as 4.30±0.05 eV. With increasing of layers number, the work function also increases (4.35 eV for 2 ML and 4.37 eV for 3 ML). These values were not presented in the literature before. Comparison with the work function and electron affinity of the bulk MoSe\(_2\) (not shown here) reveal the n-type doping of the layers.

![Figure 1](image-url)

**Figure 1.** (a) Surface potential distribution of the MoSe\(_2\) layers on the graphene. MLG and BLG are the regions with monolayer and bilayer graphene, respectively. 1-5ML indicate the number of the MoSe\(_2\) layers. (b) I-V curves measured by C-AFM by contacting a probe to the regions with different number of the MoSe\(_2\) layers. (c) PL spectra measured in the area pointed by black and red dots in figure 1(a), respectively.

To further study the electrical properties, the I-V curves were measured. For the measurement, the first contact was created to the graphene and the second was a SPM probe connected to the regions with
the different number of the MoSe$_2$ layers. Measured I-V curves are presented in figure 1 (b). From the figure it follows that the Schottky barrier between the probe and a surface is reduces with increasing of the layers quantity. For the explanation of this effect it was developed a simple model based on the work function of the probe and the data obtained by KPM (figure 1 (a)). From the model it follows that increasing of the work function leads to a decreasing of the Schottky barrier height. Such an approach paves the way to tune the metal work function for creating an ohmic contact to MoSe$_2$ monolayer.

Figure 1 (c) shows PL spectra measured on the MoSe$_2$ monolayer. Black curve was measured in the area pointed by the black dot (figure 1(a)), where the MoSe$_2$ contacted with the MLG. Red curve (red dot) was measured in the area covering the BLG. For comparison a MoSe$_2$ monolayer was also transferred to a SiO$_2$ (300nm)/Si substrate (blue curve). The spectra exhibit two broad peaks which can be attributed to A (1.58 eV) and B (1.76 eV) excitons. From the figure it follows that the MLG significantly quench the PL from MoSe$_2$, while the BLG do not affect the PL. Additionally, the ratio between the A and B peaks intensity is the same for the MoSe$_2$ on BLG and SiO$_2$, while for MLG it is changed. Such behavior is consistent with the recent results obtained on MoSe$_2$ on CVD monolayer graphene[9] and the WS$_2$ on MLG and BLG/SiC[10]. In the work[9] it was shown a PL quenching by monolayer CVD graphene. KPM and PL study of the WS$_2$ on graphene/SiC substrates reveal the quenching of the WS$_2$ PL only by MLG.

4. Conclusions
Optical and electrical properties of the MoSe$_2$/graphene heterostructures were studied by means of the scanning probe microscopy and the photoluminescence spectroscopy methods. The work function of the MoSe$_2$ monolayer was measured as 4.30±0.05 eV. With the increasing of MoSe$_2$ layers quantity the work function also increases, which leads to the reducing of the Schottky barrier height between the SPM probe and the layers. It was shown that a monolayer graphene quenches a PL Intensity of the MoSe$_2$ monolayer, while the bilayer graphene does not perturb the PL. Obtained results open the way to improve parameters of MoSe$_2$/graphene heterostructures for optoelectronic devices.

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