

VAN DER WAALS HETEROSTRUCTURES BASED ON GRAPHENE/MOS₂*

P.V. VINOKUROV, E.P. SHARIN, S.A. SMAGULOVA

¹North-Eastern Federal University, Yakutsk, Russian Federation

Vertical heterostructures based on two-dimensional materials are currently the main direction in the creation of device structures in nanoelectronics. They are created by gradually transferring layers of two-dimensional materials onto each other, when the transition into a single structure is maintained only by the van der Waals force. Such vertical van der Waals heterostructures exhibit new electronic phenomena that expand their capabilities for fundamental research and practical applications [1]. An important achievement of the developed heterostructures is the demonstration of the capabilities of new physical methods for creating device structures that different from traditional approaches in silicon electronics. Currently, graphene/MoS₂ heterostructures are of particular interest [2].

To experimentally study the interaction between graphene layers and MoS₂, a Graphene/MoS₂ heterostructure was created on a silicon substrate. Graphene and MoS₂ films were grown by chemical vapor deposition. A transfer method using polymethylmethacrylate (PMMA) was used to create the vertical heterostructure. First, MoS₂ films were transferred to a silicon substrate, then a graphene film was deposited on top by transfer. Raman spectra were collected for the graphene/MoS₂ heterostructure (Fig. 1 a). In Figure 1 a, two peaks belonging to the MoS₂ film are clearly visible: a vibrational mode in the E_{2g} plane at about 386 cm⁻¹ and a vibrational mode outside the A_{1g} plane at about 405 cm⁻¹. For a graphene film, there are two peaks characteristic of graphene: G and 2D. In addition, peak D is observed, associated with the appearance of defects in the graphene film as a result of transfer.

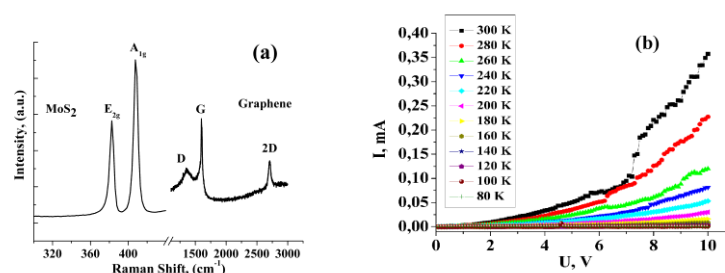


Fig.1. Raman spectrum of graphene/MoS₂ heterostructure (a). Current-voltage characteristic at T=80-300 K (b).

The current-voltage characteristics (I-V characteristics) of the graphene/MoS₂ heterostructure were measured and shown in Figure 1 b. As can be seen from Figure 1 b, the current-voltage characteristic of the graphene/MoS₂ heterostructure is similar to the current-voltage characteristic of a semiconductor diode. This type of current-voltage characteristic indicates the presence of a p-n junction at the interface between graphene and MoS₂.

This work discusses the interactions of graphene and MoS₂ layers with the properties of graphene/MoS₂ heterostructures. Theoretical calculations of the band structure and optical parameters of Gr/MoS₂ heterostructures are also presented. Electronic structure calculations were performed within the framework of density functional theory. When graphene and MoS₂ monolayer are incorporated, the internal energy of the atoms changes with the inclusion of graphene, which leads to the opening of the band gap in room K. The calculated band gap of large-scale graphene is 4 eV. The above results show that due to the formation of heterojunction optical properties, graphene/MoS₂ heterostructures undergo changes compared to single layers, which expands the possibilities of using 2D materials in optical applications.

REFERENCES

- [1] C. Li, P. Zhou, D.W. Zhang, Li, Chao, Peng Zhou, and David Wei Zhang. "Devices and applications of van der Waals heterostructures", *Journal of semiconductors*, Vol. 38, no. 3, 031005, Mar. 2017, doi: 10.1088/1674-4926/38/3/031005.
- [2] I. Lee, J. N. Kim, W. T. Kang, Y. S. Shin, B. H. Lee, W. J. Yu, Lee, Ilmin, et al. "Schottky barrier variable graphene/multilayer-MoS₂ heterojunction transistor used to overcome short channel effects", *ACS Appl. Mater. Interfaces*, Vol. 12, no. 2, pp. 2854-2861, Jan. 2019, doi: 10.1021/acsami.9b18577.

* The work was supported by the grants the Russian Science Foundation, RSF 23-79-00065.