The effect of electrical contacts to MoS_2 monolayer on its luminescence spectrum

Agata Zielińska[1], Mateusz Dyksik[1], Jonathan Eroms[2], Dieter Weiss[2], Paulina Płochocka[1,3] and Mariusz Ciorga[1,2]

[1]*Department of Experimental Physics, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland*
[2]*Institute for Experimental and Applied Physics, University of Regensburg, Universitätstraße 31, 93053 Regensburg, Germany*
[3]*Laboratoire National des Champs Magnétiques Intenses, Champs Magnétiques Pulsés, 143 Av. de Rangueil, 31400, Toulouse, France*

Semiconducting transition metal dichalcogenides (TMDCs) present new possibilities for designing novel electronic devices, including light-emitting diodes, which require an efficient contacting scheme. The latter is however challenging for TMDCs, mostly due to the typically high Schottky barrier (SB) formed between a metal and a semiconductor (SC). In theory, the barrier height is given by a difference between the work function of the metal and the electron affinity of the SC [1], but in practice, the Fermi level at the metal/SC interface is typically pinned as a result of metal-induced gap states. Recent report by Shen et al. [2] presents the possibility of obtaining ohmic contacts between semimetalic bismuth and a semiconducting TMDC layer. Due to the near-zero density of states at the Fermi level of the semimetal, the gap states are sufficiently suppresed, making possible to obtain low-resistance ohmic contacts to TMDC.

Here, we compare electrical properties of Bi and Au contacts to a MoS_2 monolayer, additionally investigating to which extent a type and quality of the electrical contact affects a photoluminescence (PL) spectrum of the sample. In case of Au contacts, the exfoliated MoS_2 layer was deposited on previously evaporated Ti/Au pads and then ironed with a tip of an AFM microscope in a contact mode. In case of Bi contacts, the MoS_2 layer was deposited on a Si/SiO_2 substrate and then Bi/Au contacts were evaporated. I-V curves of both samples were measured in the temperature range from 300 K to 2 K. Au contacts show clear Schottky characteristics, with the majority of them not conducting below 100 K, despite the calculated Schottky barriers being lower than usually reported in the literature [3]. Bi contacts, on the other hand, show ohmic behaviour from room temperature down to 80 K. Although below this temperature the ohmic behaviour is lost, the contacts still conduct down to 2 K. We calculated the contact and channel resistances in 280 K using the transfer length method and obtained a negligibly small contacts resistance compared to channel resistance (equal 46.6 $k\Omega/\mu m$).

Both samples were investigated by means of PL spectroscopy. The spectrum of the sample with Bi contacts is unusual for a MoS_2 monolayer and is significantly different from the spectrum of the sample with Au contacts. To check the effect in more details, we measured microphotoluminescence maps for both samples, with all contacts grounded. Each spectrum was integrated in 2 ranges - around 1.9 eV (trion) and around 1.8 eV (defect). We clearly observe that grounding the contacts has much more visible effect in case of the sample with Bi (ohmic) contacts, which points towards correlation between the type and quality of contacts and the observed luminescence spectrum.

[1] A. Allain, J. Kang, K. Banerjee, and A. Kis, *Nature Materials* **14**, 1195–1205 (2015).
[2] P.-C. Schen et al., *Nature* **593**, 211–217 (2021).
[3] D. S. Schulman et al., *Chemical Society Reviews* **47**, 3037 (2018).