Optimization of Contacts for van der Waals heterostructures by AFM ironing

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Semiconducting transition metal dichalcogenides (TMDCs) like MoS_2, $MoSe_2$, WS_2 and WSe_2 offer many new possibilities of structure engineering from the spintronics' point of view and are, therefore, attractive for future novel electronic devices. Integration of any device with an external circuitry requires, however, an efficient contacting scheme, which is challenging for TMDCs. Between a metal and a semiconductor (SC) the Schottky barrier (SB) is typically formed, which is theoretically dependent on the difference between the work function of the metal and the electron affinity of the SC [1]. In practice, the Fermi level at the metal/SC interface is typically pinned as a result of metal-induced gap states. This problem can be ommited by introducing a tunnel barrier in the form of an additional interlayer, e.g., hBN layer, between the metal and the TMDC, which limits the wavefunction spreading from the metal into the TMDC [2]. Transfer techniques commonly used to stack individual 2D layers into vdW structures can lead to inhomogeneities due to contaminants trapped between a 2D layer and a substrate or a metal layer [3]. One of the recently suggested methods to circumvent this problem is the so-called AFM ironing, when a contact-mode AFM scan is used to remove any possible imperfections like organic residues, bubbles or wrinkles, and improve adjacency of layers and, therefore, contact's resistance. This method has been used with success in many experiments [4-6].

Here, we investigate the effect of AFM ironing on the quality of Ti/Au contacts to MoS_2. MoS_2 flakes were produced by means of mechanical exfoliation and deposited on Si/SiO_2 substrates. Apart from investigating the direct metal/MoS_2 contacts, we studied also the influence of a thin hBN layer, acting as a tunnel barrier between the metal and the MoS_2 flake, on contact parameters. To study the influence of AFM ironing on the quality of such prepared contacts, the electrical and optical properties of the ironed and the non-ironed samples were compared using transport measurements and photoluminescence spectroscopy, respectively.

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