Epitaxial 2D $HfSe_2$ Semiconductor/$TaSe_2$ Metal van der Waals Heterostructure

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The formation of low resistance electrical contacts on 2D semiconductors remains a challenge and is one of the bottlenecks for their application in devices. Although some successful attempts have been reported [1], the standard contact fabrication by metal deposition often induces defects and damages to the 2D materials, which degrade their intrinsic properties. One way to circumvent that relies on the use of a metallic 2D material allowing a van der Waals interface with the 2D semiconductor. In this work, we focus on such a system involving a metallic ($TaSe_2$) and a semiconducting ($HfSe_2$) transition metal dichalcogenide (TMD). $HfSe_2$ seems promising due do its predicted high carrier mobility [2] whereas $TaSe_2$ clearly exhibits a metallic character in its 2H phase [3]. Interestingly, a high work function has been reported for both materials and make their association appealing for contact realization [4].

We first optimize the growth of $TaSe_2$ and $HfSe_2$ layers on Se-terminated $GaP(111)_B$ substrates. The layers are prepared by MBE under excess Se with a typical growth rate in the 3-4 ML/h range. $HfSe_2$ crystallizes in the 1T phase whose structural quality is rather independent on the growth temperature within the explored range (250-500°C). By contrast, multilayers $TaSe_2$ mostly exhibit the 3R and 2H polytypes with an improvement of the film crystallinity with increasing growth temperature and the layers grown between 250°C and 500°C have a resistivity comparable to those reported for bulk $TaSe_2$. In both cases, diffraction techniques clearly evidence the epitaxial relationships between the GaP substrate and the TMD layer. These latter are preserved during the growth of the $HfSe_2$/$TaSe_2$ heterostructure (Fig. 1) and the respective polytypes of each material are clearly identified in the stacking using scanning transmission electron microscopy (Fig. 2). Finally, photoelectron spectroscopy measurements show a n-type doping in $HfSe_2$ and a small work-function mismatch with $TaSe_2$ (Fig. 3).

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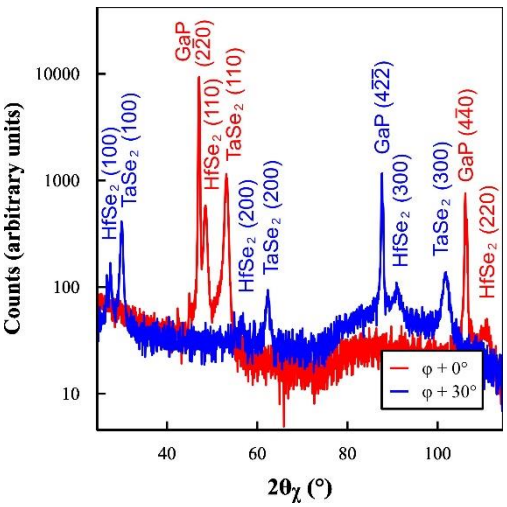

Fig. 1: In-plane grazing incidence X-ray diffraction pattern of a $TaSe_2/HfSe_2$/GaP heterostructure. The $HfSe_2$ [1 0 0] // $TaSe_2$ [1 0 0] // [2-1-1] GaP epitaxial relationship is verified.

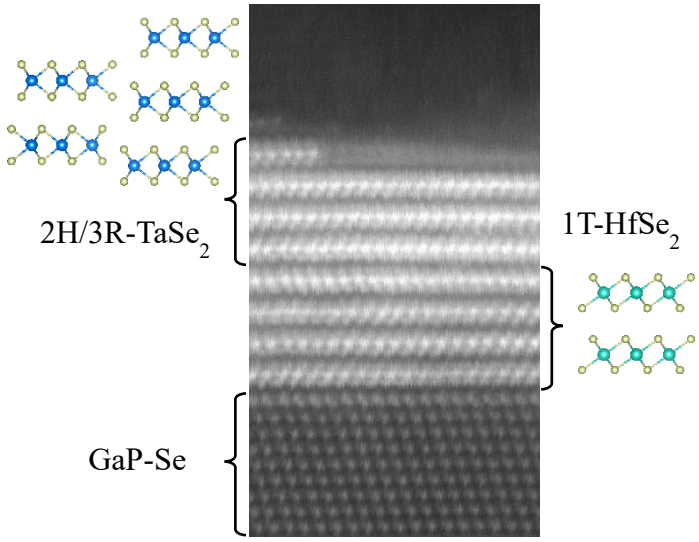

Fig. 2: Scanning transmission electron microscopy of a $TaSe_2/HfSe_2$/GaP heterostructure.

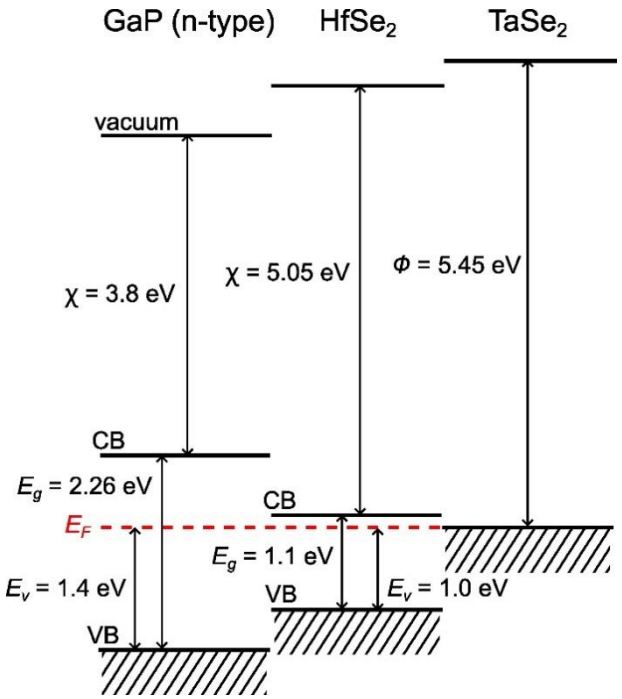

Fig. 3: Band alignments in a $TaSe_2/HfSe_2$ heterostructure grown on n-type GaP substrates, as derived from X-ray and ultra-violet electron spectroscopy measurements. The GaP electron affinity and band gap energies are from the literature [5,6].

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