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Nano-ARPES investigation of twisted bilayer WS_2

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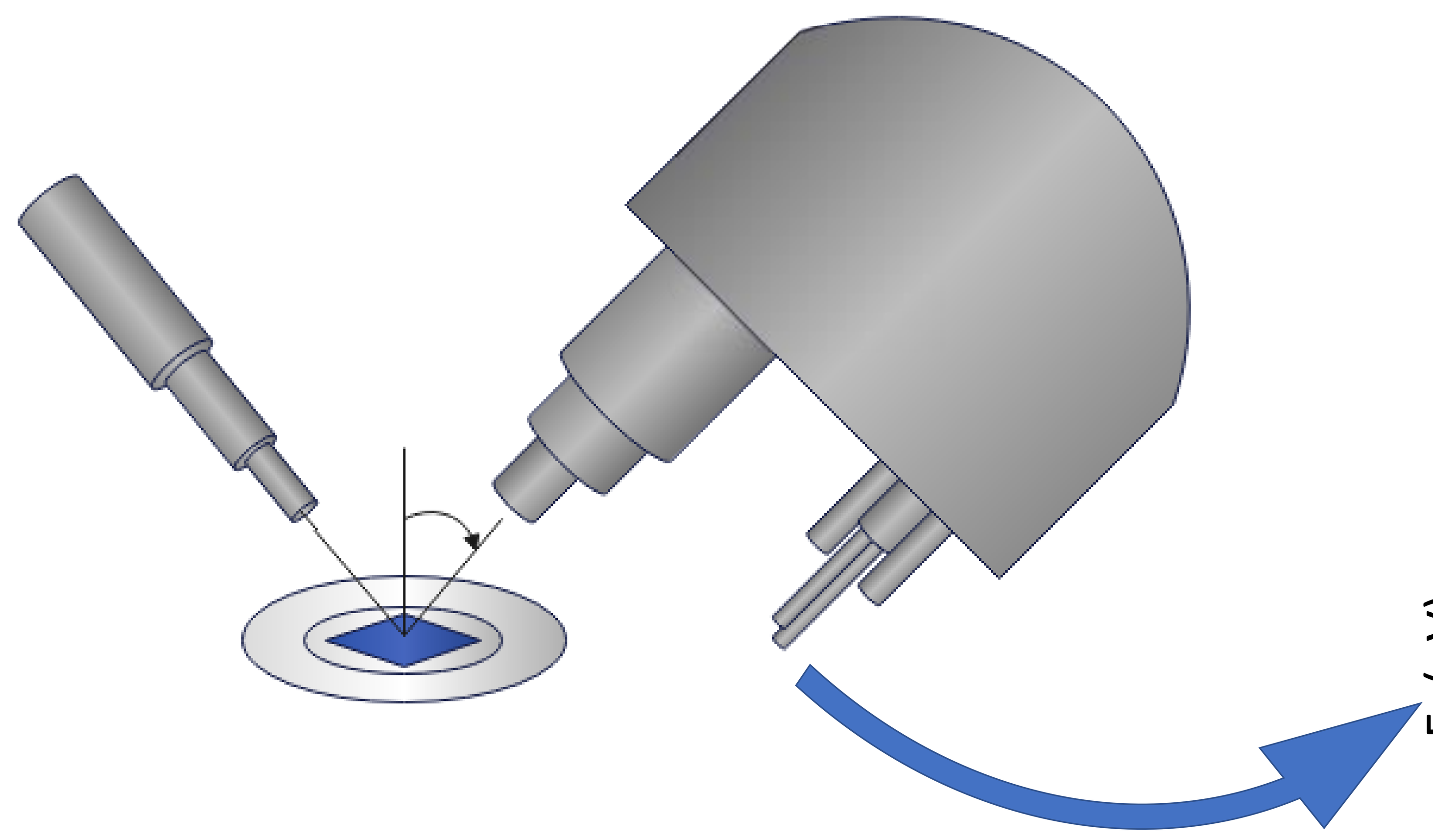
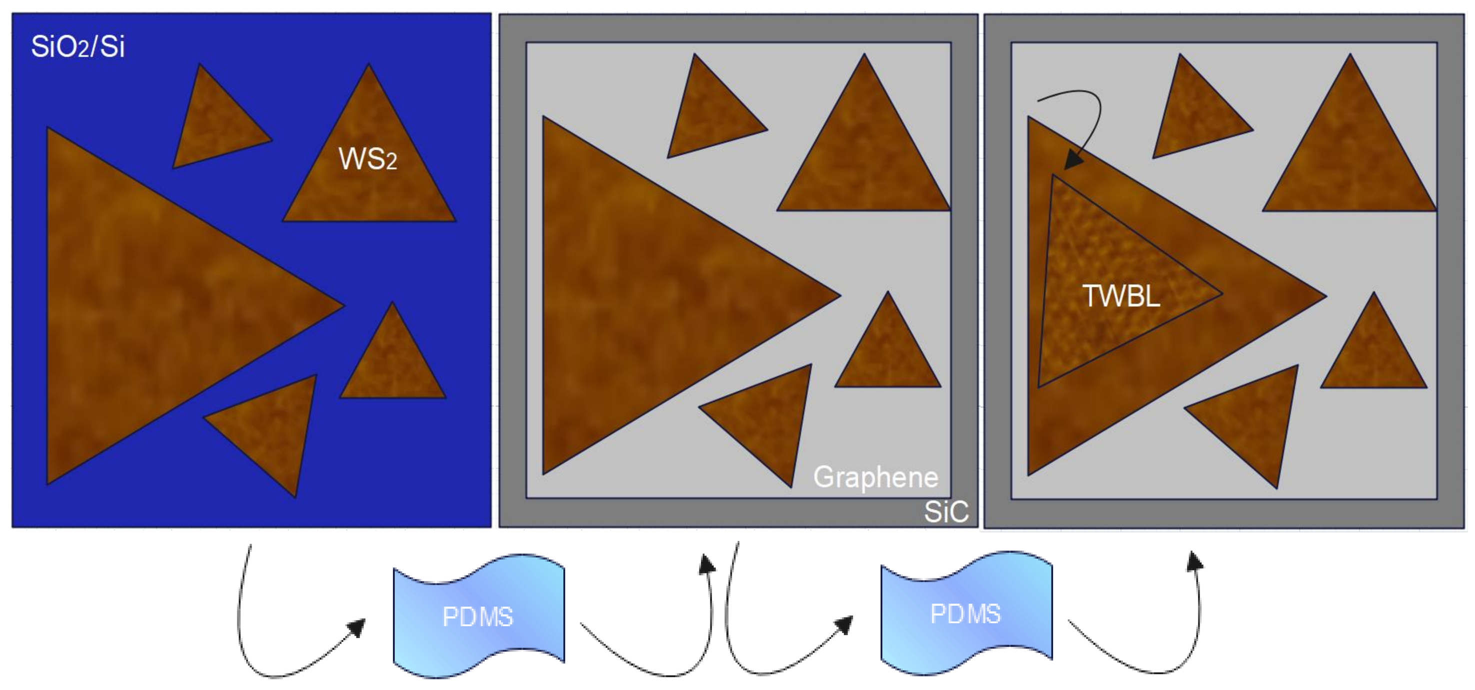
Abstract

The interesting phenomena occurring in twisted bilayer graphene lead to a better understanding of strongly correlated systems [1]; it is important to continue the research on this field by analyzing the behaviour of other twisted bilayers such as transition metal dichalcogenides (TMDs). In the last decade TMD monolayers have been widely studied both from the fundamental point of view and for applications in various fields. In particular WS_2 seems to be a good candidate for the next generation of electronic devices.[2] Despite the interest, very few results are published regarding the band structure of this material when two layers are stacked one on top of the other at a certain angle because of the difficulty in realizing this structure in a large enough size to be investigated spectroscopically. In this project we performed a nano-ARPES study at the SOLEIL synchrotron that revealed the band structure of twisted bilayer WS_2 with a twist angle of 3.6°. The experimental results are compared with the theoretical simulation made by DFT calculations considering the spin orbit coupling corrections for the single layer, the bilayer and the bulk crystal along the major symmetry directions Γ-K and Γ-M.



Sample preparation: WS_2 was prepared by chemical vapour deposition on a SiO_2/Si substrate and transferred on top of a graphene/SiC substrate by using PDMS. Atomic force microscopy (AFM) measurements were performed to visualize the Moiré superstructure and determine the twist angle.

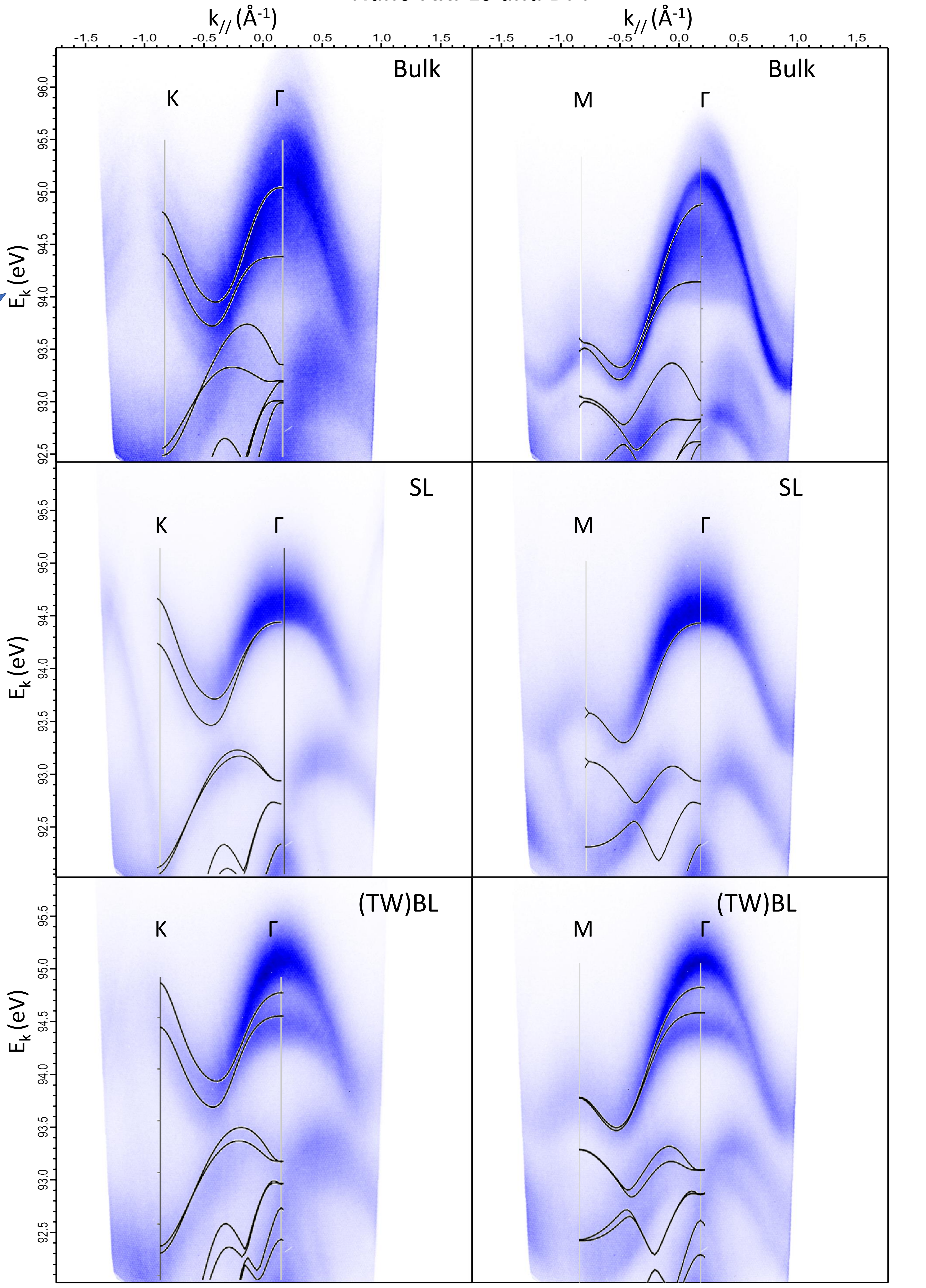


Why Graphene/SiC as substrate? The roughness of the substrate can affect the resolution of the bands. Graphene on SiC is flat at the nanometer scale and allows for a good anglar resolution. The preparation of the substrate is a combination of the sublimation growth in Ar atmosphere and the usage of a polymer as additional carbon source.[3] The polymer is deposited by spin coating and then heated up before the graphene deposition.

Conclusions

The theoretical calculation is in good agreement with the experimental measurements regarding the number of branches and their energy. In the case of the TWBL the simulation considered an untwisted bilayer, hence they show significative discrepancy with respect to the experimental results.

Nano-ARPES and DFT



References

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