The Influence of the Twist Angle on the Properties of Transition Metal Dichalcogenide Bilayers

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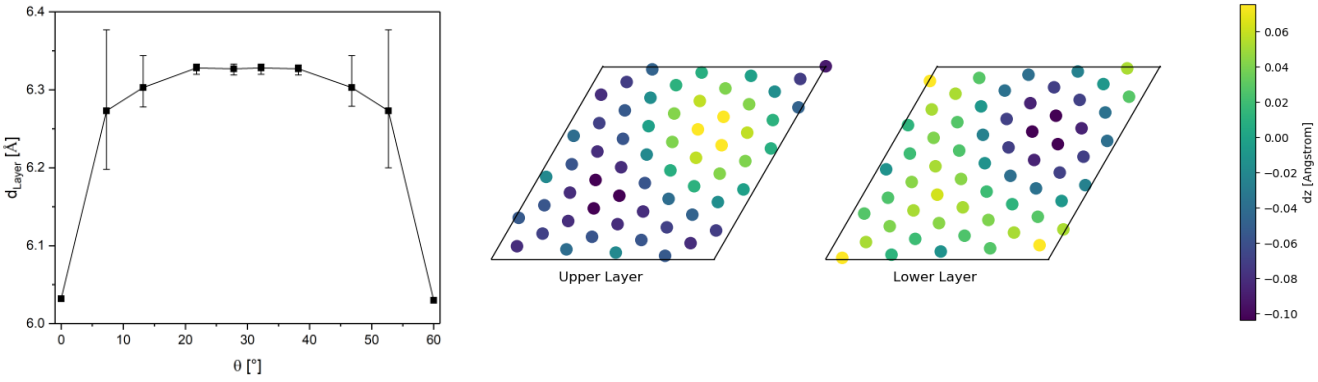
The stacking of single layer 2D crystals like transition metal dichalcogenides creates a new class of materials: van der Waals heterostructures. [1] In these materials a variety of structures can be realised by controlling the stacking order and the twist angle between adjacent layers. In this work the influence of the twist angle on MoS2 bilayers was studied using reactive force field (ReaxFF) calculations. The most prominent structural effect upon interlayer twisting is the formation of moiré patterns of rapidly increasing size for small twist angles, resulting in huge simulation cells that can be only studied using force fields. [2] Also there is a change in the interlayer distance with minima for twist angles of 0° and 60°. A more subtle effect is the formation of an interlayer waviness as shown in the figure. It could be shown that the amplitude of the waviness is strongest for small twist angles and that the general features of the interlayer waviness can be linked to other structural properties within the bilayers. Based on these findings the effect of the twist angle on the structural and physical properties of the semiconducting van der Waals bilayers was studied.

References

[1] A. K. Geim, I. V. Grigorieva, Nature, 499 (2013) 419.
[2] G. C. Constantinescu, N. D. Hine, Physical Review B, 91 (2015) 195416

Figures



(a) (b)

Figure 1: (a) Mean interlayer distance for different twist angles with maximum amplitude of the interlayer waviness indicated as bars. (b) Visualisation of the interlayer waviness of a MoS_2 bilayer with a twist angle of 7.3°. Out of plane deviation from the mean layer position is indicated for the Mo atoms using a colormap. The symmetry between upper and lower layer become clearly visible.