Temperature-driven rotation epitaxy of monolayer TaS_2 on bilayer graphene

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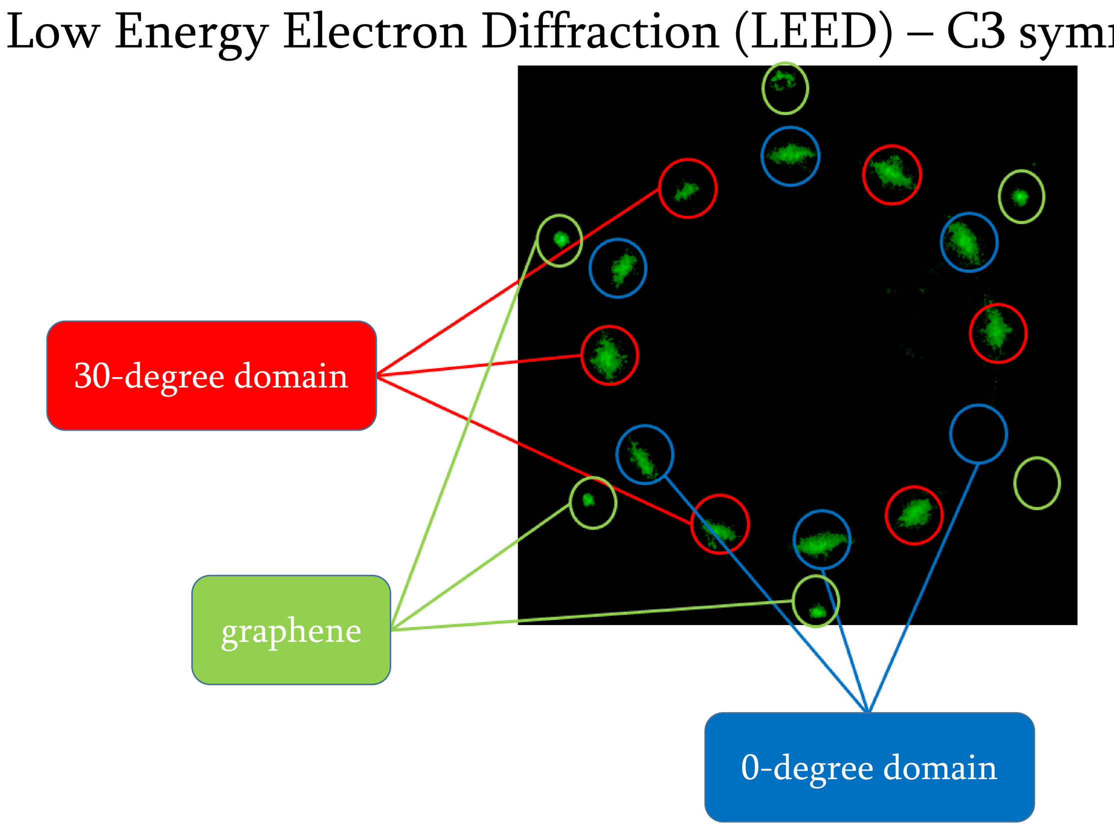
Introduction

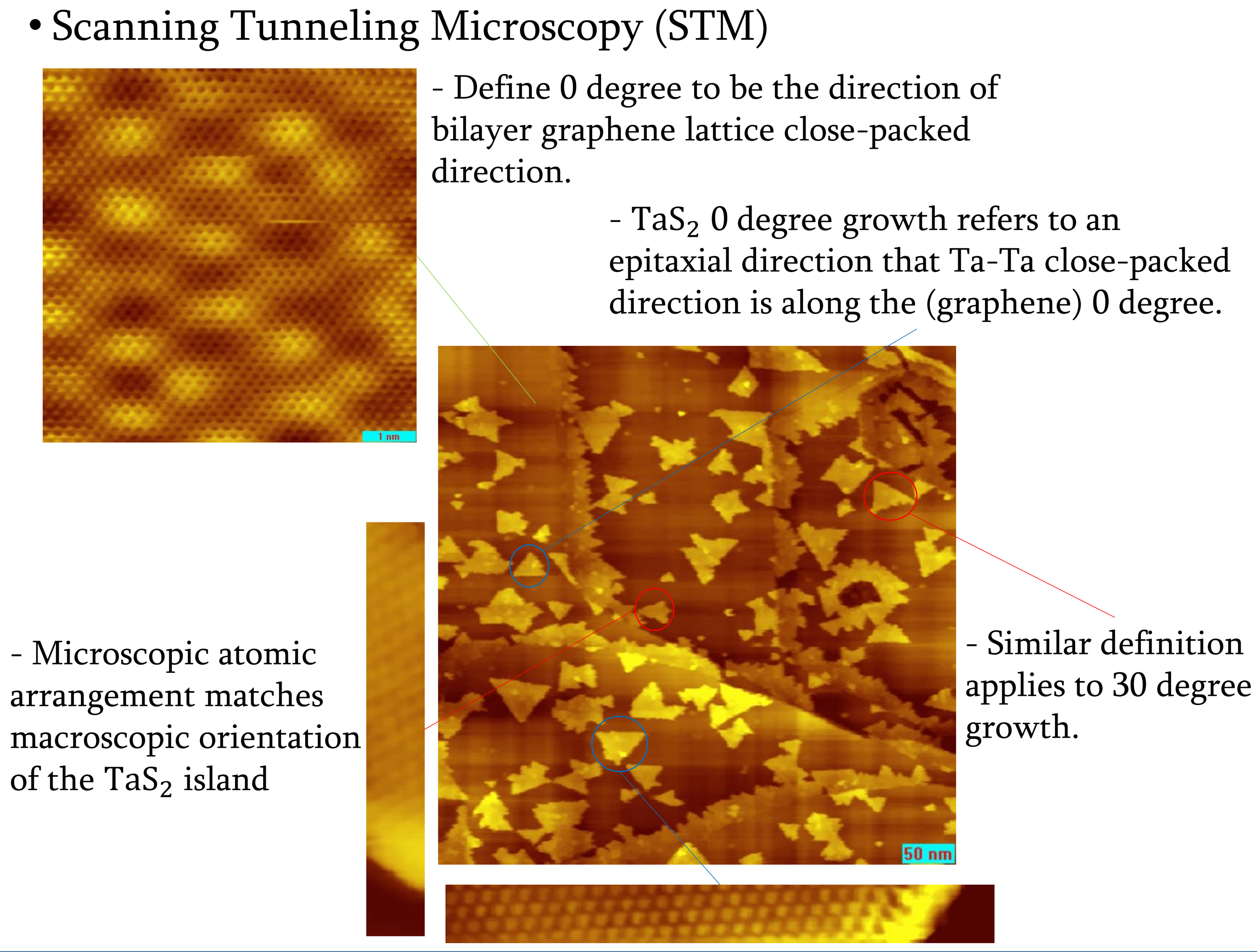
•In our studies, we observed unexpected epitaxial rotation of monolayer H-phase TaS_2 on bilayer graphene as the growth temperature varies.
•This is not an observation of coexistent orientations (often observed in TMD monolayers), but an observation that shows the preferred epitaxial orientation changes with the growth temperature.
•What we observed is an uncommon large angle change of preferred epitaxial orientation.
•A plausible explanation of the mechanism is the large differential thermal expansion.

Domain Identification

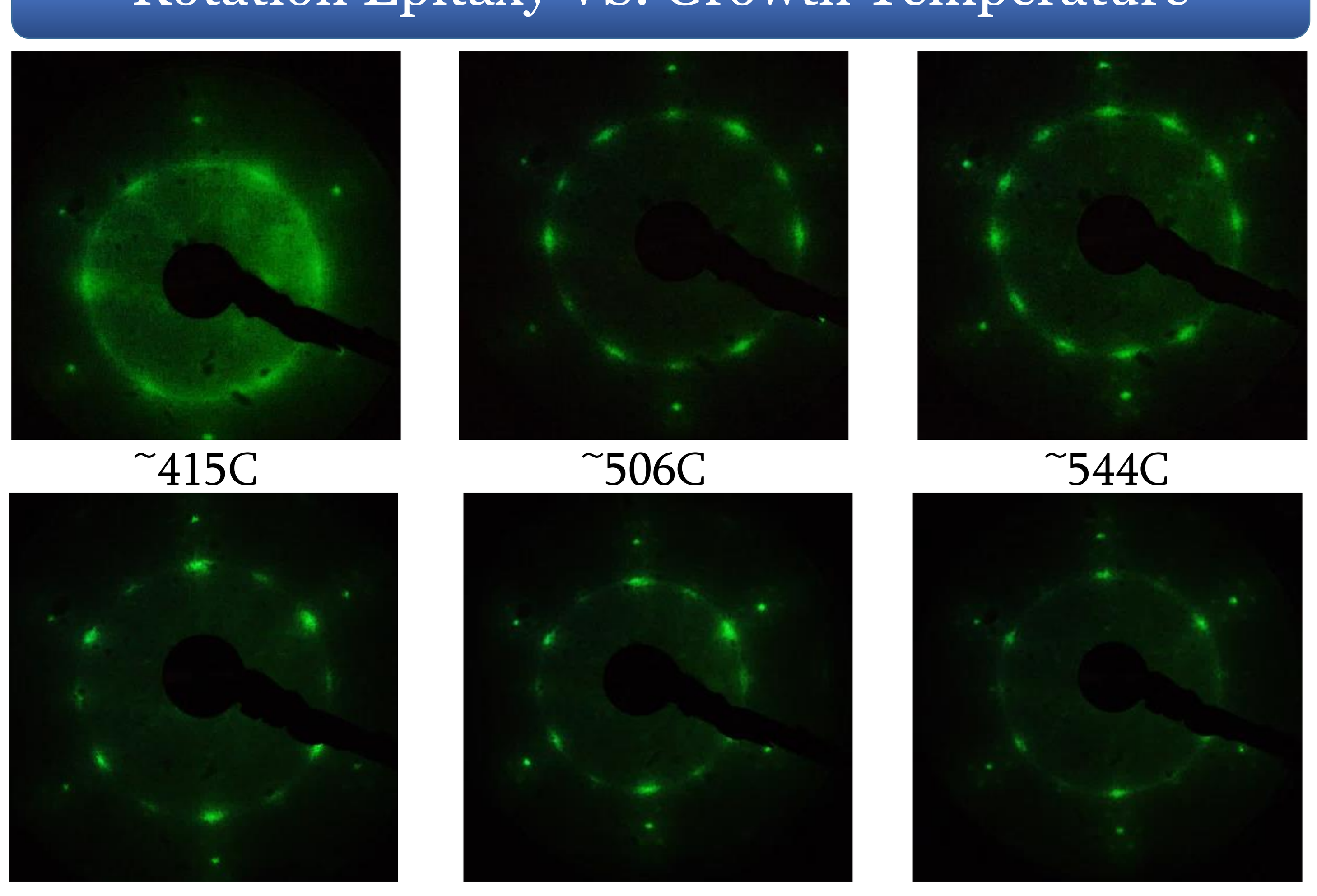
• Low Energy Electron Diffraction (LEED) – C3 symmetry



• Scanning Tunneling Microscopy (STM)

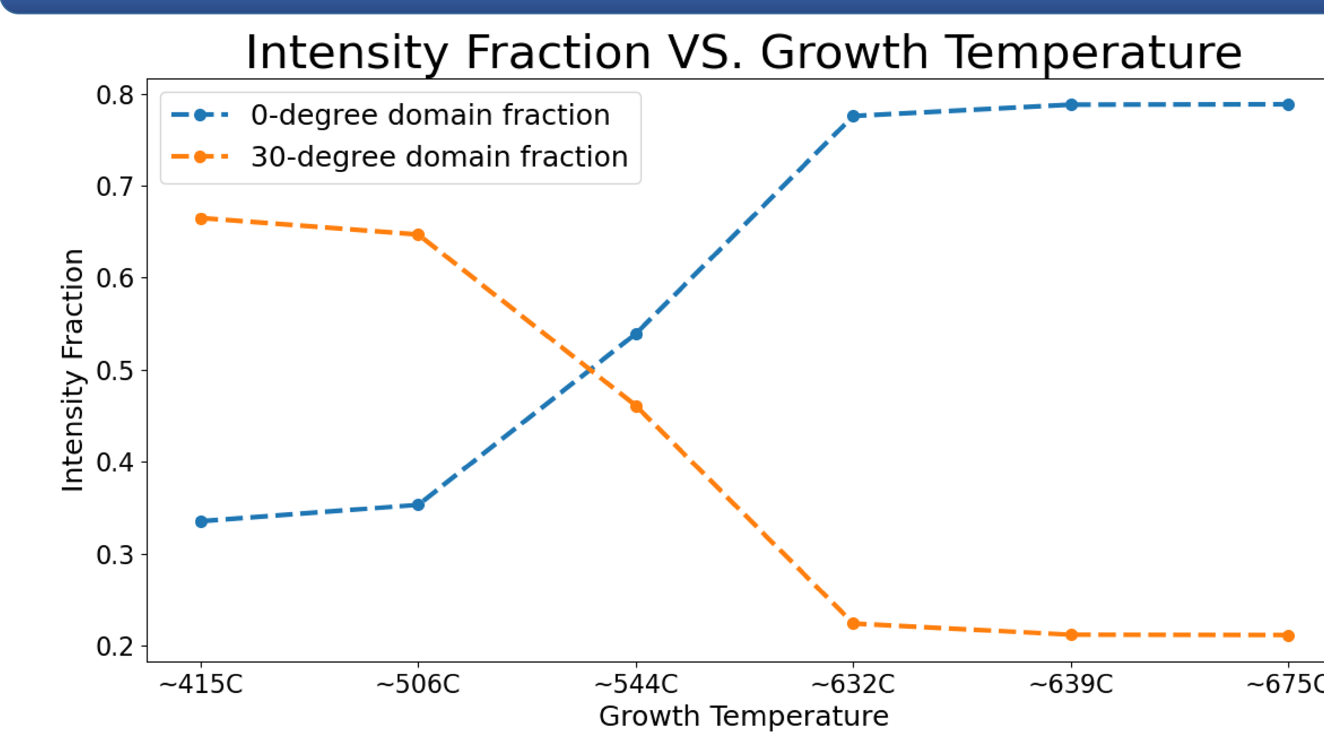


Rotation Epitaxy VS. Growth Temperature



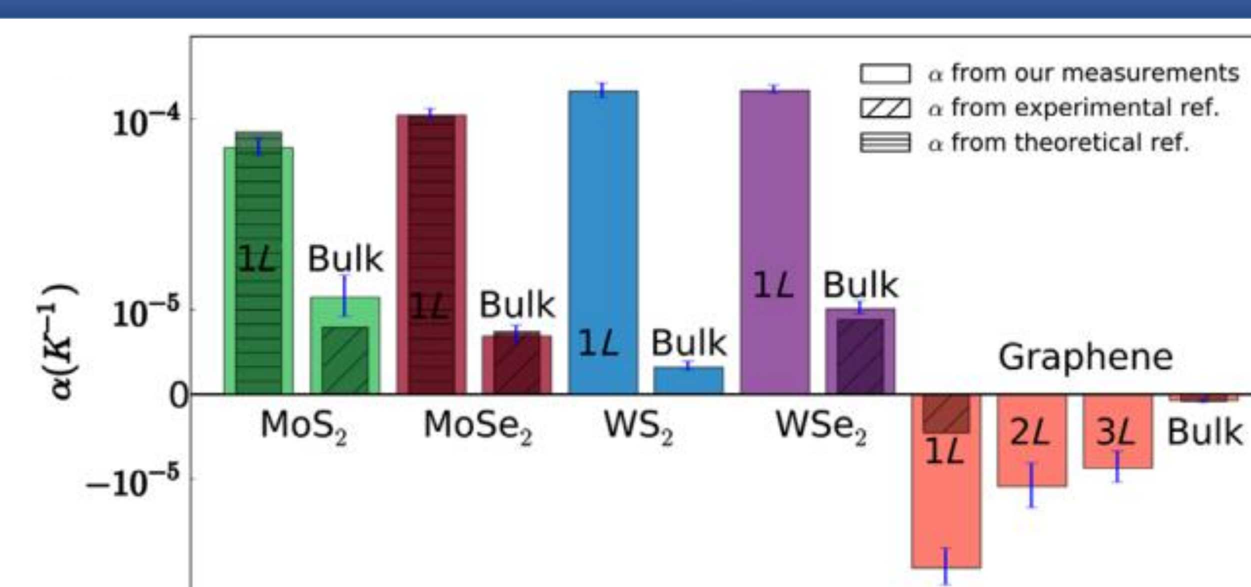
•At low temperature, TaS_2 prefers 30 degree growth.
•At median temperature, TaS_2 adopts competing strength of 0 degree and 30 degree growth.
•At high temperature, TaS_2 prefers 0 degree growth.

Intensity Fraction Evolution



- Intensity fraction is extracted through spot profile gaussian fitting.

A Possible Explanation



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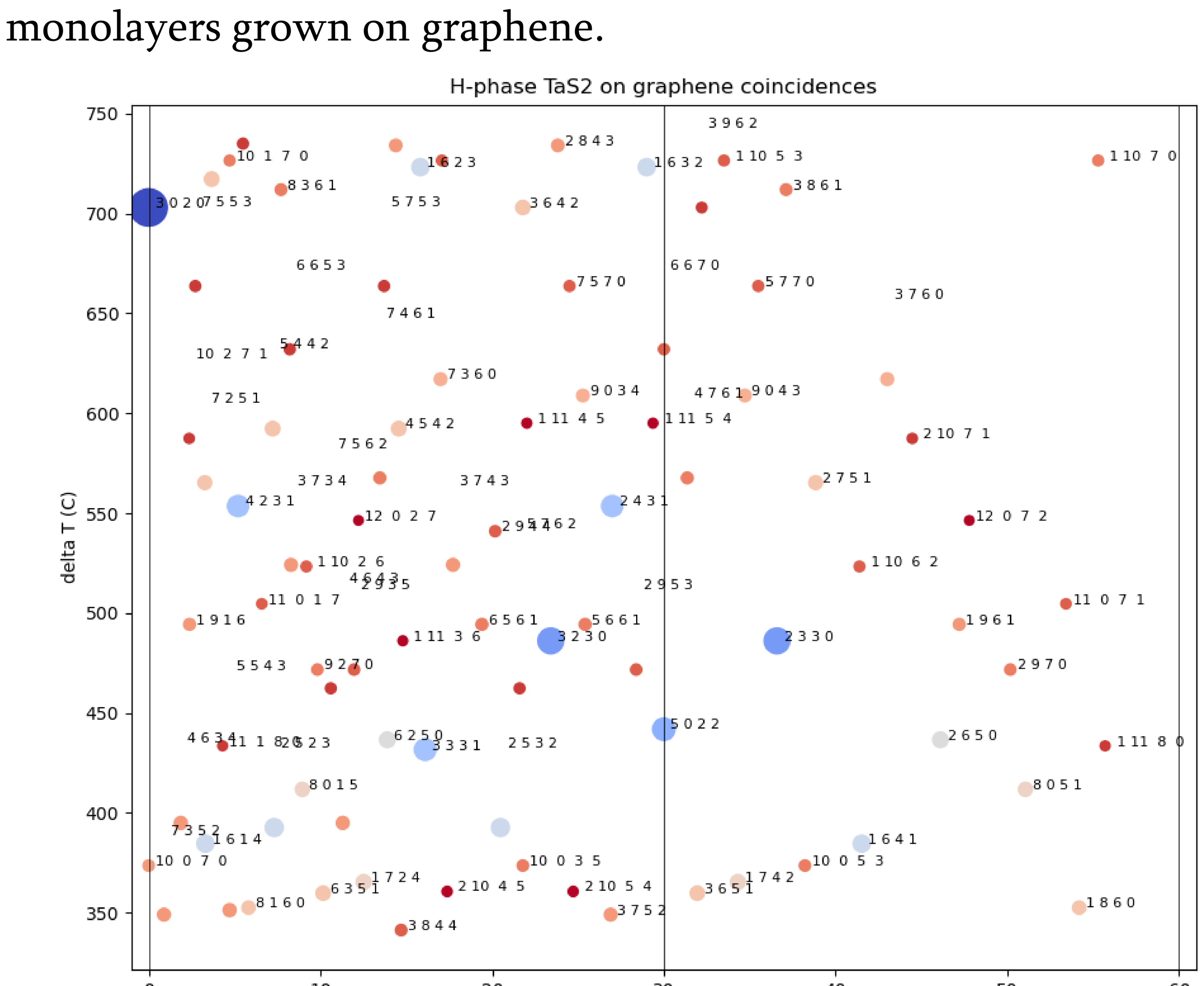
•2D monolayer typically has a much larger linear thermal expansion coefficient (LTEC) than its bulk form
•Graphene has a negative thermal expansion coefficient over a wide temperature range
•Given the above, one can argue that a large temperature-driven thermal expansion difference will be present in cases of TMD monolayers grown on graphene.



•Lattice coincidence matching
- two hexagonal lattices will form a coincidence if one superlattice matches the other superlattice by the following relation: $a_1{}^2(i^2+ij+j^2) = a_2{}^2(k^2+kl+l^2)$
- coincidence can be visualized after rotating the second lattice by: $\theta = arctan2\left(\frac{\sqrt{3}}{2}j, i+\frac{1}{2}j\right) - arctan2\left(\frac{\sqrt{3}}{2}l, k+\frac{1}{2}l\right)$

•Issues
- We used WS_2 LTEC (no experimental data for TaS2 monolayers)
- a seemly inconsistency between the simulation and experimental observation: optimal matching does not fall exactly at 0 or 30 degrees. This may be amended if the assumed rigid lattice is allowed to relax

Contributions & Acknowledgements

H.K.C. performed MBE growth, LEED and STM measurements, and data analysis. D.M. performed data analysis and modeling. A.D.C. performed bilayer graphene preparation. W.W.P. and S.J.T. interpreted the data and led the project.
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