首届致远学术节
学生科研成果展示

# Strain Induced Effects On Monolayer Graphene And Transition Metal Dichalcogenide

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## Introduction

Strain engineering proves to be effective in tuning electronic and optical properties in various 2D materials such as graphene and molybdenum disulfide($MoS_2$). Its massive potential application in electronics and valleytronics attracts enormous interest mainly in two aspects: (i) what effect does strain induced and (ii) how do we induce desired effect by optimizing the magnitude and distribution applied strain.

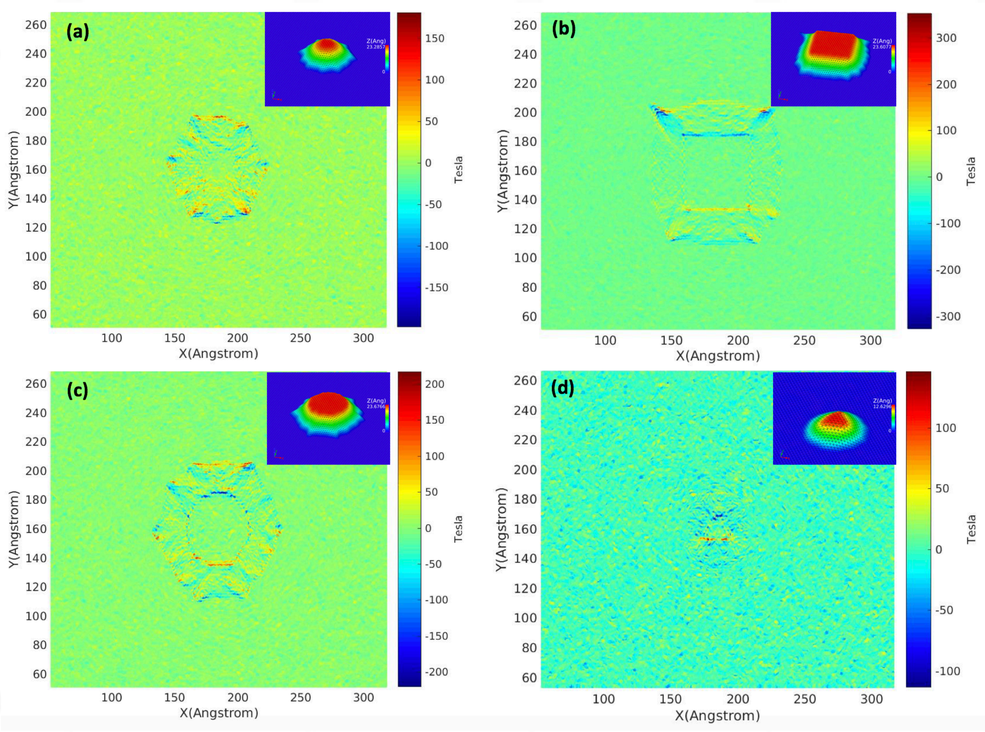
For the first aspect, previous strain engineering studies on graphene, strain can induce additional Raman features, strong gauge field and hence pseudo-magnetic field over 300T is observed. In $MoS_2$, besides the Raman shift observed in experiments, *ab initio* calculations shows by forming ripple structure in zig-zag direction, the band gap can be tuned and a direct-to-indirect gap transition is predicted when curvature of the ripple structure increases. In addition, recent discoveries of that electron with different valley index reacting oppositely to pseudo-magnetic field indicates a new potential application of strain engineering.

For the second aspect, a common way is to prepare nanostructured substrate by E-Beam Lithography(EBL) and Focus Ion Beam Lithography(FIBL) For example, when a graphene sheet is placed on a nanostructured substrate, due to the van der Waals force between carbon atoms and substrate atoms, the graphene will fit to the shape of the nanostructure and hence the strain on graphene is induced. Therefore, by making nanostructure of different shape, we can apply different non-uniform strain on graphene hence induce different distribution of pseudo-magnetic field.

Therefore, we carried out molecular dynamics(MD) simulations to predict strain distribution on graphene and $MoS_2$ induced by nanostructured substrate, which can be essentially helpful in valleytronic device fabricating.

## Strain engineering on monolayer graphene

Large-scale Atomic/Molecular Massively Parallel Simulator(LAMMPS) with its built in AIREBO potential is used in our MD simulations. In the simulations, I introduced strain on graphene monolayer by placing the graphene monolayer on a nanostructured substrate and then relaxing the system for a sufficient long time. We compare our simulation results with topography data obtained using Atomic Force Microscopy(AFM) by Goncalves et al[1]. Specifically, I simulate a semi-sphere nanoparticle with radius of r=2.5nm on gold substrate with four combination of different boundary conditions and different substrate. By scaling AFM data down, we find our simulation presents close results.



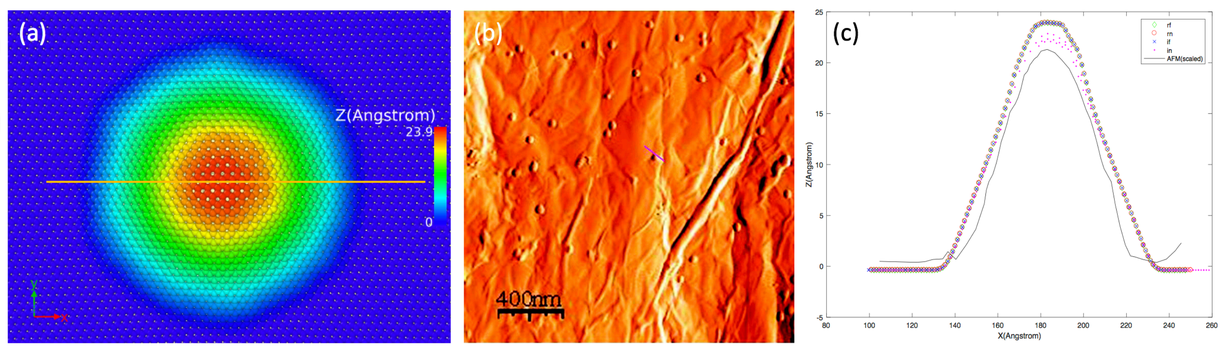




Figure 1: Comparison between simulation with different substrate or boundary condition setting and scaled AFM line cut data obtained by Goncalves et al[1]. **(a)** Typical simulation result with line cut direction marked in orange line; **(b)** AFM image obtained by Goncalves et al with line direction marked in purple; **(c)** Comparison between five line-cut data. rf = real substrate with fixed boundary condition; rn = real substrate with free boundary condition; if = imaginary substrate with fixed boundary condition; in = imaginary substrate with free boundary condition. Imaginary substrate is a LAMMPS implanted technique to accelerate the calculation without losing significant amount of precision.

Nanostructure of different shape will induced different pseudo-magnetic field distribution on the graphene monolayer. Therefore, I investigate spherical, cubic, cylindrical and tetrahedral nanostructure. Results are shown in the Figure 2. In the case of spherical and cylindrical, I obtain pseudo-magnetic field with six fold symmetry, which is in accordance with Qi et al [2], who induces strain by pushing graphene sheet towards substrate with hole of different shape. In Figure 2(b), where the shape of nanoparticle is cube, I observe same pyramid structure as Neek-Amal et al [3]. In addition, I observe the shape of the area, which is pushed up by the nanoparticle, presents a hexagonal shape which is also in accordance with Neek-Amal et al [3].

Figure 2: Top view of z-component of pseudo-magnetic field induced by nanoparticle with shape of **(a)** sphere (radius of 2.4nm), **(b)** cube (side length of 4.8nm), **(c)** cylinder (radius of 2.4nm), **(d)** tetrahedron (edge length of 2.4nm with top rounded with radius of 1.2nm). The topography in real space is shown in up-right panel in each graph with color coding of z position of each atom. X-axis is the direction of zig-zag.

## Strain engineering on molybdenum disulfide

Similar to simulation on graphene, we relax a monolayer $MoS_2$ on imaginary nanostructured substrate with free boundary condition for sufficient amount of time. Then we calculated the displacement field and local strain tensor based on the final and initial position of the atom. The result indicates that while the Mo layer and the upper S layer is stretched like graphene, the lower S layer is actually compressed. However, the pseudo-magnetic field calculation of $MoS_2$ is different from graphene therefore requires further investigation.

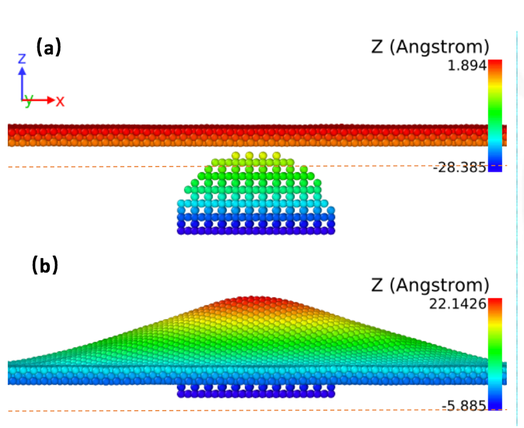



Figure 3: **(a)-(b)** Cross-section view of initial and final state of the simulation respectively. Orange line marked the plane where imaginary substrate was created.

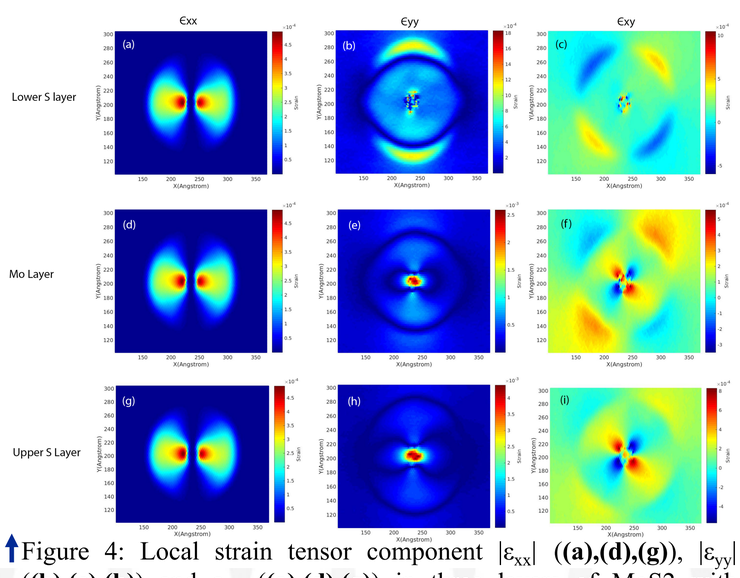



Figure 4: Local strain tensor component $|\varepsilon_{xx}|$ **((a),(d),(g))**, $|\varepsilon_{yy}|$ **((b),(e),(h))** and $\varepsilon_{xy}$ **((a),(d),(g))** in three layers of MoS2 with magnitude colored.

## References

[1] G. Goncalves, et al. *Chemistry of Materials* 21.20 (2009)
[2] Z. Qi, et al. *Physical Review B* 90.12 (2014)
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