Dislocation network structures in 2D bilayer system

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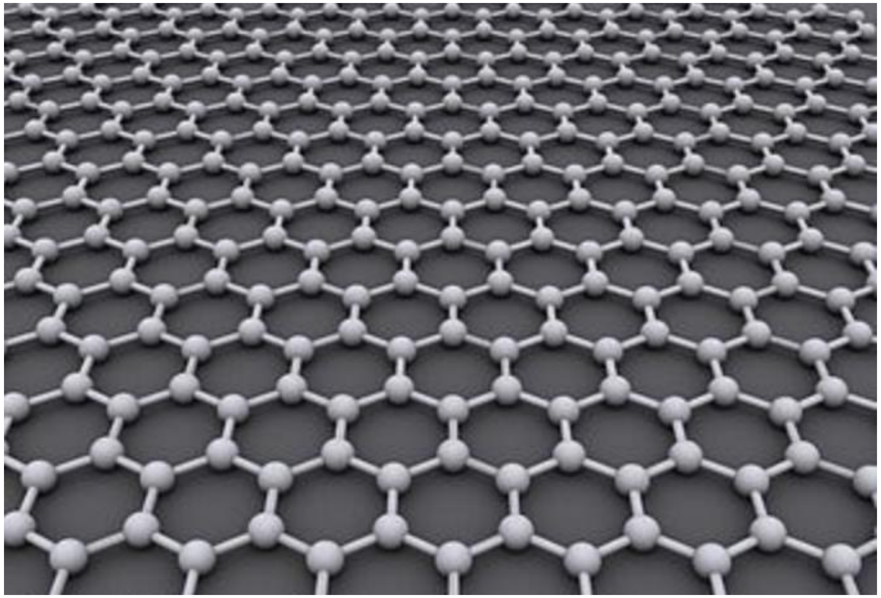
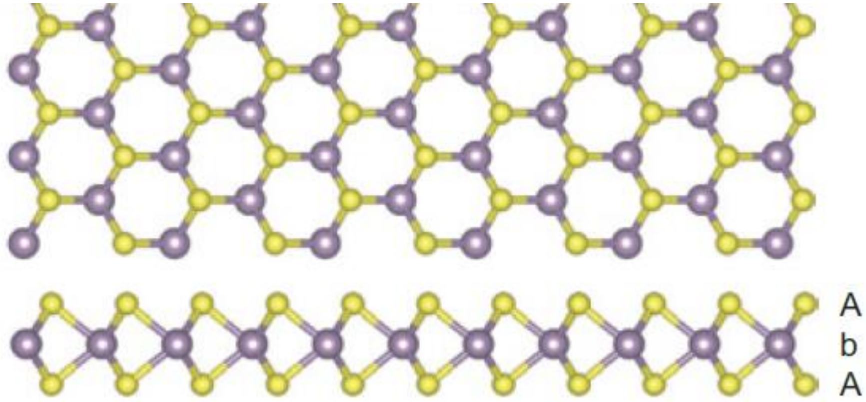
Prof. David SROLOVITZ, UPENN

Low-dimensional materials

- 2D Monolayer materials: graphene,
  hexagonal boron nitride (hBN),
  transition-metal dichalcogenides (e.g., MoS_2), …





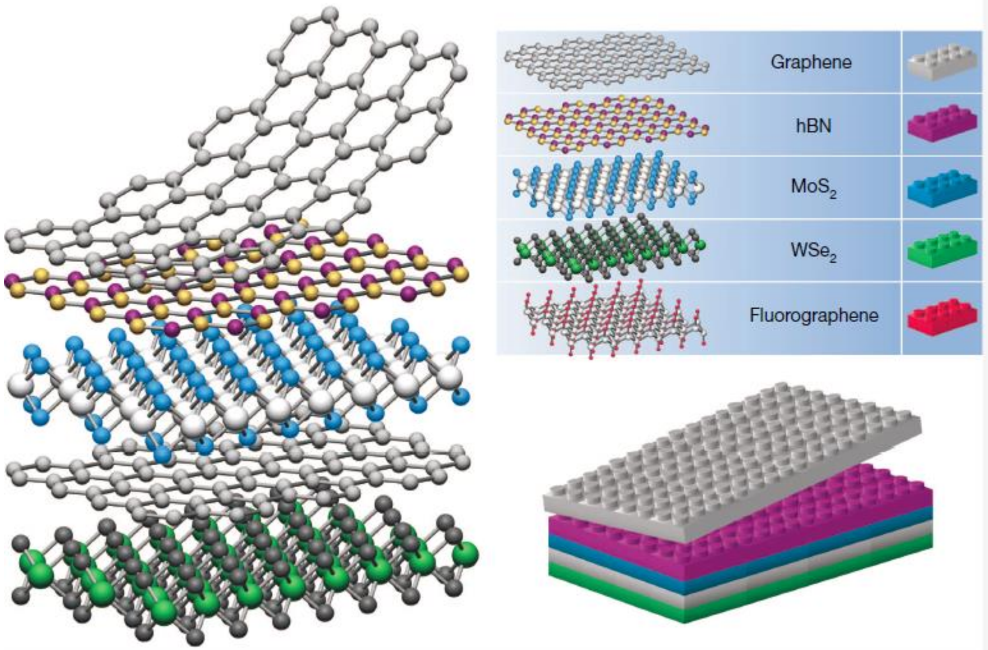
Low-dimensional materials: Bilayers

- Monolayer materials: graphene, hBN, MoS2, …

  ↓ van der Waals (vdW) interaction

- Bilayers: identical layers w/ or w/o a twist or different layers → tunable electronic behavior

Van der Waals Homo-/Hetero-structure



[A. K. Geim *et. al.* Nature, (2013)]

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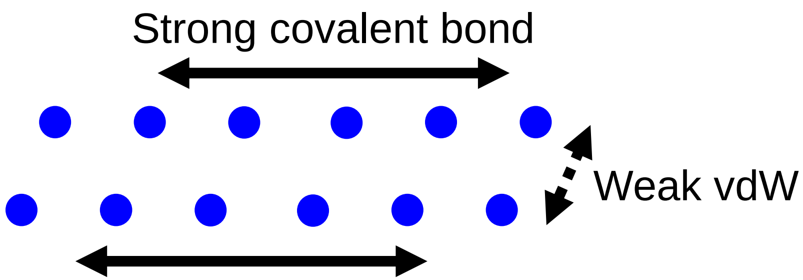

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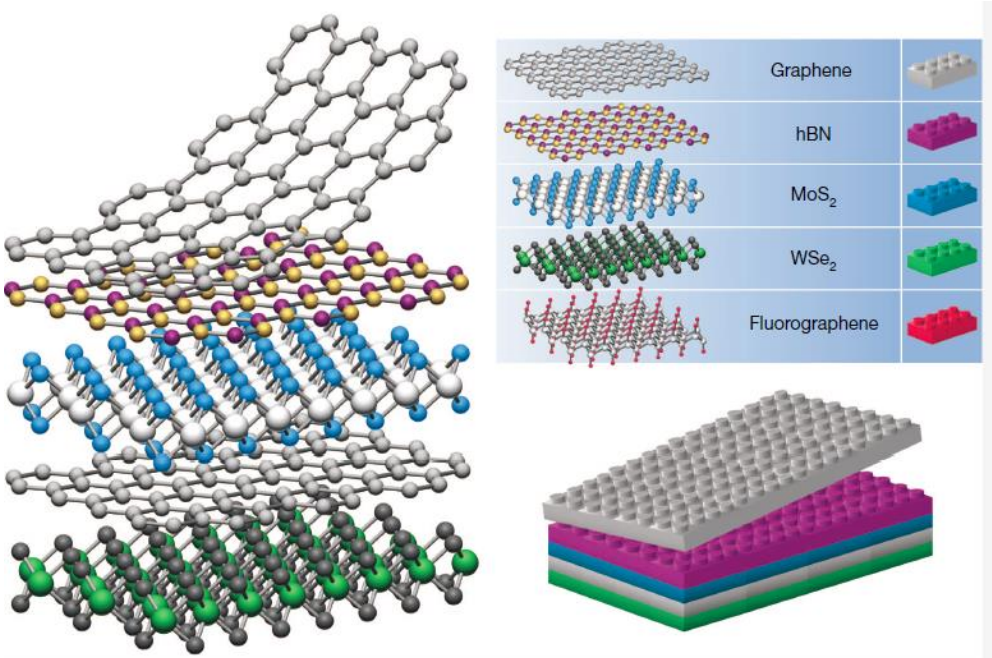

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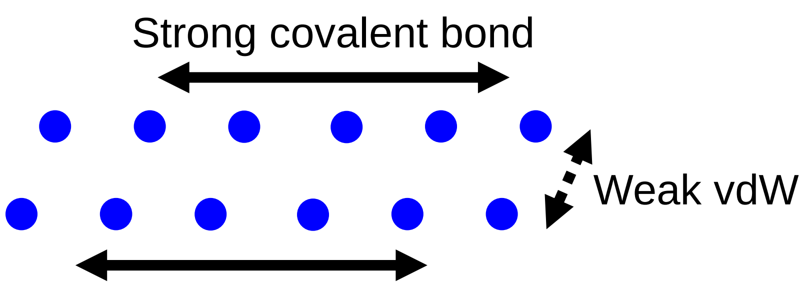


Weak vdW interaction

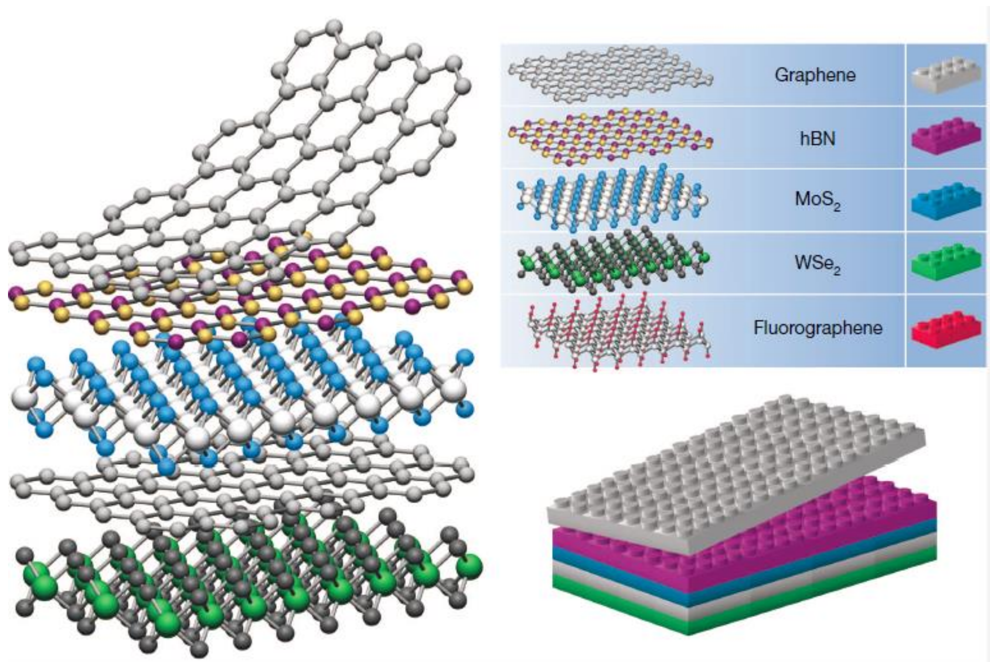
+

Small bending rigidity

↓

Interlayer defect

Van der Waals Homo-/Hetero-structure



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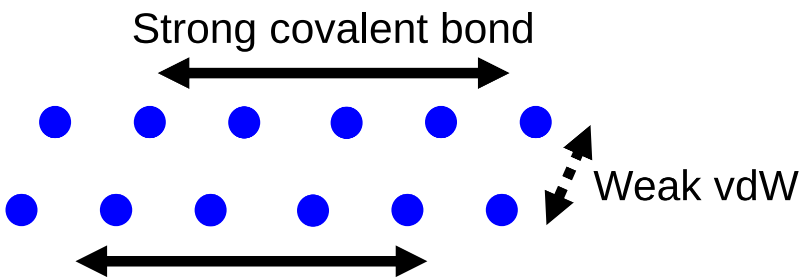

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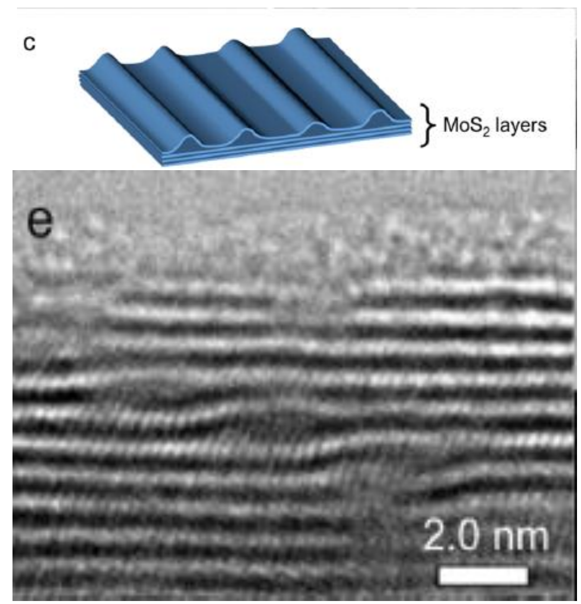
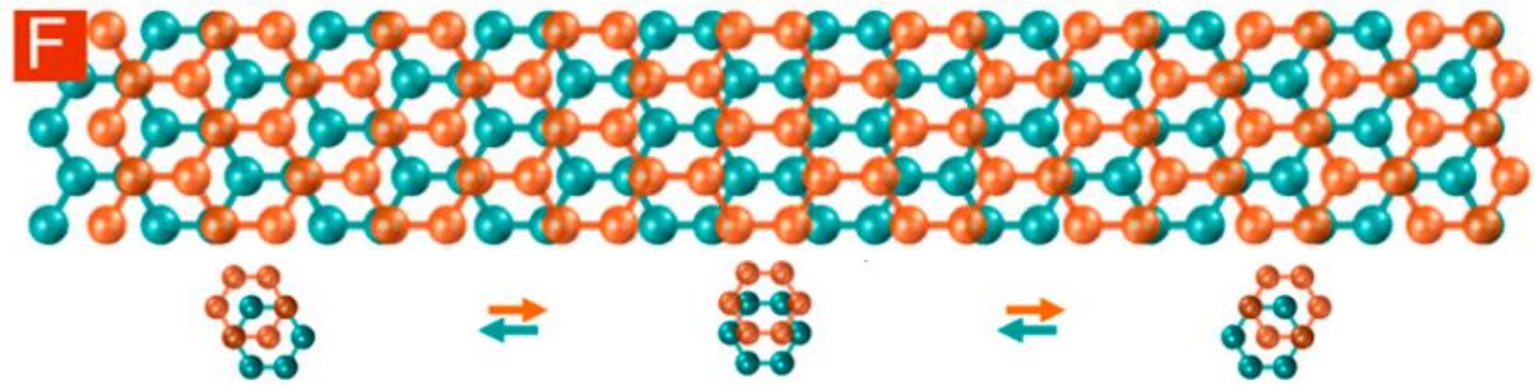


[A. Kushima *et al.*, Nano Lett., (2015)]

Defect types I

Interlayer defects: Shift top layer w.r.t. bottom layer

AB stacking   Interlayer dislocation   AC stacking



[J. Alden, et. al., PNAS, (2013)]

Interlayer dislocation: line defects that separate regions with different shifts

Defect types I

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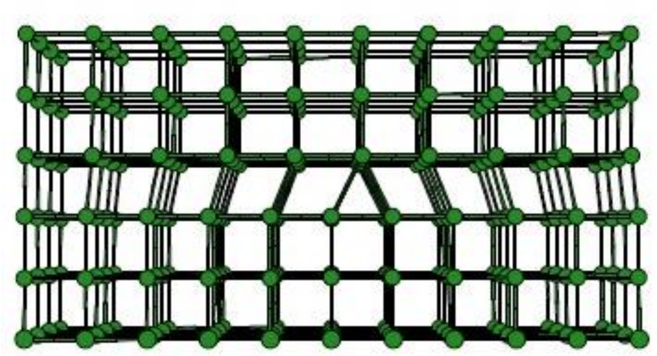
Dislocation:



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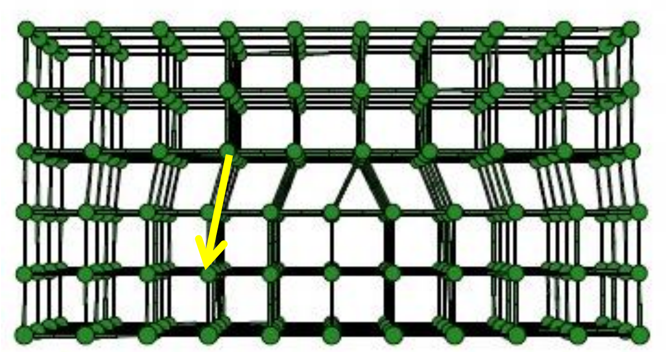

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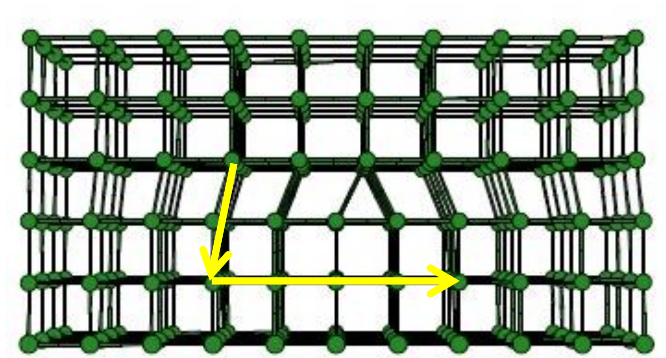

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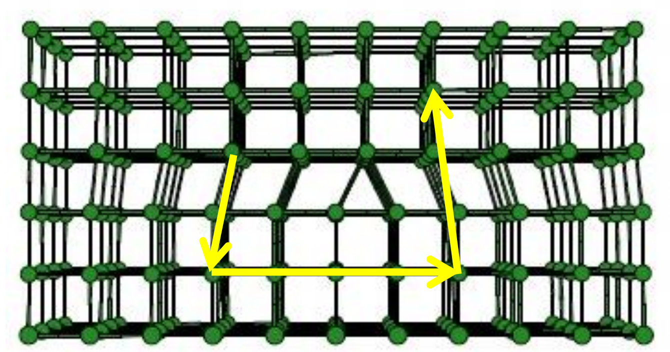

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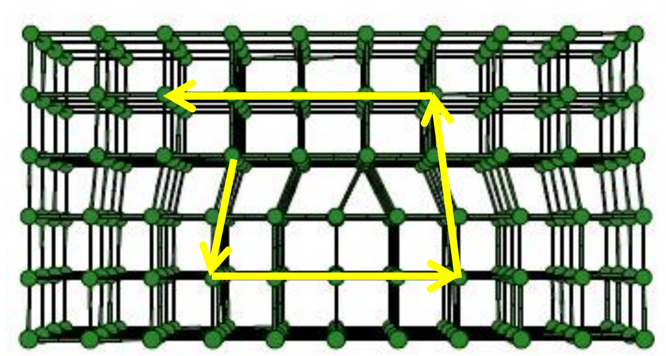

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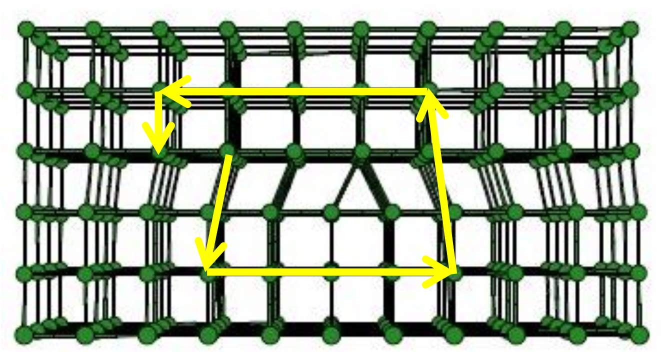

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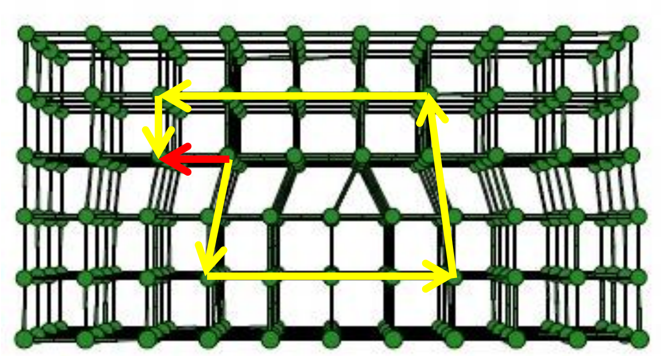

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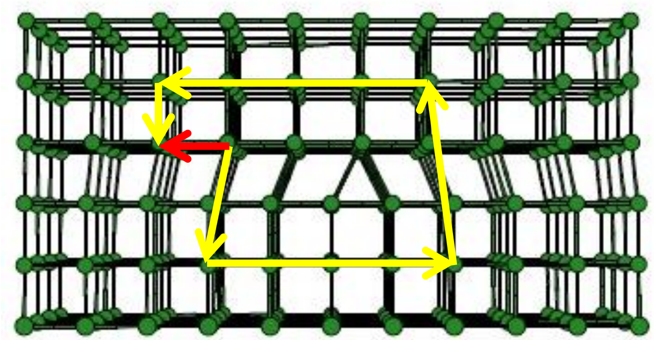
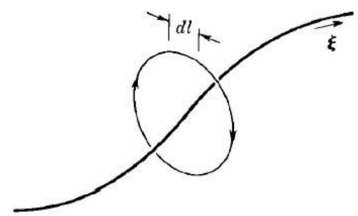


Burgers vector $\vec{b}$: characterize the dislocation



$$\oint_L d\vec{u} = \vec{b}$$

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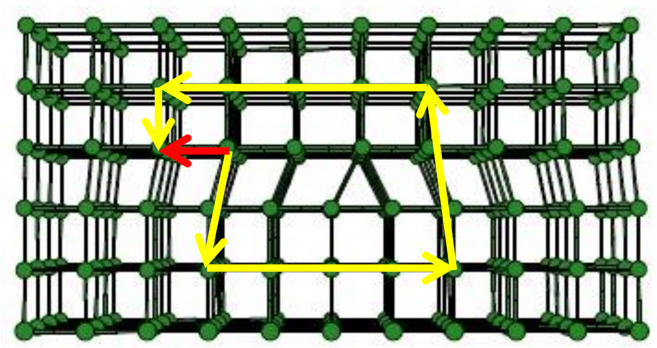

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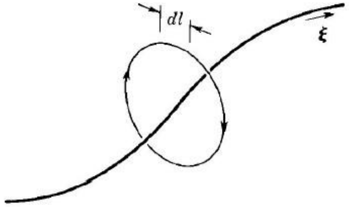

$$\oint_L d\vec{u} = \vec{b}$$

Dislocation energy $\propto \vec{b}^2$

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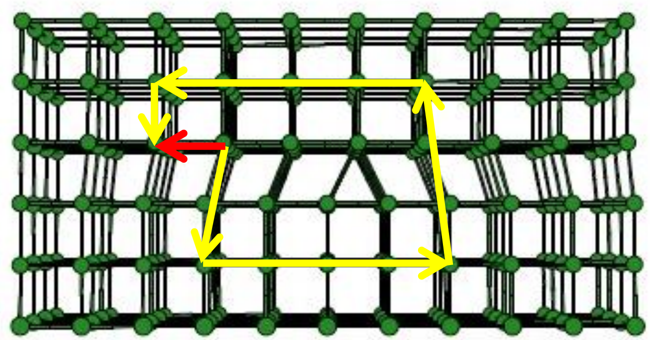

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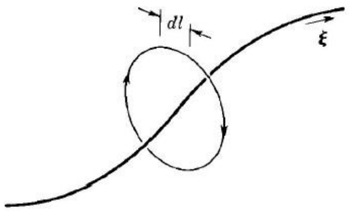

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Angle between $\vec{\xi}$ and $\vec{b}$ determines the type of dislocation:
edge (90^o), screw (0^o), or mixed (0^o~90^o)

Defect types I

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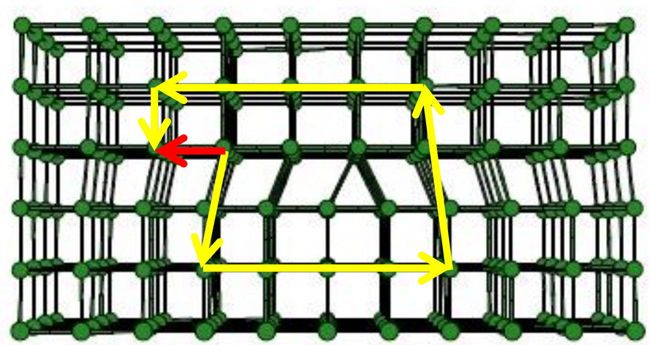
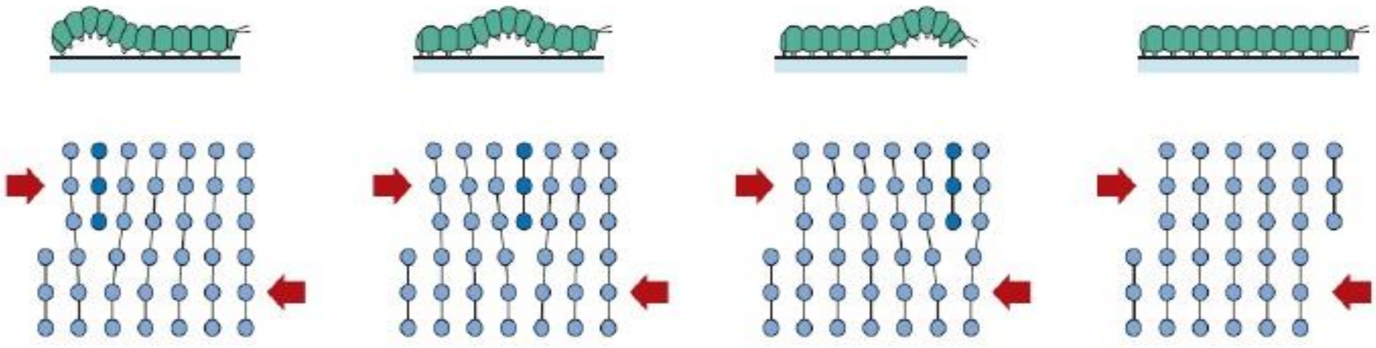
Dislocation:



Dislocations are main carriers of plastic deformation

Glide motion – Dislocation moves in response to a shear stress applied in a direction perpendicular to its line



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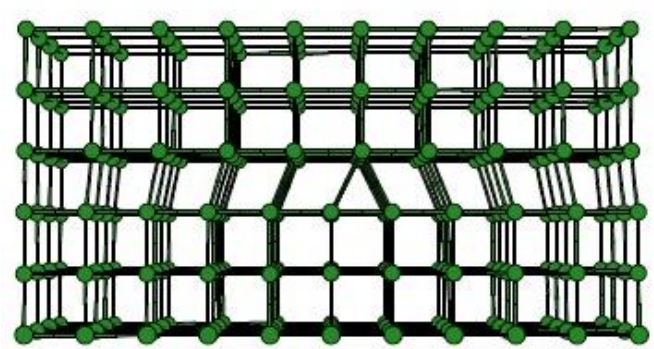
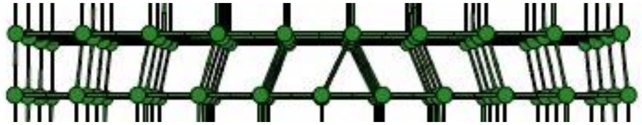
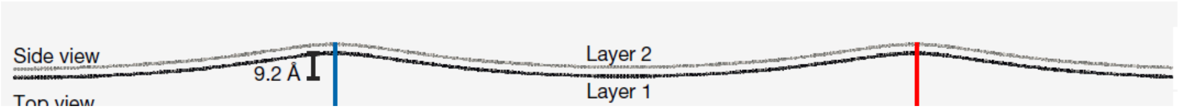


Dislocations are main carriers of plastic deformation

Dislocation in 2D structure:



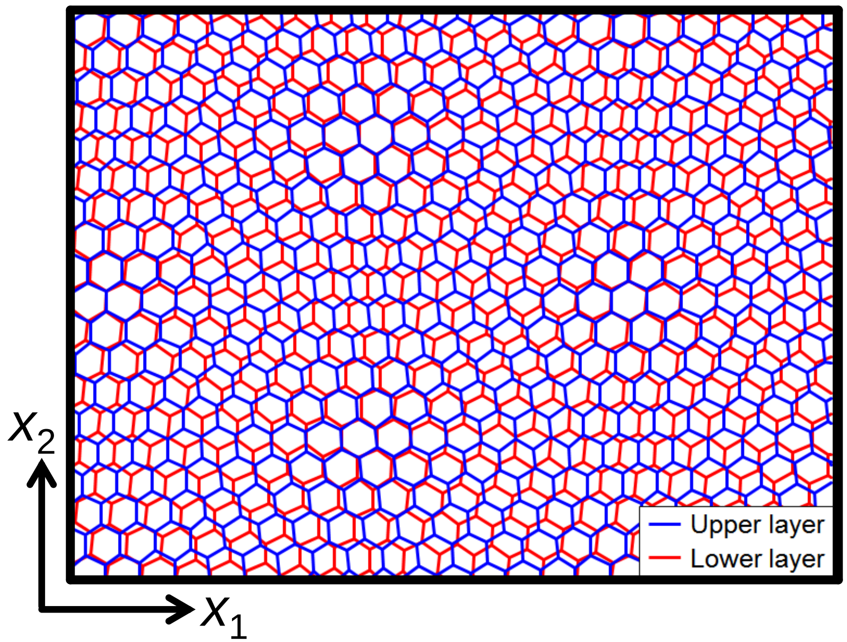


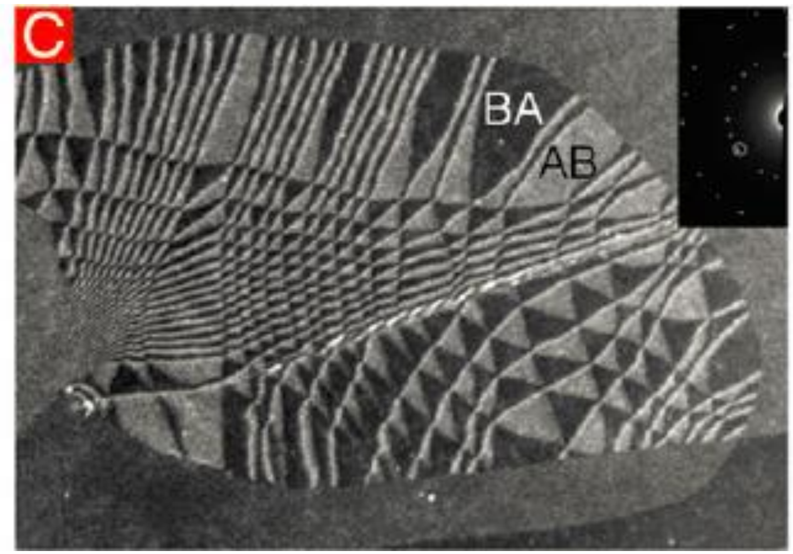
[B. Butz, *et. al.*, Nature, (2014)]

Defect types II

Interlayer defects: rotate top layer w.r.t. bottom layer (twist)

Moiré pattern





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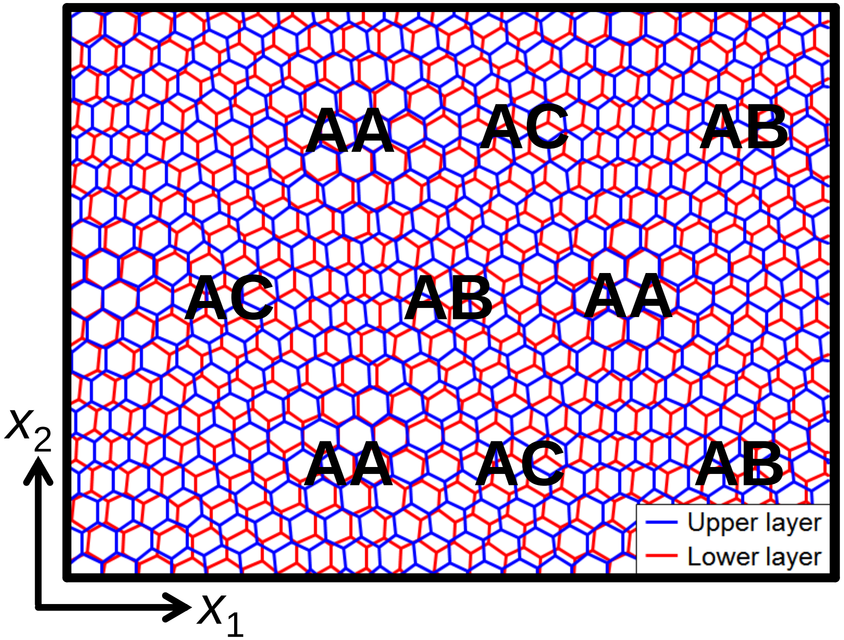

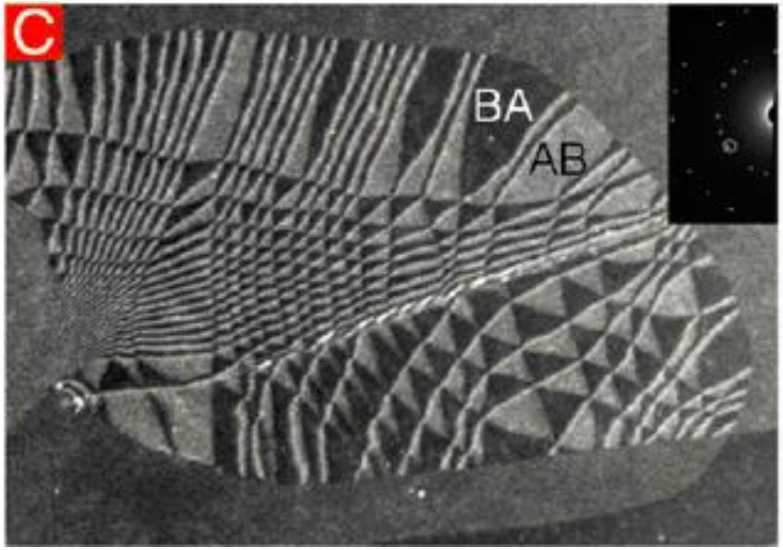

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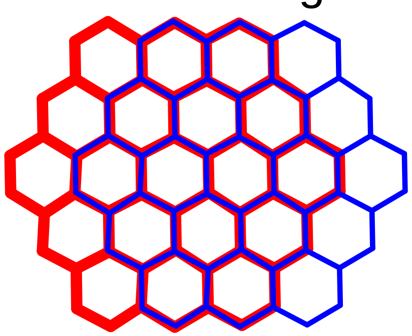
AA stacking



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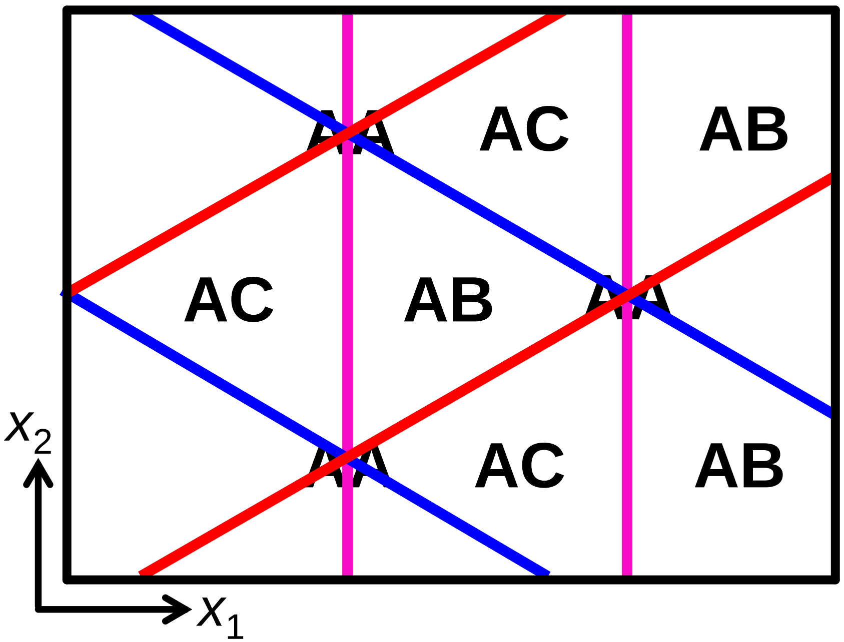

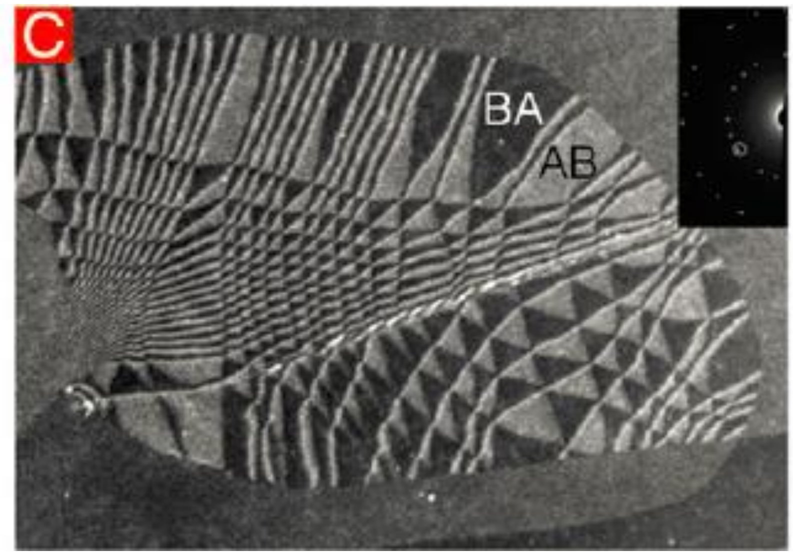

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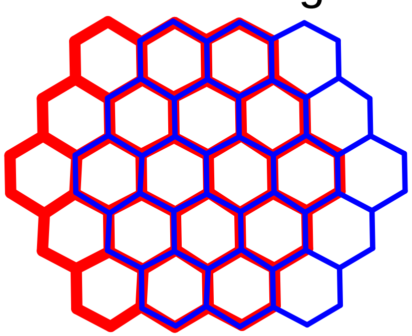
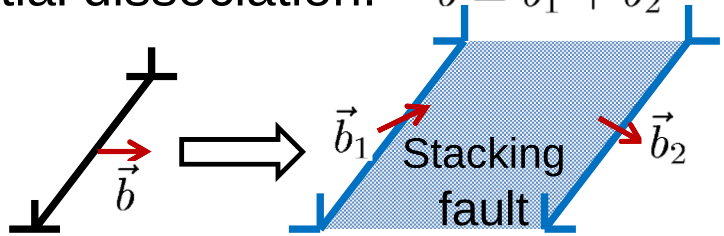


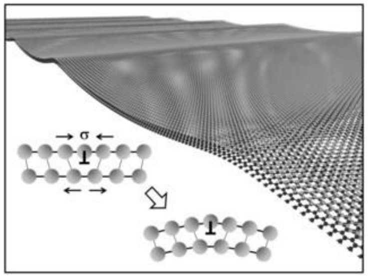
Twisted bilayer: Interlayer dislocation network

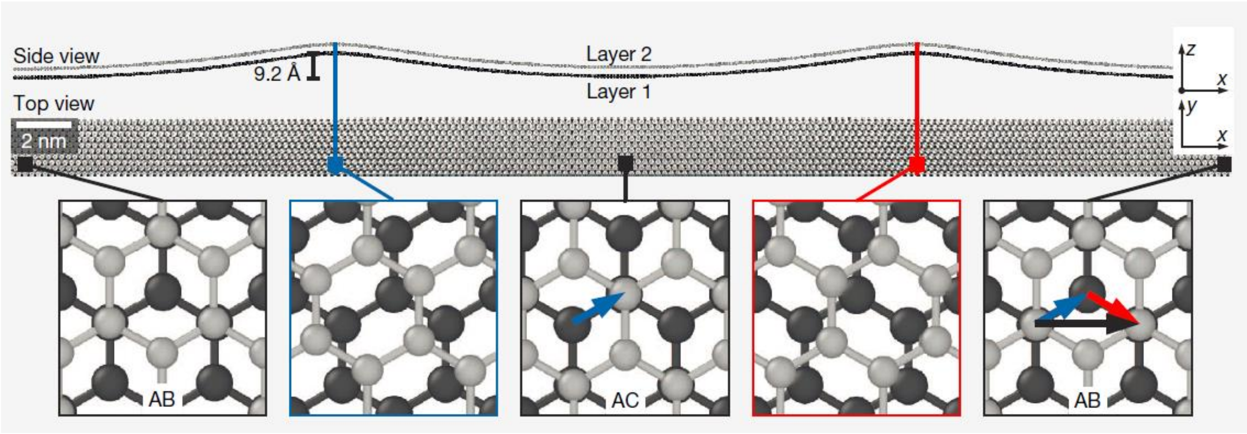
Why multiscale

Bilayer structure: local relaxation + bending

Partial dissociation: $\vec{b} = \vec{b}_1 + \vec{b}_2$







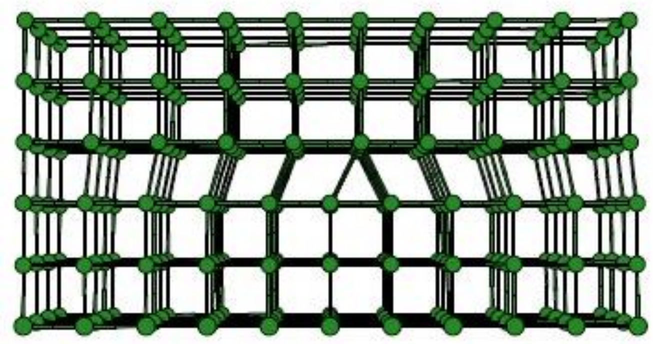
[B. Butz, *et. al.*, Nature, (2014)]

Intralayer: strong chemical bond – elastic sheet

Interlayer: weak vdW interaction – atomistic information

Multiscale

General multiscale model



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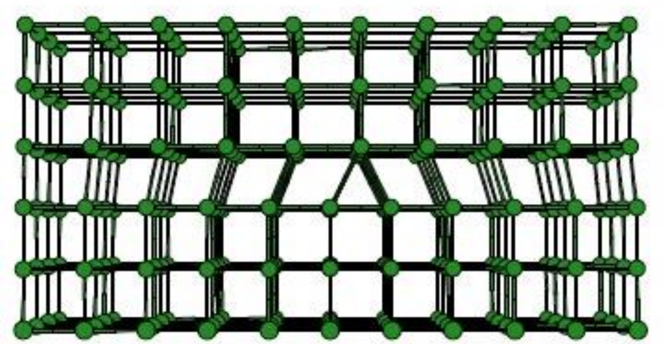

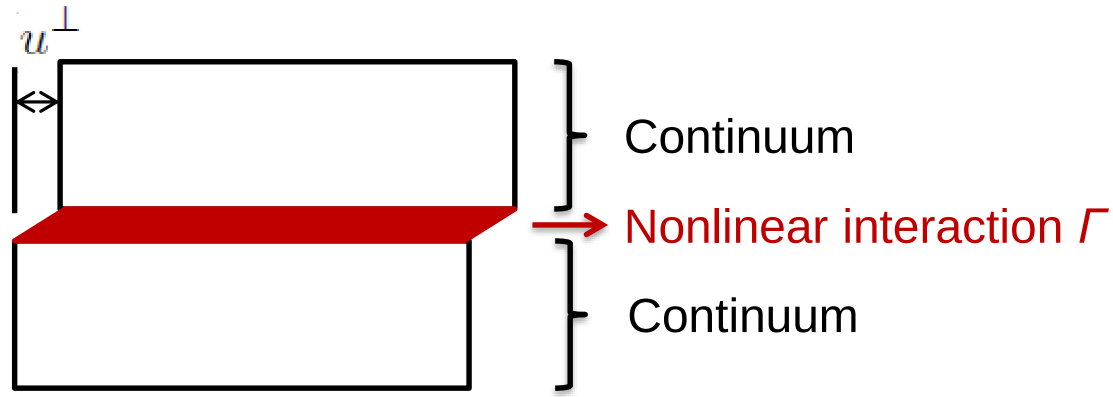

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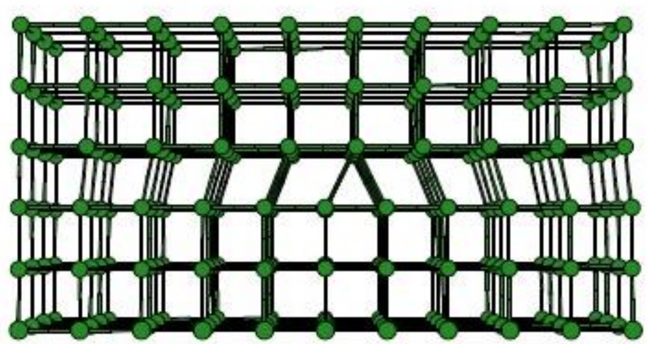
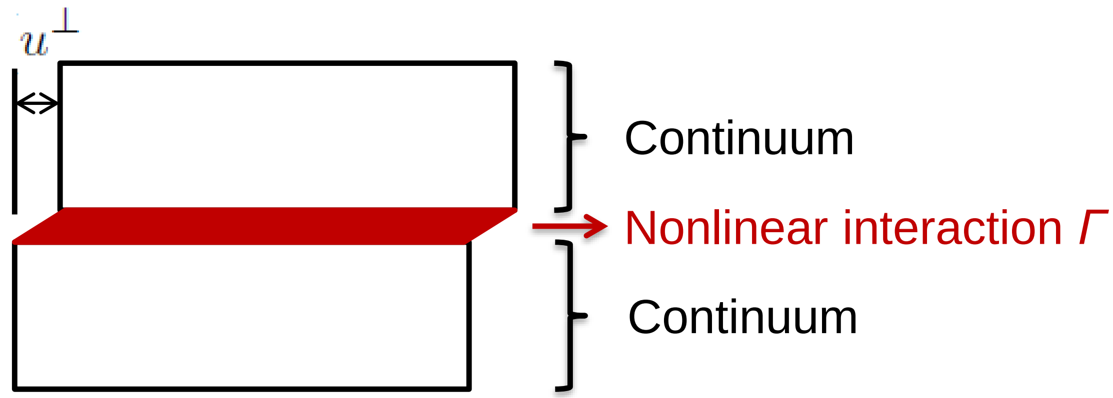




- Total energy: $E = E_{\text{elastic}} + E_{\text{misfit}}$

$$E_{\text{elastic}} = \frac{1}{2}\int \sigma_{13}(x)u^\perp(x)dx$$

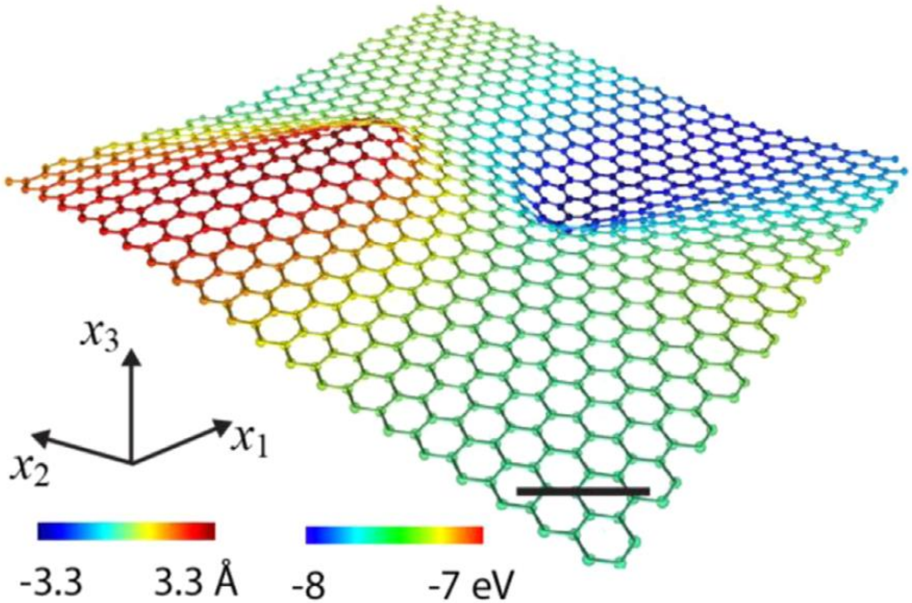
$$E_{\text{misfit}} = \int \Gamma\left(u^\perp(x)\right)dx$$

  – E_{elastic}: Continuum level
  – E_{misfit}: First-principle

- Equilibrium dislocation distribution:

Elastic contribution (Intralayer)

$$\overbrace{\text{In-plane + Out-of-plane}}^{\text{Elastic deformation}}$$



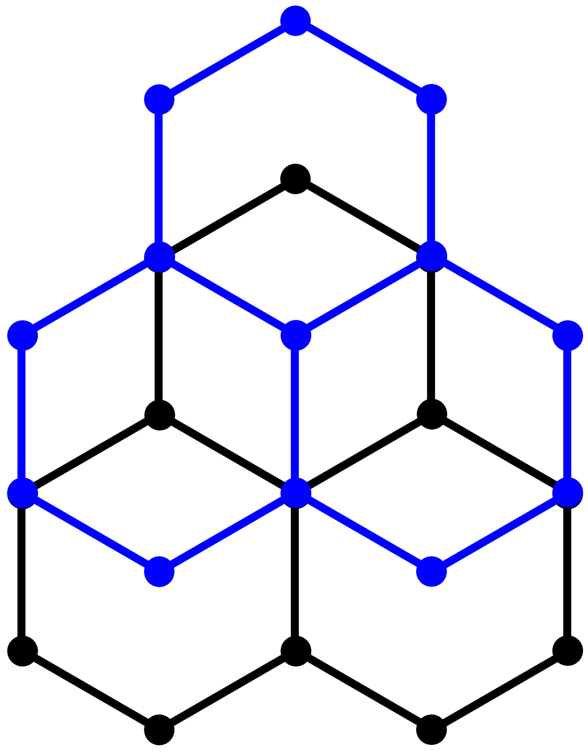
T. Zhang *et. al.*, JMPS, 2014

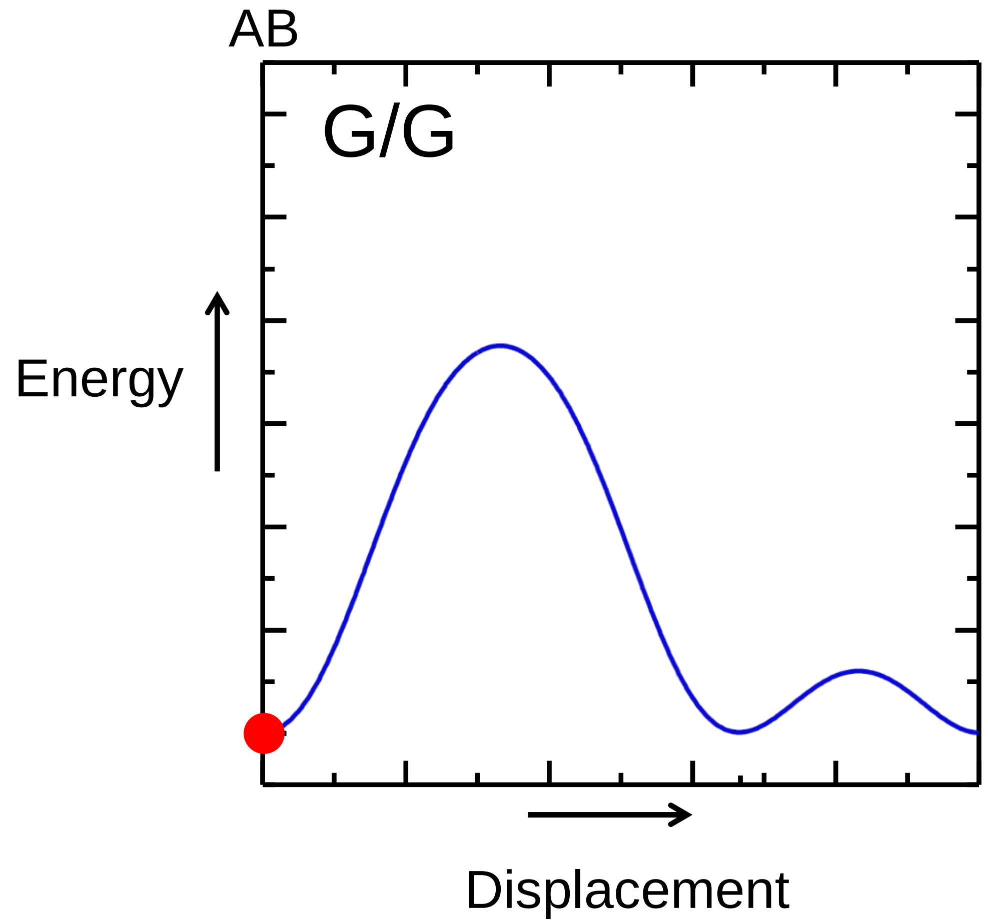
$$\varepsilon_{ij}=\frac{1}{2}\left(u_{i,j}+u_{j,i}+w_{,i}w_{,j}\right), \quad i,j=1,2,$$

$$H=\nabla\bullet\left(\frac{\nabla w}{\sqrt{1+|\nabla w|^2}}\right), \quad \kappa_G=\frac{\det(w_{,ij})}{\left(1+|\nabla w|^2\right)^2},$$

$$E=\int\int\frac{1}{2}\frac{Eh}{1+\nu}\left(\varepsilon_{ij}\varepsilon_{ij}+\frac{\nu}{(1-2\nu)}\varepsilon_{kk}\varepsilon_{kk}\right)dx_1\,dx_2+\int\int\left(\frac{1}{2}BH^2+B_G\kappa_G\right)dx_1\,dx_2,$$

Misfit contribution (Interlayer)





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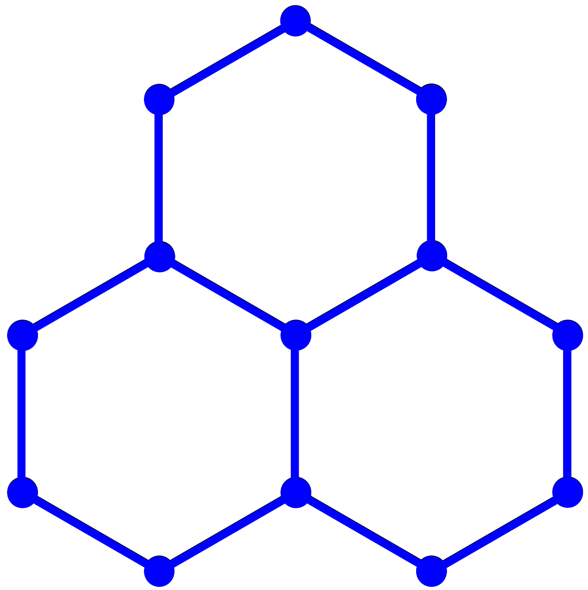

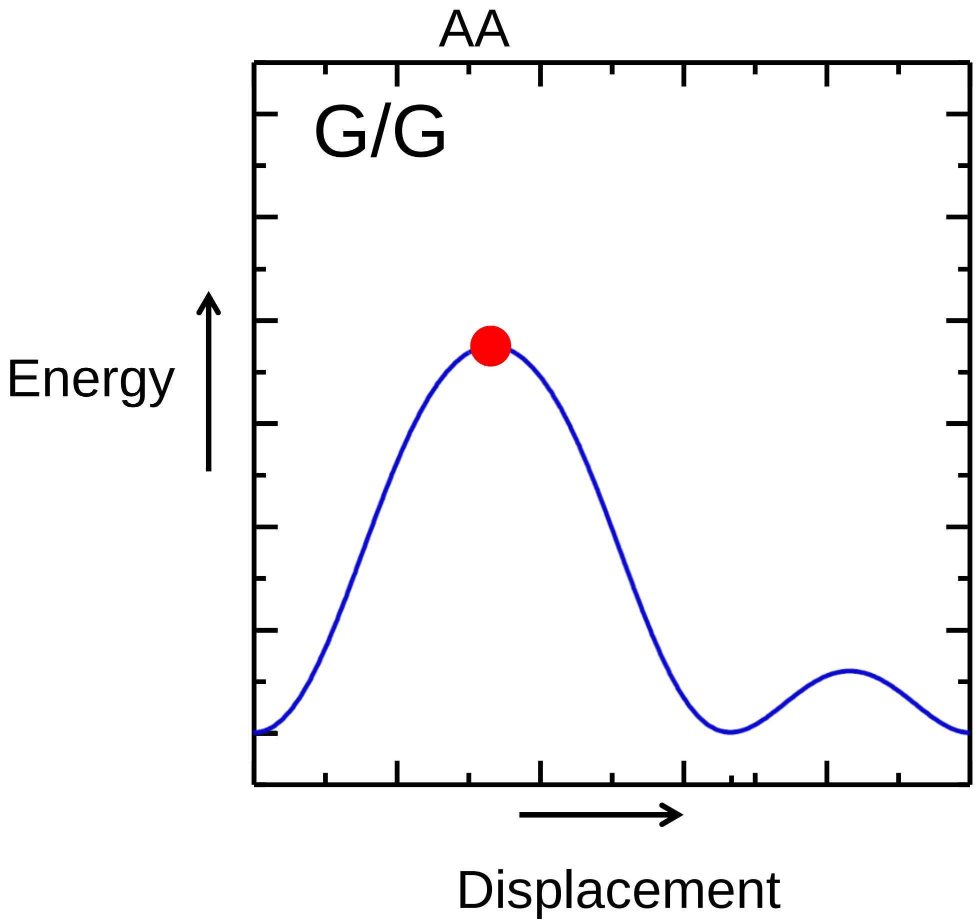

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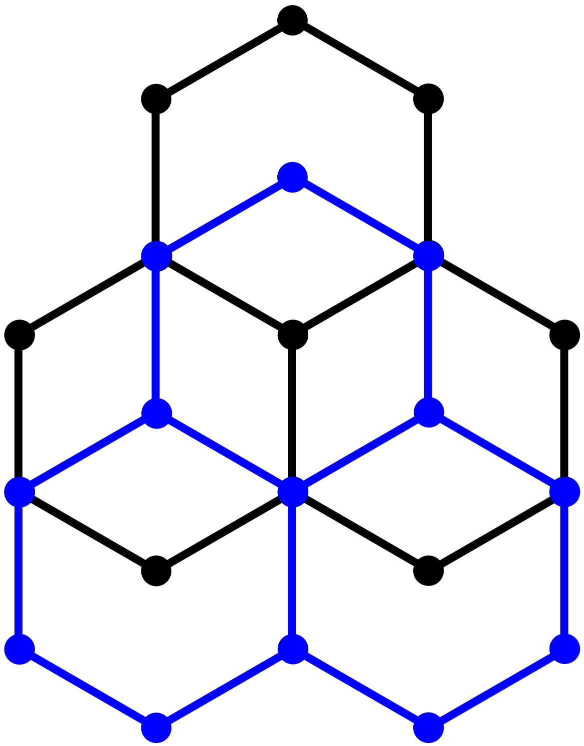

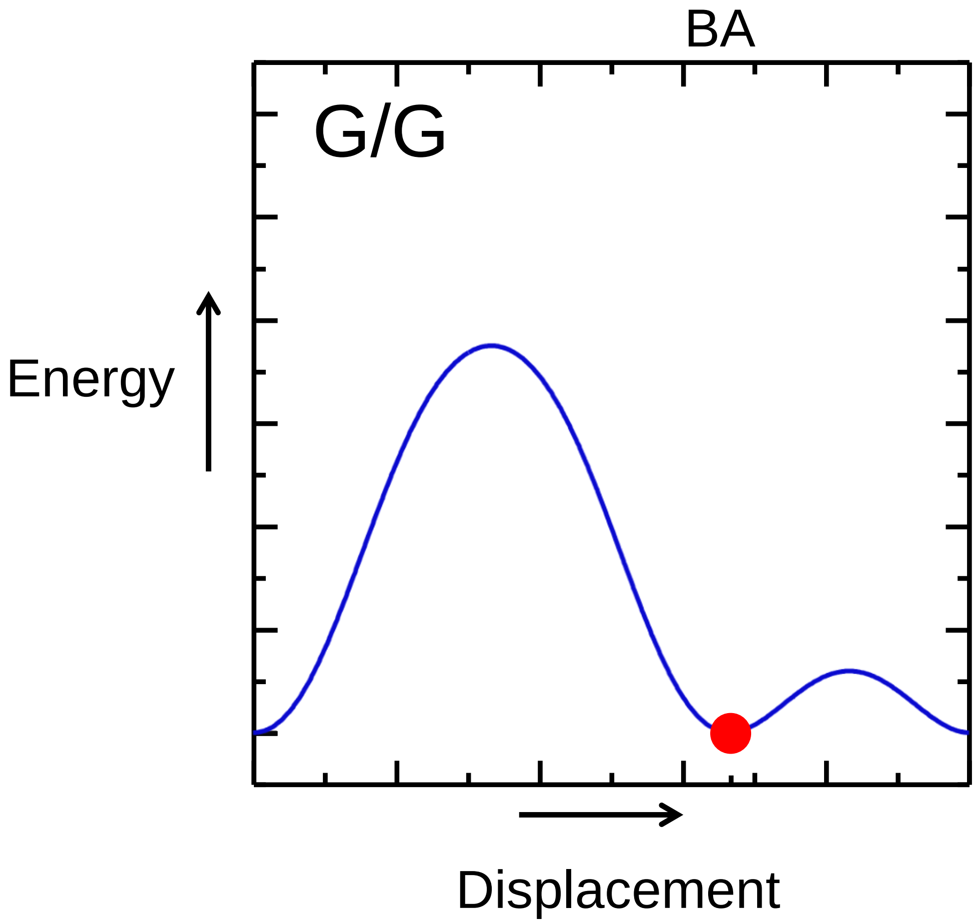

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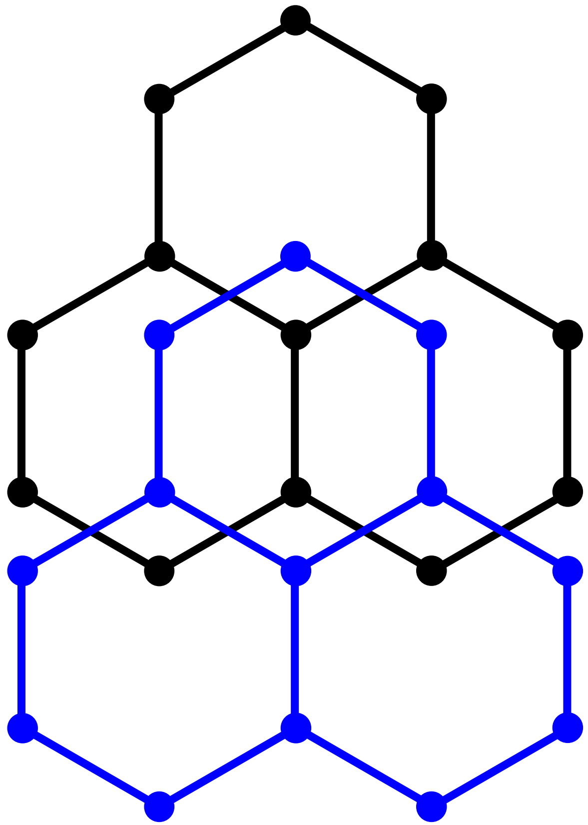

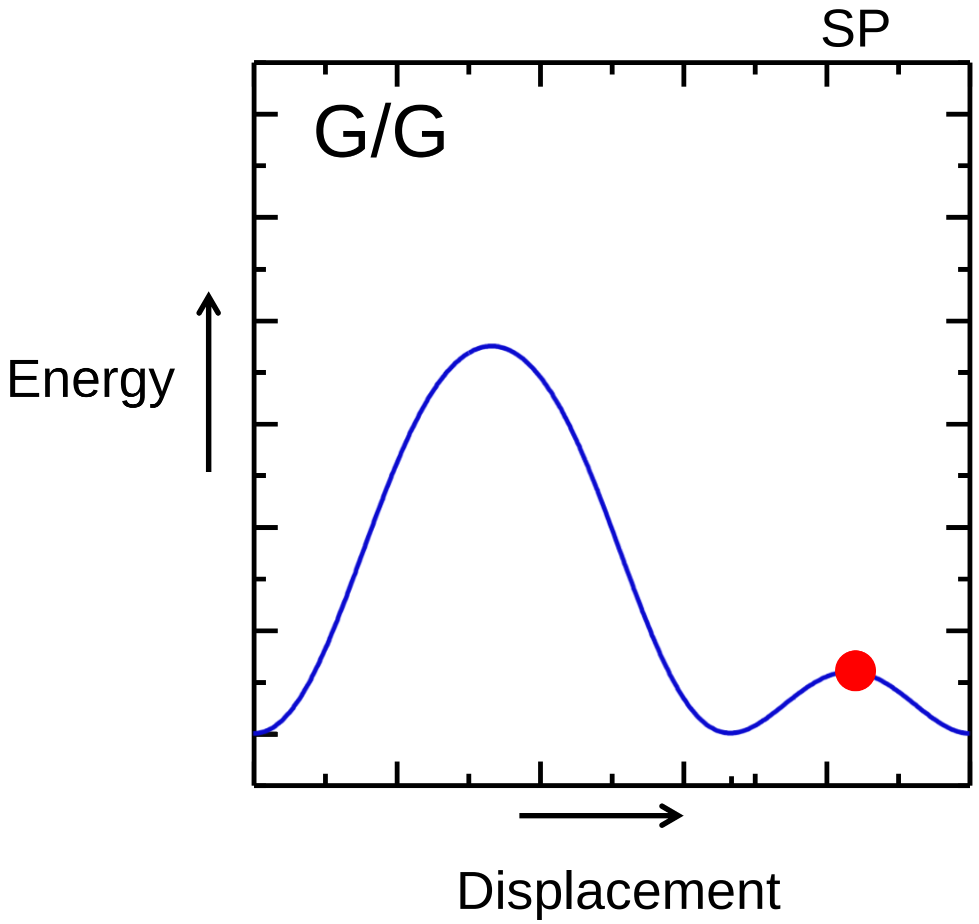

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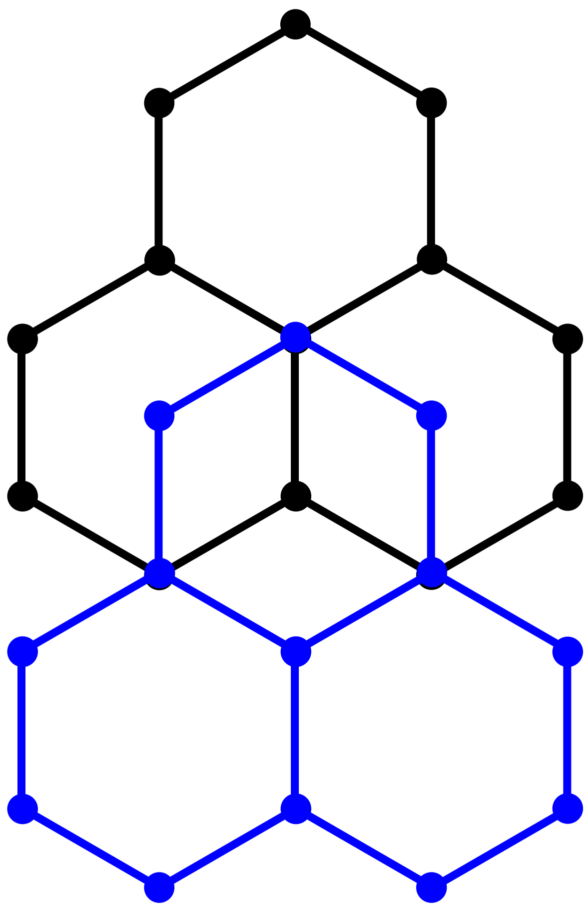

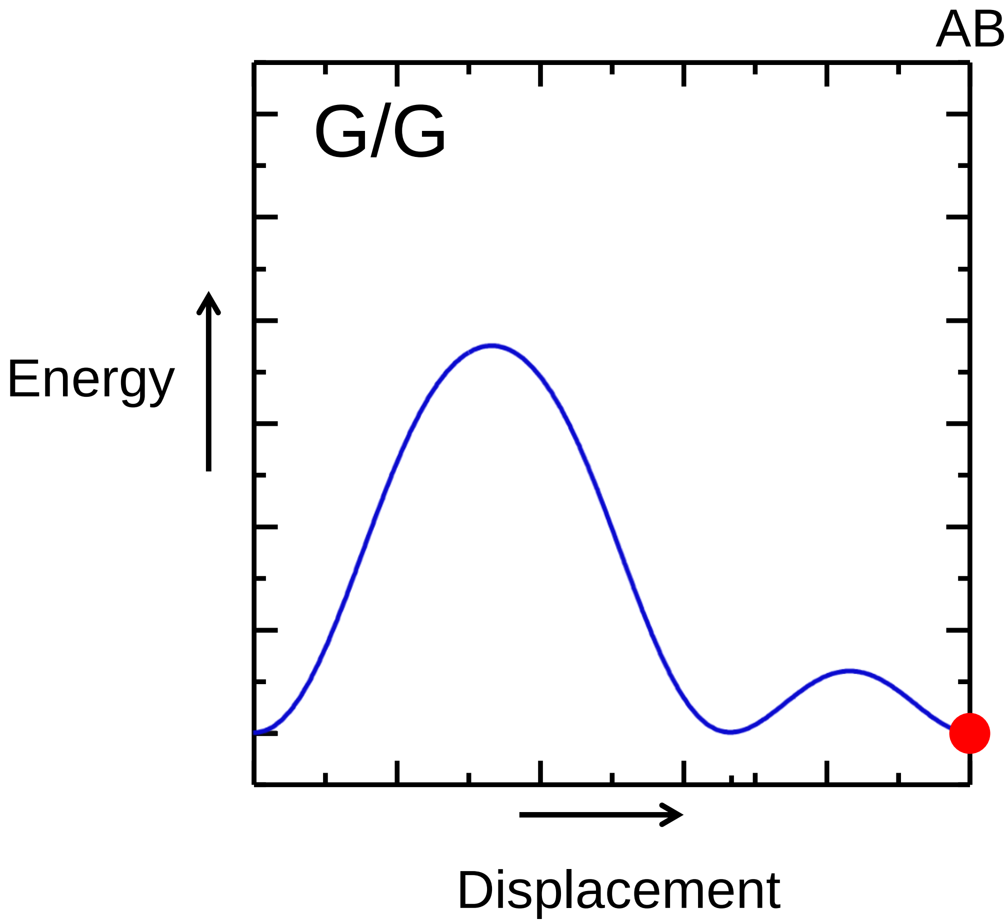

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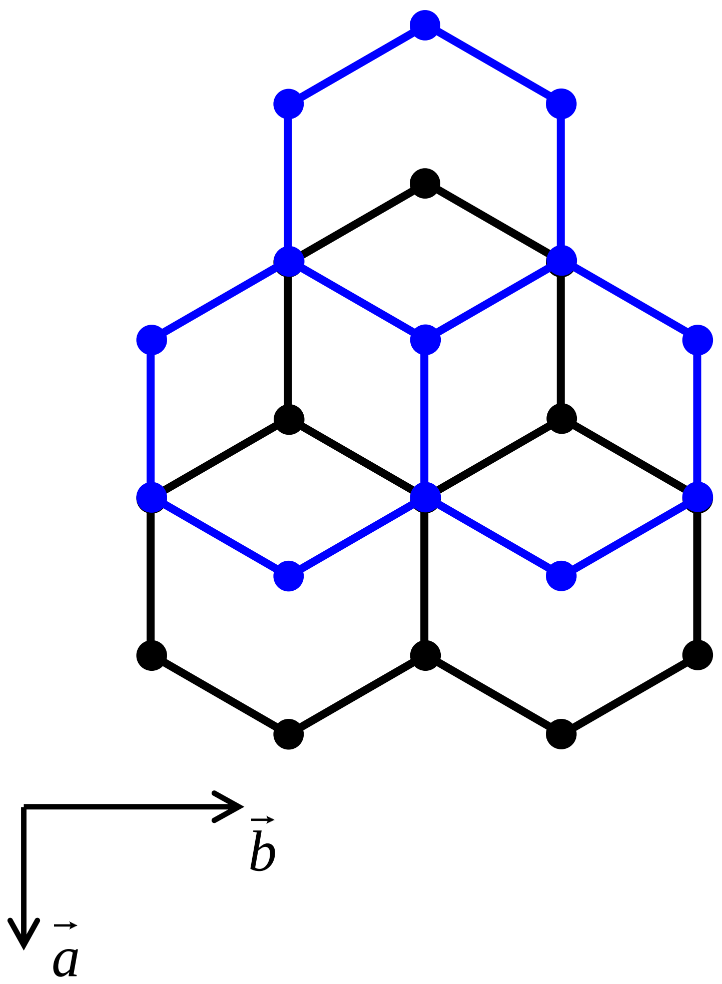
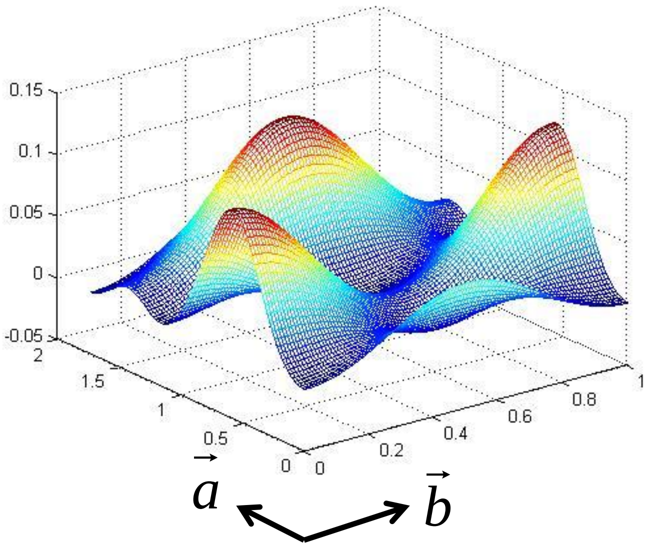
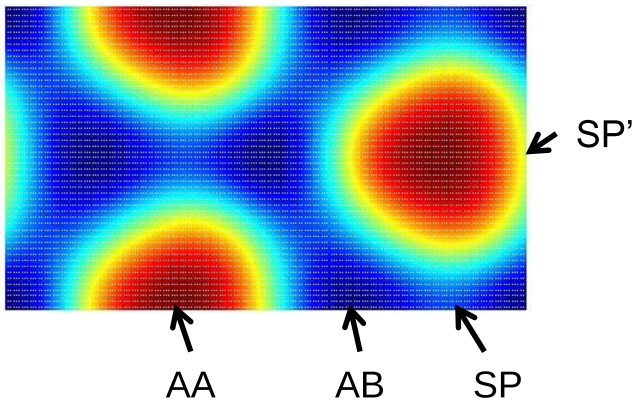
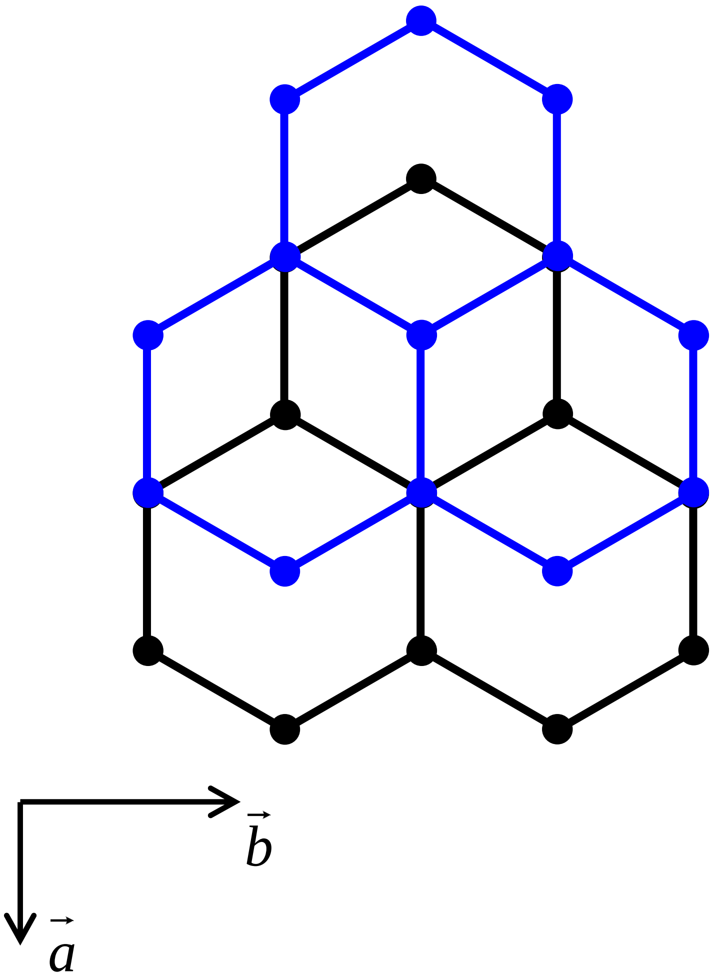


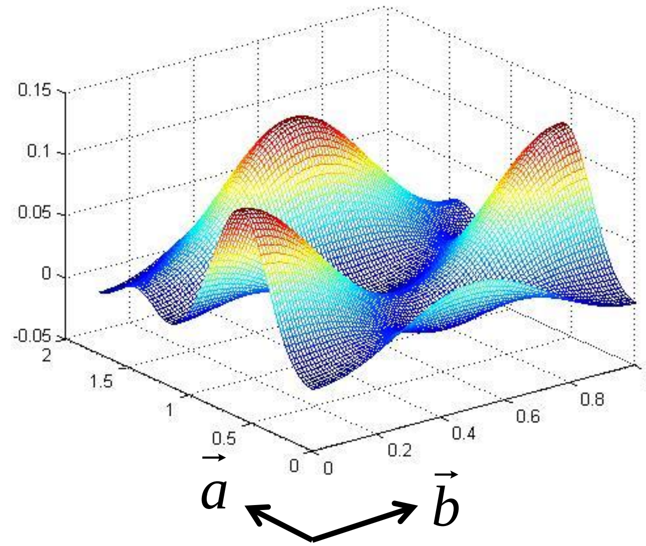




Misfit contribution (Interlayer)

2D Generalized Stacking Fault Energy (GSFE)





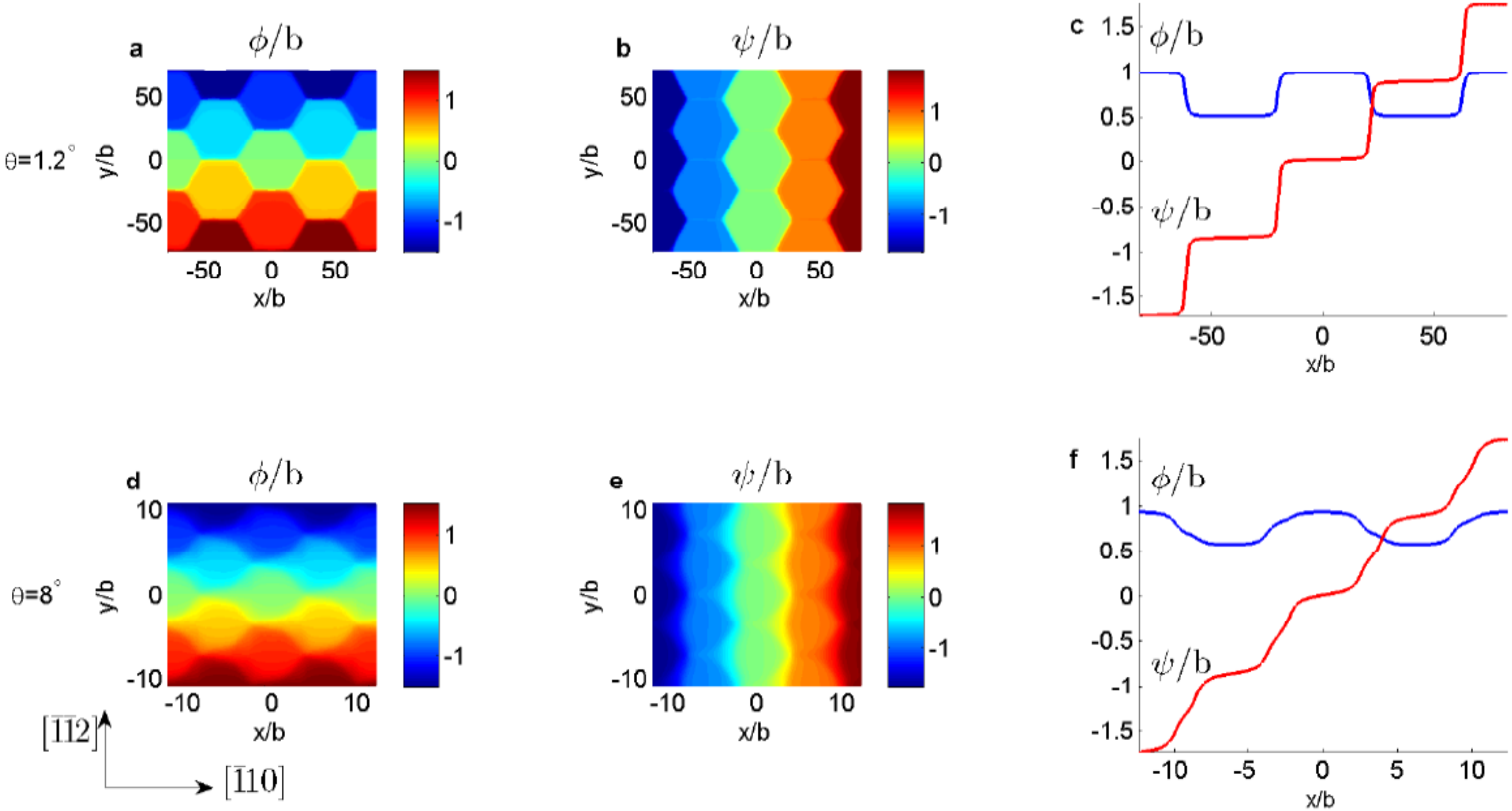
$$
\begin{aligned}
\gamma\left(u_1^{\perp}, u_2^{\perp}\right) = {} & \\
c_0 + c_1 & \left[\cos\frac{2\pi}{a_0}\left(u_1^{\perp} + \frac{u_2^{\perp}}{\sqrt{3}}\right) + \cos\frac{2\pi}{a_0}\left(\phi - \frac{u_2^{\perp}}{\sqrt{3}}\right) + \cos\frac{4\pi u_2^{\perp}}{\sqrt{3}a_0}\right] \\
+ c_2 & \left[\cos\frac{2\pi}{a_0}\left(u_1^{\perp} + \sqrt{3}u_2^{\perp}\right) + \cos\frac{2\pi}{a_0}\left(u_1^{\perp} - \sqrt{3}u_2^{\perp}\right) + \cos\frac{4\pi u_1^{\perp}}{a_0}\right] \\
+ c_3 & \left[\cos\frac{2\pi}{a_0}\left(2u_1^{\perp} + \frac{2u_2^{\perp}}{\sqrt{3}}\right) + \cos\frac{2\pi}{a_0}\left(2u_1^{\perp} - \frac{2u_2^{\perp}}{\sqrt{3}}\right) + \cos\frac{8\pi u_2^{\perp}}{\sqrt{3}a_0}\right] \\
+ c_4 & \left[\sin\frac{2\pi}{a_0}\left(u_1^{\perp} - \frac{u_2^{\perp}}{\sqrt{3}}\right) - \sin\frac{2\pi}{a_0}\left(u_1^{\perp} + \frac{u_2^{\perp}}{\sqrt{3}}\right) + \sin\frac{4\pi u_2^{\perp}}{\sqrt{3}a_0}\right] \\
+ c_5 & \left[\sin\frac{2\pi}{a_0}\left(2u_1^{\perp} - \frac{2u_2^{\perp}}{\sqrt{3}}\right) - \sin\frac{2\pi}{a_0}\left(2u_1^{\perp} + \frac{2u_2^{\perp}}{\sqrt{3}}\right) + \sin\frac{8\pi u_2^{\perp}}{\sqrt{3}a_0}\right],
\end{aligned}
$$

General multiscale model

Applied to twist Grain Boundaries

[Dai *et. al.*, Acta Mat., 2013]

ϕ and ψ for Al



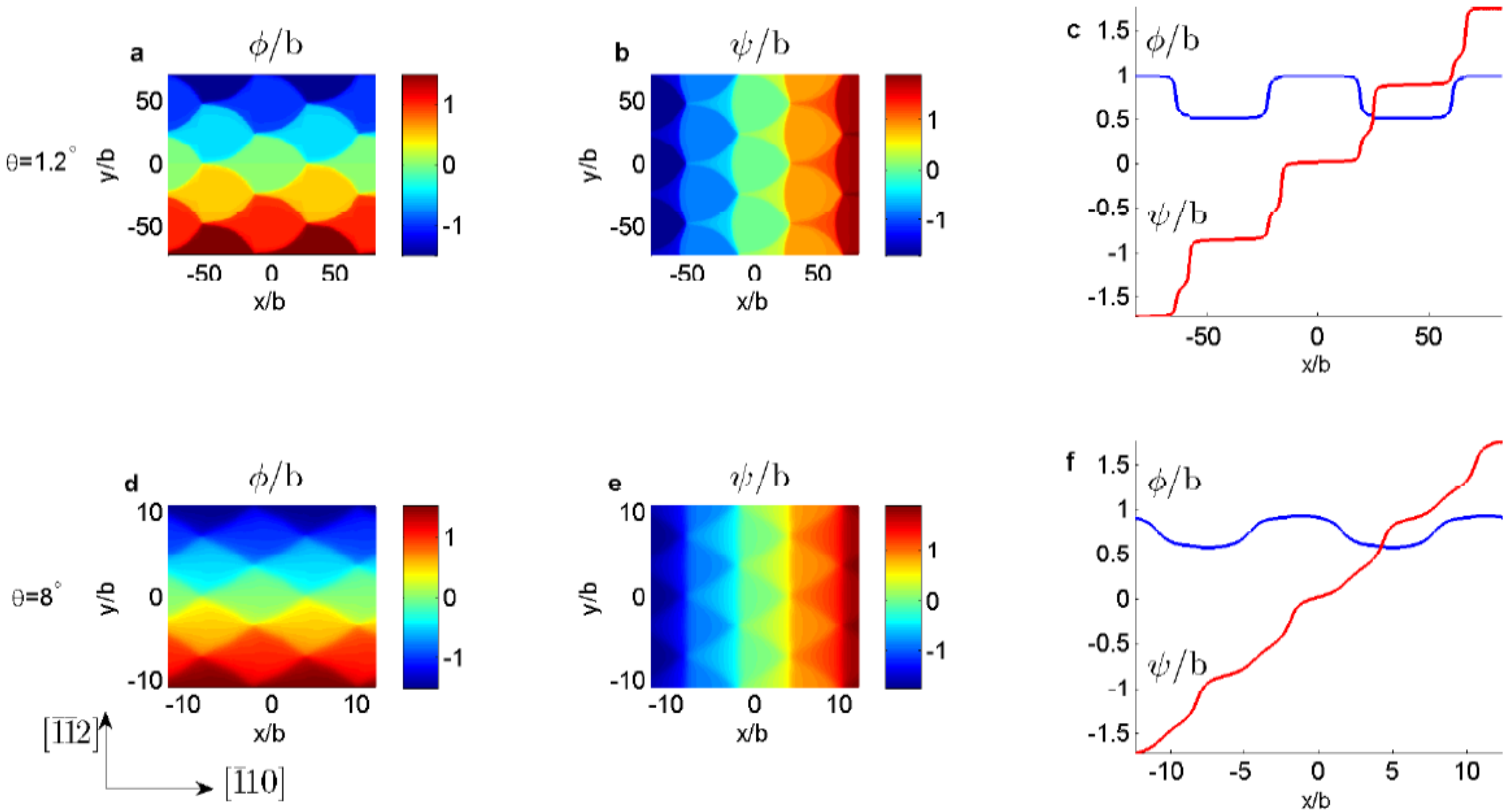
Profiles along $y = -L_y/4$

General multiscale model

Applied to twist Grain Boundaries

[Dai *et. al.*, Acta Mat., 2013]

ϕ and ψ for Cu



Profiles along $y = -L_y/4$

General multiscale model

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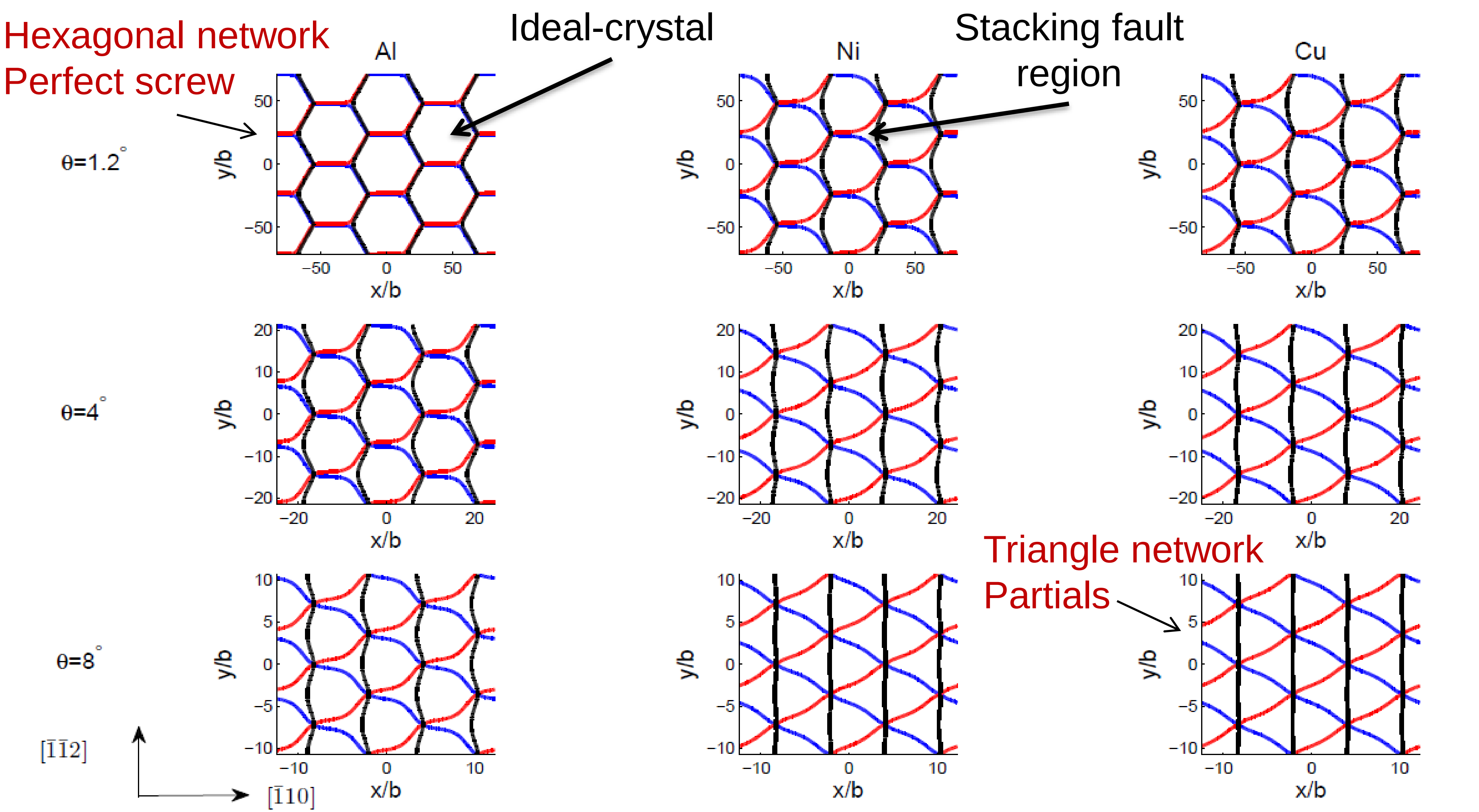

General multiscale model

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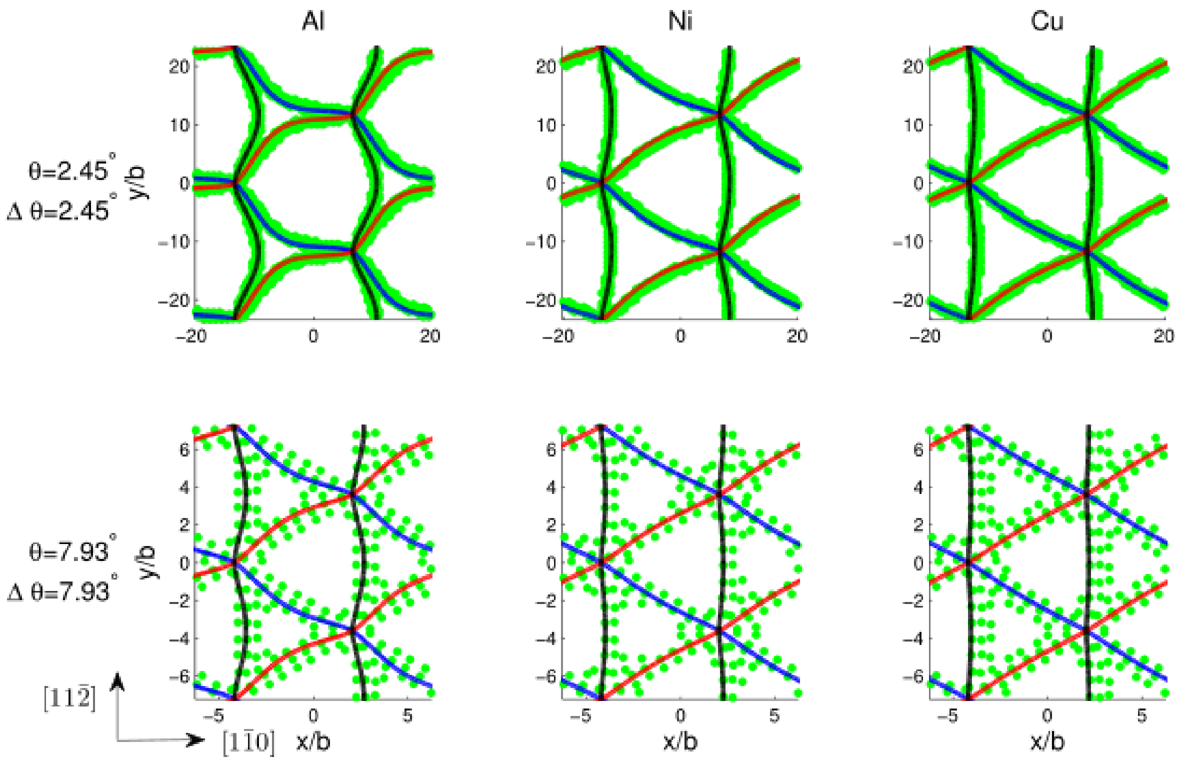
[Dai *et. al.*, Acta Mat., 2013]

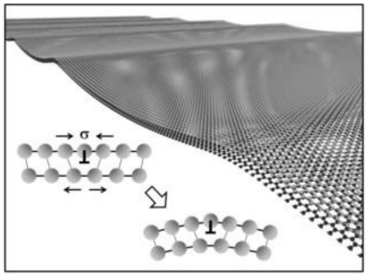


Green dots: atoms within dislocation cores obtained in molecular simulation.

Solid curves: dislocation network obtained in our model.

Misfit contribution (Interlayer)

Interlayer separation effect



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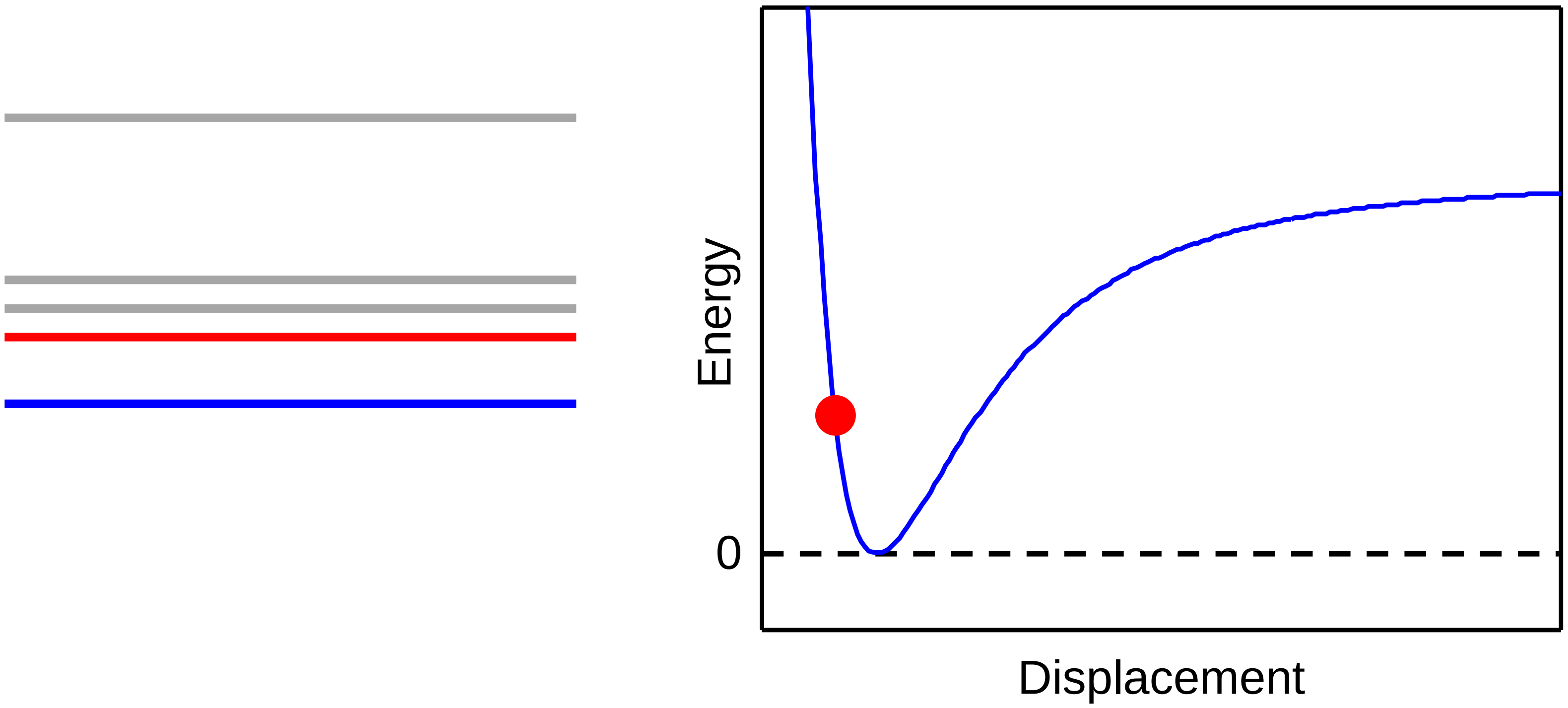
Interlayer separation effect



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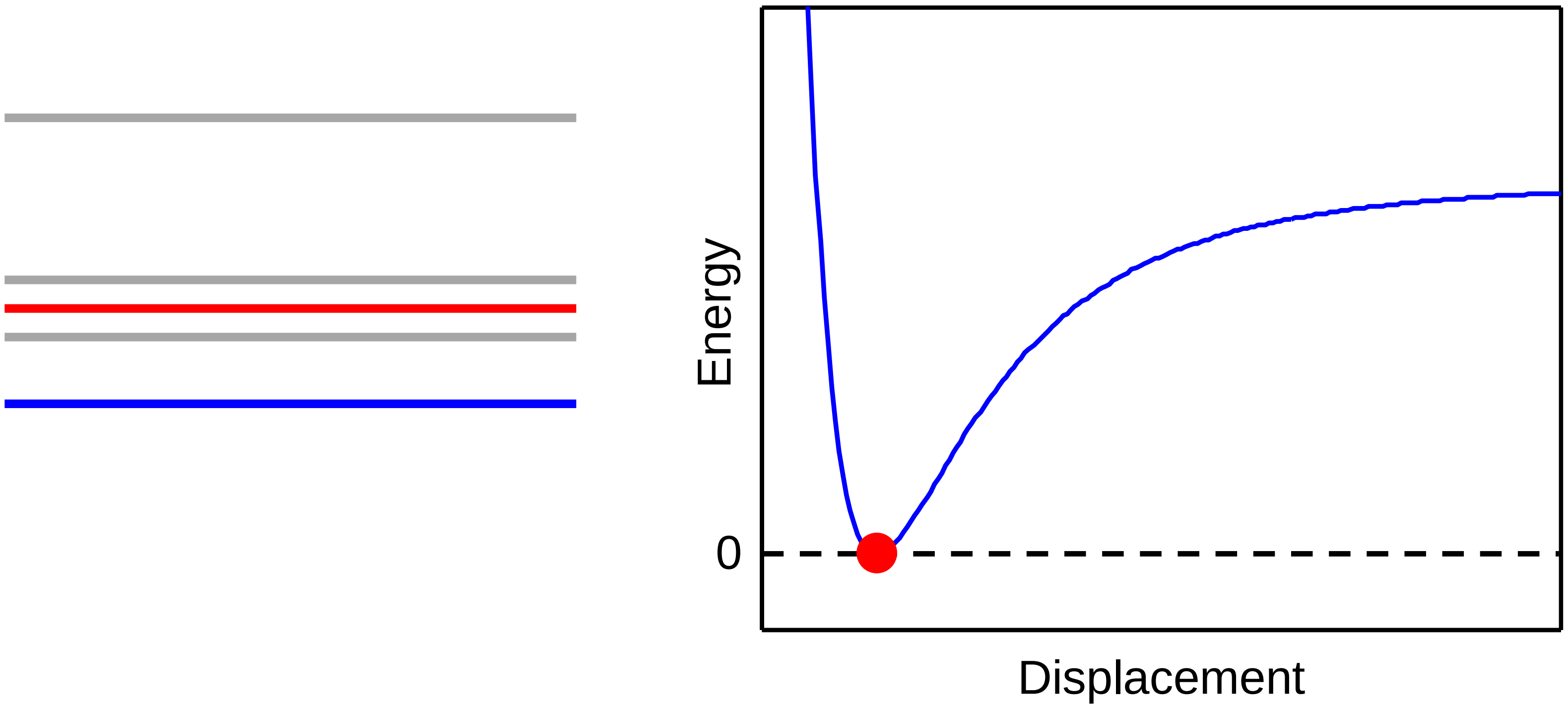
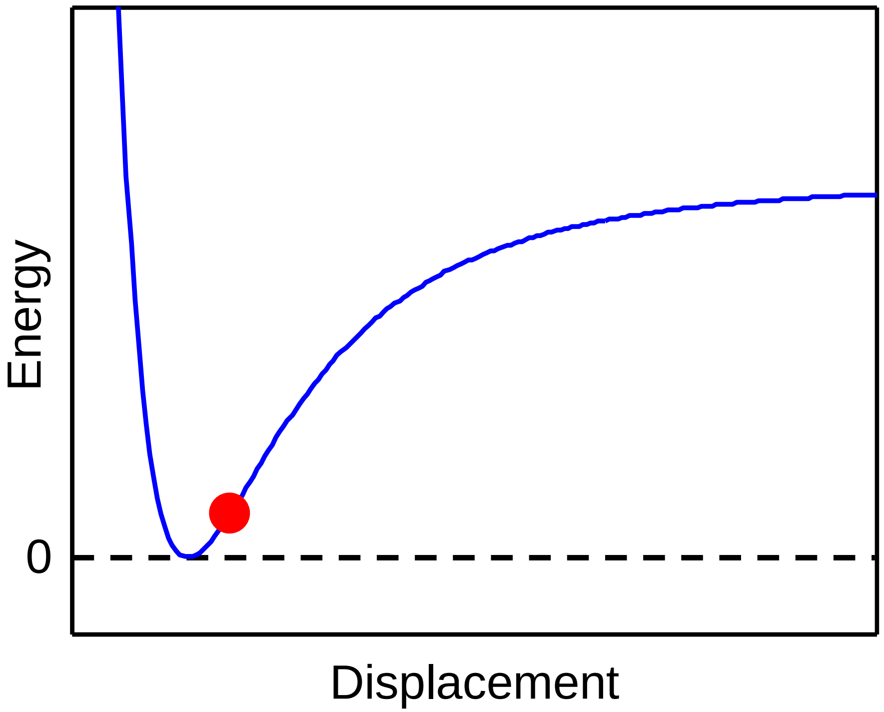
Interlayer separation effect



Misfit contribution (Interlayer)

Interlayer separation effect



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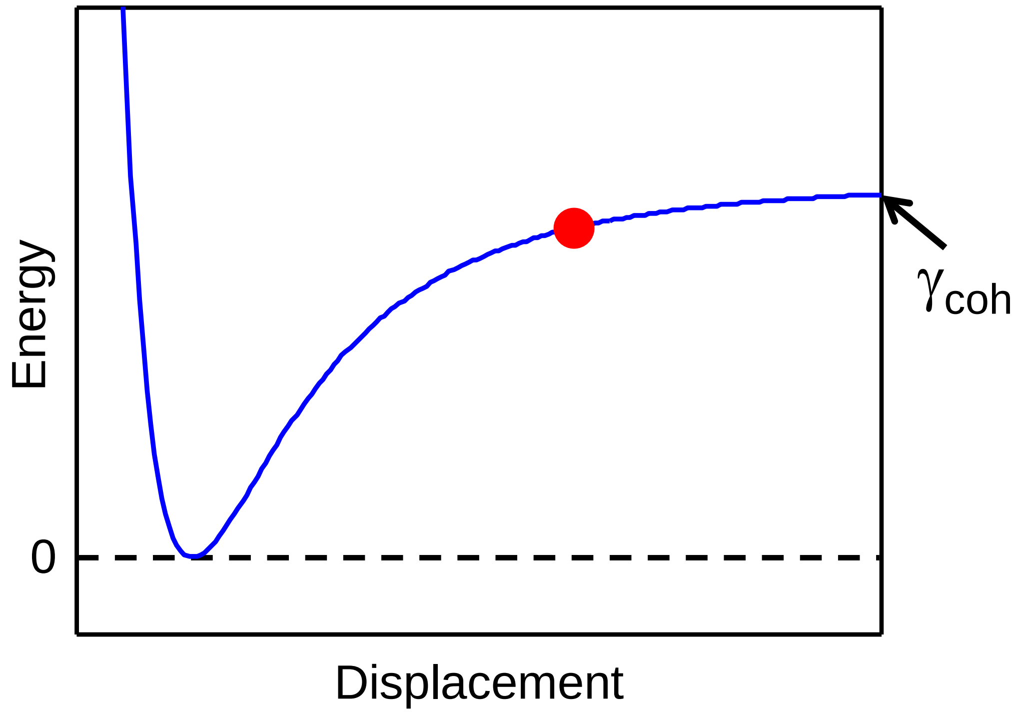
Interlayer separation effect



Misfit contribution (Interlayer)

3D Generalized Stacking Fault Energy (3D GSFE)

$$\Gamma(u_1^{\perp}, u_2^{\perp}, \delta) = A \exp(-\alpha\delta) - B\left(\frac{d}{\delta}\right)^4 + \gamma_{\mathrm{coh}},$$

δ is the interlayer spacing

from Morse-potential

convergence to long-range vdW interaction

Γ should satisfies:

- $$\left.\begin{aligned} &\Gamma(u_1^{\perp}, u_2^{\perp}, \delta = d(u_1^{\perp}, u_2^{\perp})) = \gamma(u_1^{\perp}, u_2^{\perp}), \\ &\left.\frac{\partial \Gamma(u_1^{\perp}, u_2^{\perp}, \delta)}{\partial \delta}\right|_{\delta = d(u_1^{\perp}, u_2^{\perp})} = 0, \end{aligned}\right\}$$ Equivalent to the 2D GSFE

- $$\left.\frac{\partial^2 \Gamma(u_1^{\perp}, u_2^{\perp}, \delta)}{\partial \delta^2}\right|_{\delta = d(u_1^{\perp}, u_2^{\perp})} = \frac{C_{nn}(u_1^{\perp}, u_2^{\perp})}{d(u_1^{\perp}, u_2^{\perp})} \equiv \kappa(u_1^{\perp}, u_2^{\perp})$$ additional condition related to elastic modulus

$\downarrow$

Expressions for $\alpha, A,$ and B

$$\begin{aligned} \alpha = &\Big\{ -\left[\kappa d^2 - 20(\gamma - \gamma_{\mathrm{coh}})\right] \\ &+ \sqrt{\left[\kappa d^2 - 20(\gamma - \gamma_{\mathrm{coh}})\right]^2 + 64\kappa d^2(\gamma - \gamma_{\mathrm{coh}})}\Big\} \\ &/\left[8d(\gamma - \gamma_{\mathrm{coh}})\right], \\ A = &\left[4(\gamma - \gamma_{\mathrm{coh}}) \exp(\alpha d)\right] / (4 - \alpha d), \\ B = &\left[\alpha d(\gamma - \gamma_{\mathrm{coh}})\right] / (4 - \alpha d). \end{aligned}$$

Misfit contribution (Interlayer)

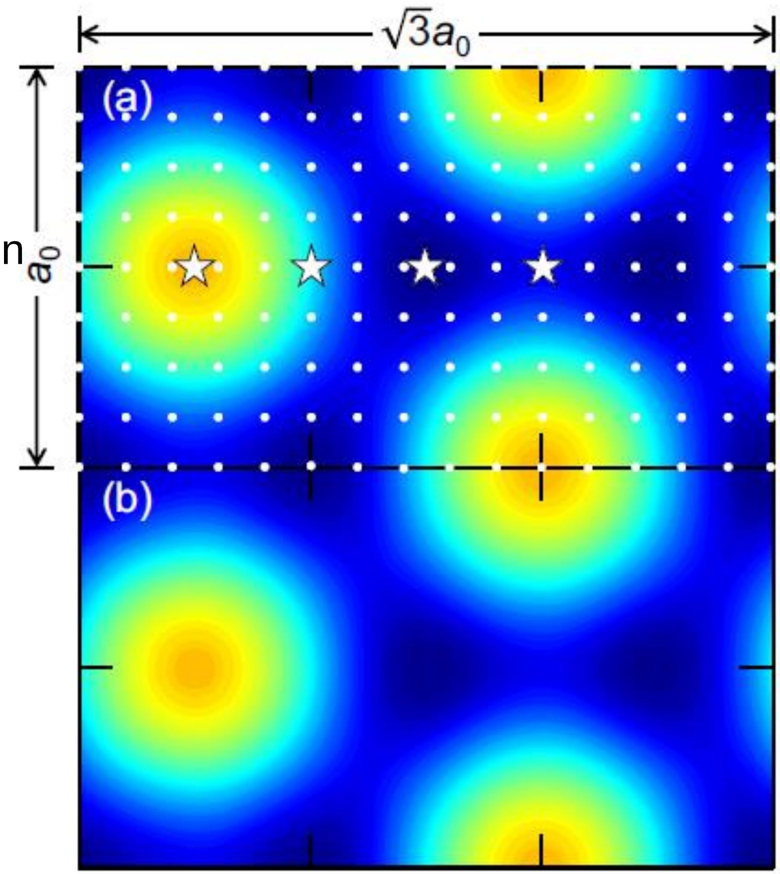
3D Generalized Stacking Fault Energy (3D GSFE)

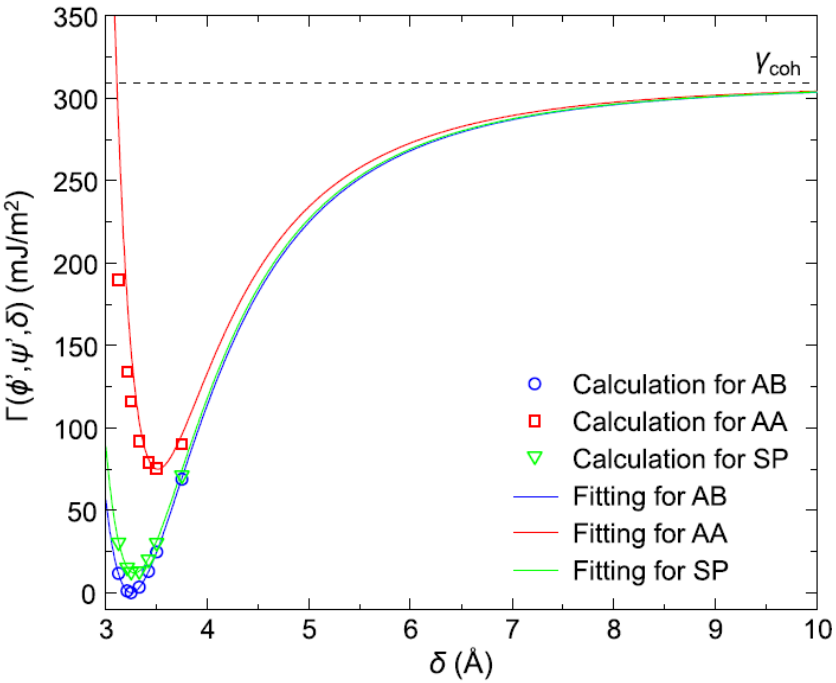
Interlayer shift

Interlayer separation

Calculation

Fitting



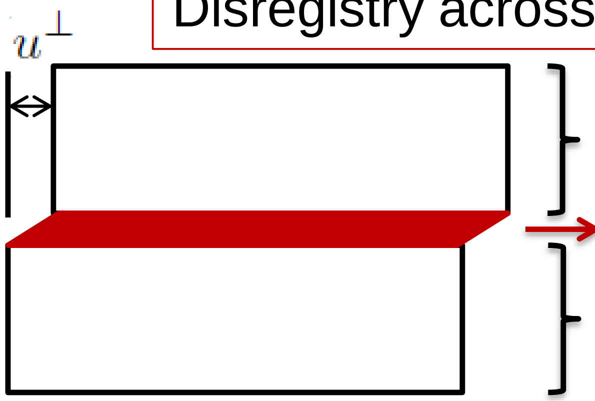


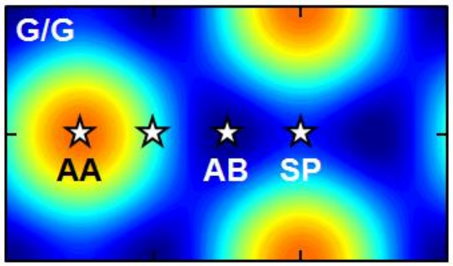
[S. Zhou *et. al.*, PRB, 2015]

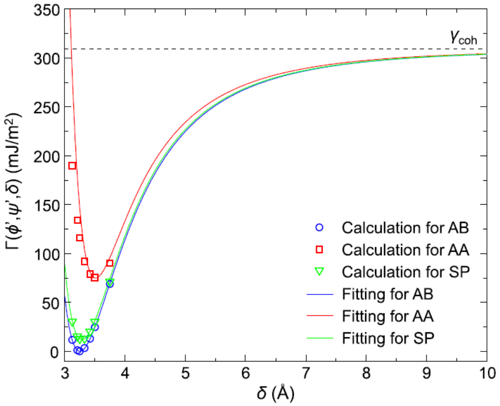
General multiscale model

Generalized Peierls-Nabarro model + 3D GSFE

Disregistry across slip plane: $u^{\perp}$







- Total energy: $E = E_{\text{elastic}} + E_{\text{misfit}}$

$$E_{\text{elastic}} = \frac{1}{2}\int \sigma_{13}(x)u^{\perp}(x)dx$$

$$E_{\text{misfit}} = \int \Gamma\left(u^{\perp}(x)\right)dx$$

  - E_{elastic}: Continuum level
  - E_{misfit}: First-principle

Γ = *Γ*(u_1, u_2, *d*)

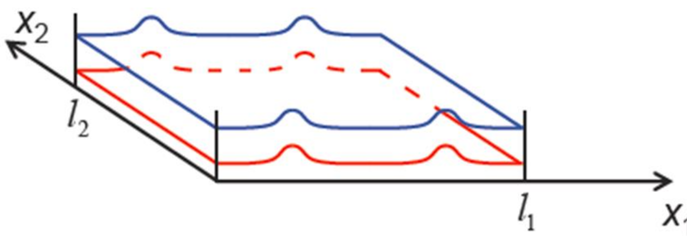
- Equilibrium dislocation distribution: $\frac{\partial E}{\partial u^{\perp}} = 0$

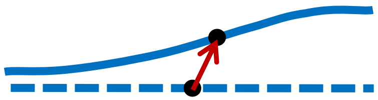
General multiscale model

Variables

Displacements

- Upper (+): $(u_{1+}(x_1,x_2),\ u_{2+}(x_1,x_2),\ f_+(x_1,x_2))$
- Lower (−): $(u_{1-}(x_1,x_2),\ u_{2-}(x_1,x_2),\ f_-(x_1,x_2))$





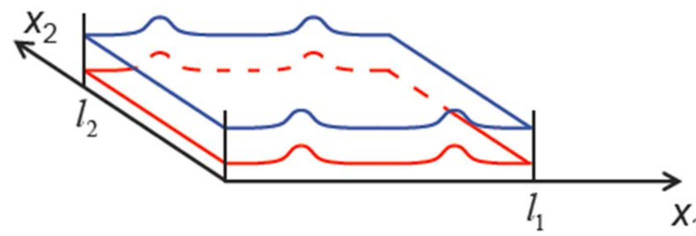
Flat state to Buckled state

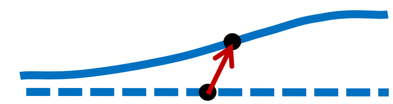
General multiscale model

Variables

Displacements

- Upper (+): ($u_{1+}(x_1,x_2)$, $u_{2+}(x_1,x_2)$, $f_+(x_1,x_2)$)
- Lower (−): ($u_{1-}(x_1,x_2)$, $u_{2-}(x_1,x_2)$, $f_-(x_1,x_2)$)





Flat state to Buckled state

Total energy functional

Like in the Peierls-Nabarro model for dislocations, we write the total energy as the sum of the elastic energy (due to the elastic deformation) and misfit energy (due to the interactions between layers)

$$E_{\text{total}} = E_{\text{elas}} + E_{\text{misfit}} = E_{\text{elas}+} + E_{\text{elas}-} + E_{\text{misfit}}$$

Elastic energy
$$\begin{cases} E_{\text{strain}\pm} = \dfrac{1}{2}\displaystyle\int C_{ijkl}\varepsilon_{ij}\varepsilon_{kl}\,dx_1dx_2 \\ E_{\text{bend}\pm} = \dfrac{1}{2}\displaystyle\int (\kappa H^2 + \kappa_G K)\,dx_1dx_2, \end{cases}$$

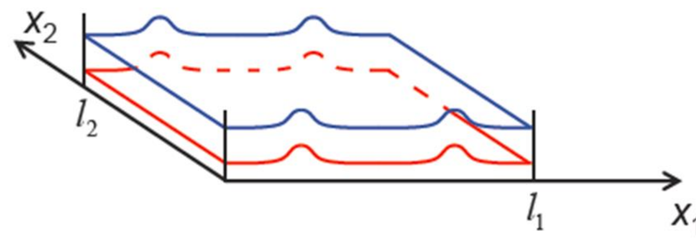
Misfit energy
$$E_{\text{misfit}} = \int \Gamma(u_1^{\perp}, u_2^{\perp}, f^{\perp})\,dx_1dx_2,$$

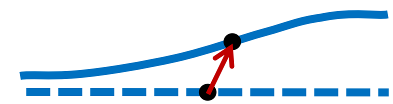
General multiscale model

Variables

Displacements

- Upper (+): $(u_{1+}(x_1,x_2),\ u_{2+}(x_1,x_2),\ f_+(x_1,x_2))$
- Lower (−): $(u_{1-}(x_1,x_2),\ u_{2-}(x_1,x_2),\ f_-(x_1,x_2))$





Flat state to Buckled state

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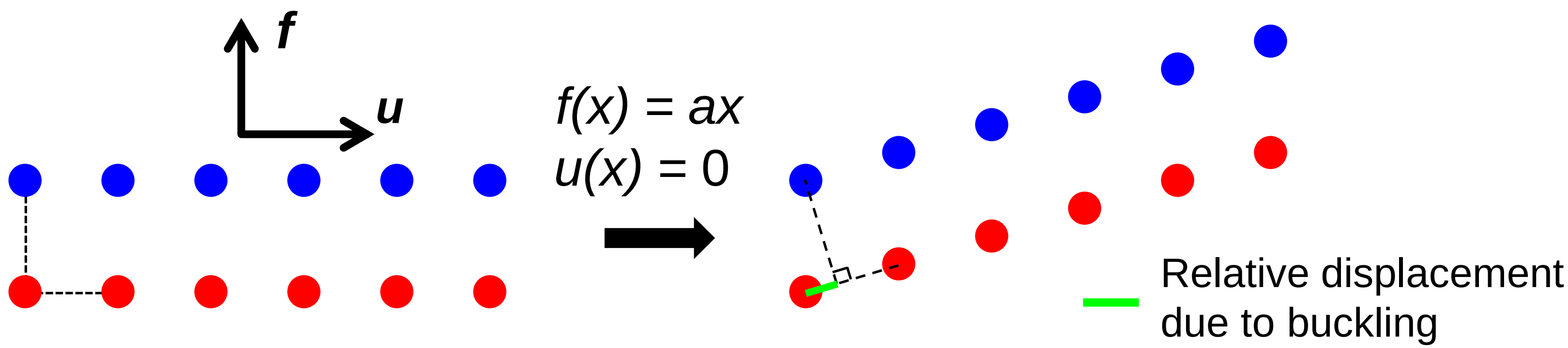
Misfit energy
$$E_{\text{misfit}} = \int \Gamma(u_1^\perp, u_2^\perp, f^\perp)\,dx_1dx_2,$$

Relative displacements

General multiscale model

Relative Displacement

1. Buckling change the local coordinate system
2. The deformation of the neutral plane is approximated by the average of the displacements of the upper layer and the lower layer



Relative displacements between layers:

$$u_1^{\perp} = (\varepsilon_{11+}^0 - \varepsilon_{11-}^0)x_1 + u_{1+} - u_{1-} + \frac{1}{2}(\frac{\partial f_+}{\partial x_1} + \frac{\partial f_-}{\partial x_1})(d + f_+ - f_-)$$

$$u_2^{\perp} = (\varepsilon_{22+}^0 - \varepsilon_{22-}^0)x_2 + u_{2+} - u_{2-} + \frac{1}{2}(\frac{\partial f_+}{\partial x_2} + \frac{\partial f_-}{\partial x_2})(d + f_+ - f_-)$$

$$f^{\perp} = f_+ - f_-$$

General multiscale model

Equilibrium structure:

The equilibrium equations:

$$\frac{\delta E_{\text{total}}}{\delta u_{i\pm}} = -\frac{1}{2}C_{ijkl\pm}\left[\frac{\partial^2 u_{k\pm}}{\partial x_l \partial x_j} + \frac{\partial^2 u_{l\pm}}{\partial x_k \partial x_j} + \frac{\partial}{\partial x_j}\left(\frac{\partial f_\pm}{\partial x_k}\frac{\partial f_\pm}{\partial x_l}\right)\right] \pm \frac{\partial \Gamma}{\partial u_i^\perp} = 0,$$

$$\frac{\delta E_{\text{total}}}{\delta f_\pm} = -C_{ijkl\pm}\frac{\partial}{\partial x_i}\left[\frac{\partial f_\pm}{\partial x_j}\left(\varepsilon_{kl}^0 + \frac{1}{2}\left(\frac{\partial u_{k\pm}}{\partial x_l} + \frac{\partial u_{l\pm}}{\partial x_k}\right) + \frac{1}{2}\frac{\partial f_\pm}{\partial x_k}\frac{\partial f_\pm}{\partial x_l}\right)\right] + \kappa \Delta^2 f_\pm$$

$$-\frac{1}{2}\frac{\partial^2 \Gamma}{\partial u_i^\perp \partial u_j^\perp}\frac{\partial u_j^\perp}{\partial x_i}(d + f_+ - f_-) \pm \frac{\partial \Gamma}{\partial u_i^\perp}\frac{\partial f_\mp}{\partial x_i} \pm \frac{\partial \Gamma}{\partial f^\perp} = 0.$$

Numerically, the minimum energy state can be found by iterating

$$\frac{\partial u_{i\pm}}{\partial t} = -\frac{\delta E_{\text{total}}}{\delta u_{i\pm}}$$

$$\frac{\partial f_\pm}{\partial t} = -\frac{\delta E_{\text{total}}}{\delta f_\pm}$$

until the energy does not change (to numerical precision)

General multiscale model

Inputs: Applied to bilayer graphene (BLG)

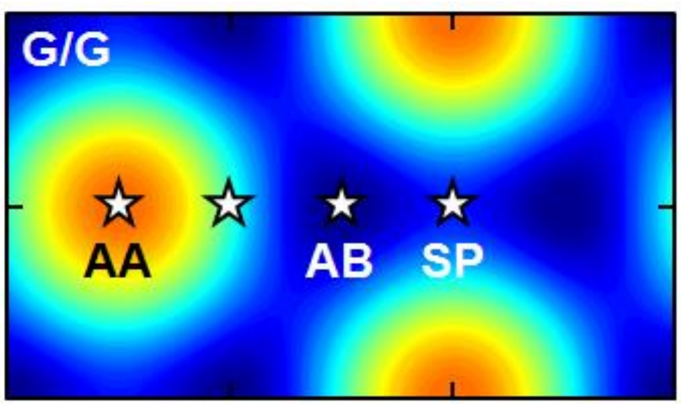
1. Elastic constants and bending rigidity [S. Chen *et. al*., PRB, (2011)]

   Elastic modulus: C_{11} = 312.45J/m^2; C_{12} = 91.65J/m^2; C_{44} = 110.4J/m^2.
   Bending rigidity: κ = 22.08×10^{-20}J

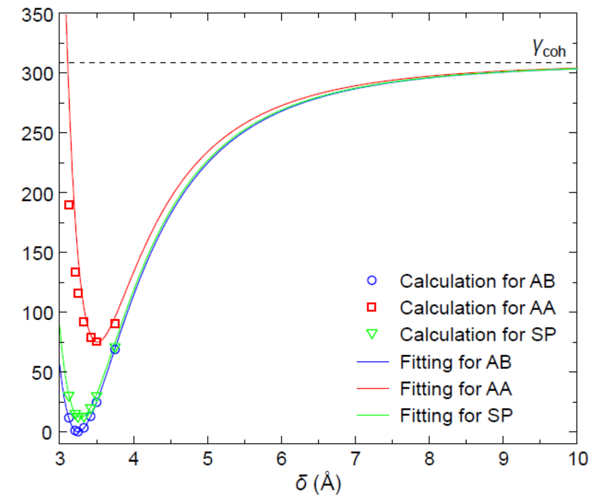
2. 3D Generalized Stacking-Fault Energy (3D GSFE): calculated based on ACFDT-RPA [S. Zhou *et. al.*, PRB, (2015)]

$$\Gamma(u_1^{\perp}, u_2^{\perp}, \delta) = A\exp\left(-\alpha\delta\right) - B\left(\frac{d}{\delta}\right)^4 + \gamma_{\mathrm{coh}},$$

$\Gamma(u_1^{\perp}, u_2^{\perp}, \delta \equiv \delta_0)$

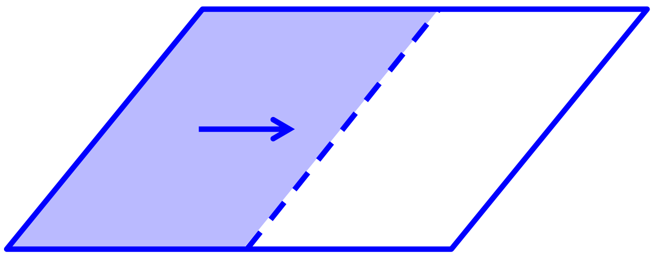


$\Gamma(u_1^{\perp} \equiv u_1^0, u_2^{\perp} \equiv u_2^0, \delta)$

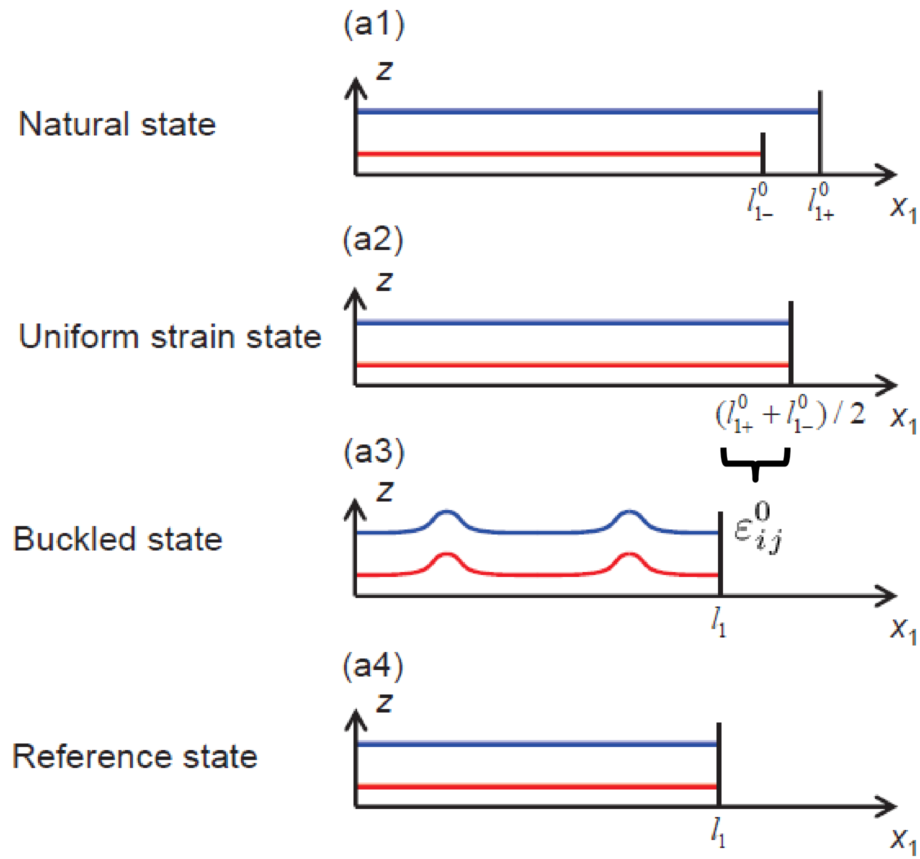


Interlayer dislocation in Bilayer Graphene (BLG)

Edge dislocation:



Generate an edge dislocation
(only show upper layer)

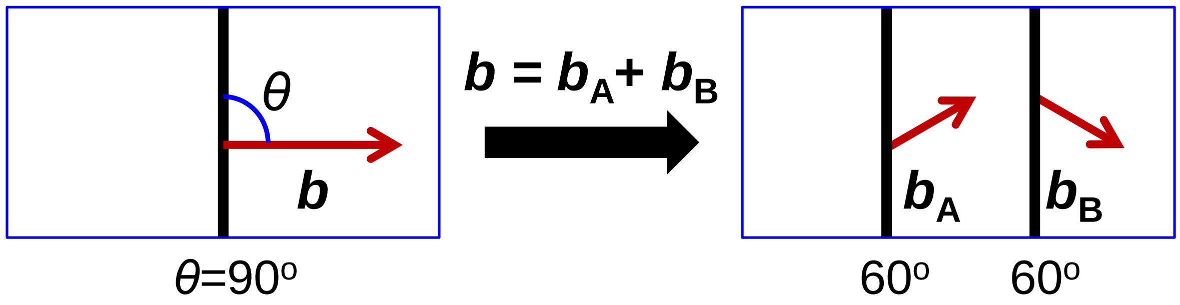


Define pre-existed strains:

$$\varepsilon^0_{ii\pm} = (l_i - l^0_{i\pm})/l_i \ (i = 1, 2)$$

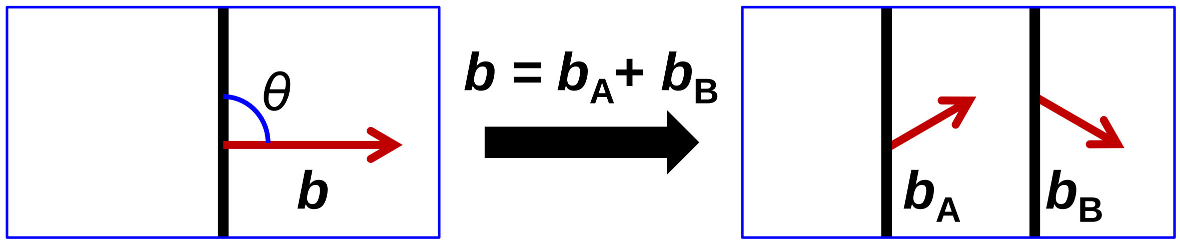
Interlayer dislocation in Bilayer Graphene (BLG)

Edge dislocation:

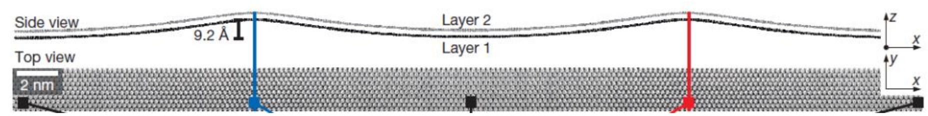


Interlayer dislocation in Bilayer Graphene (BLG)

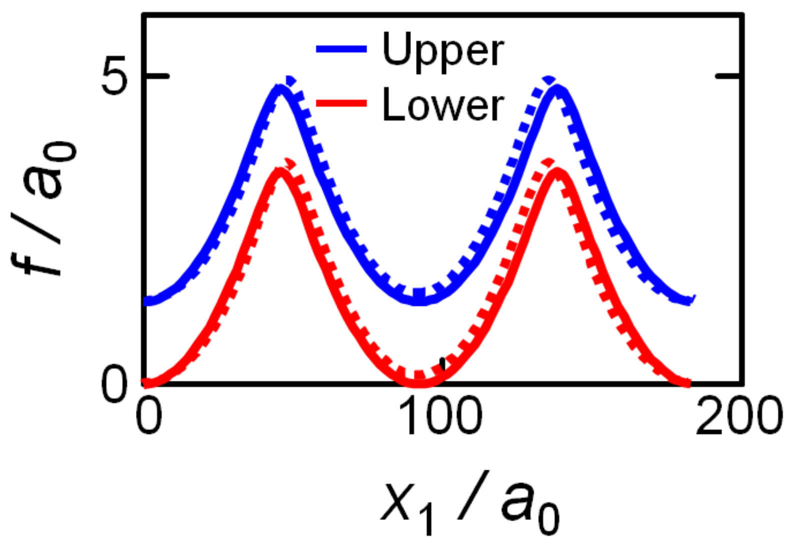
Edge dislocation: - breaks into 2 partial dislocation
- agrees with MD results (dashed curves)



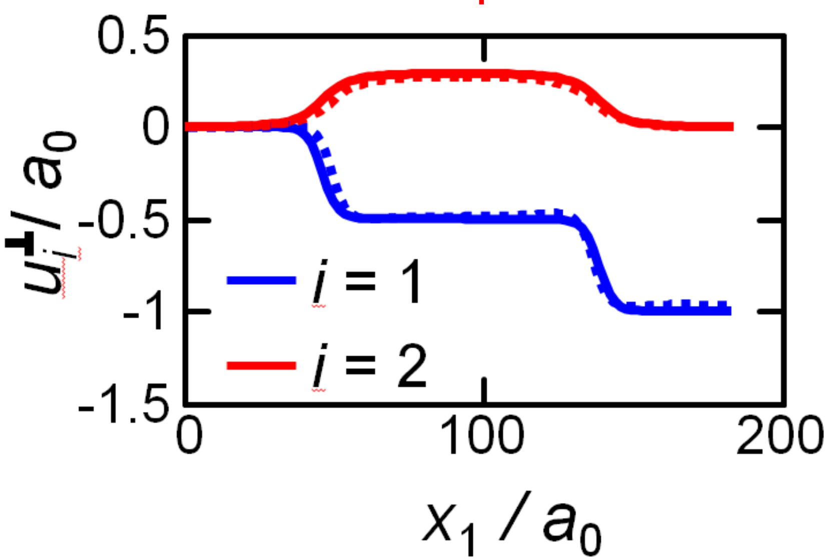
θ=90º 60º 60º



Out-of-plane displacements (Bilayer shape)



Relative displacements



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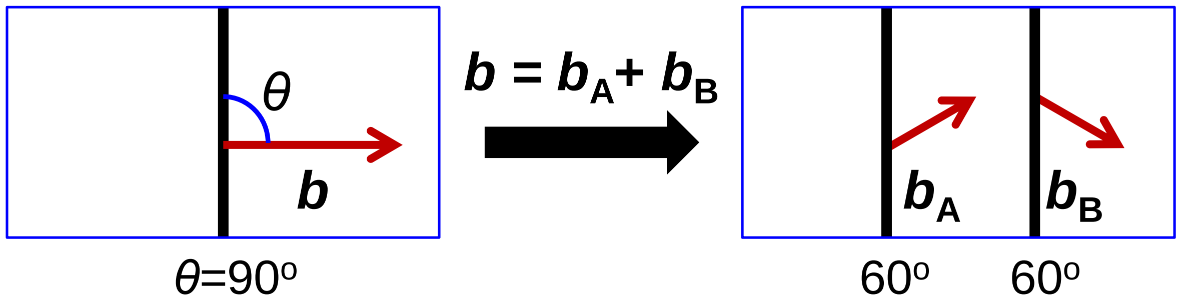

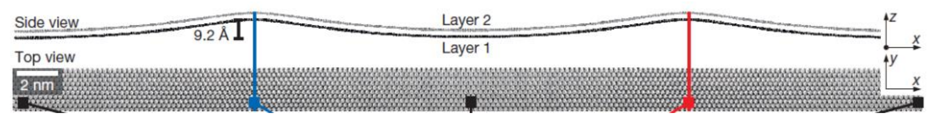

Out-of-plane displacements
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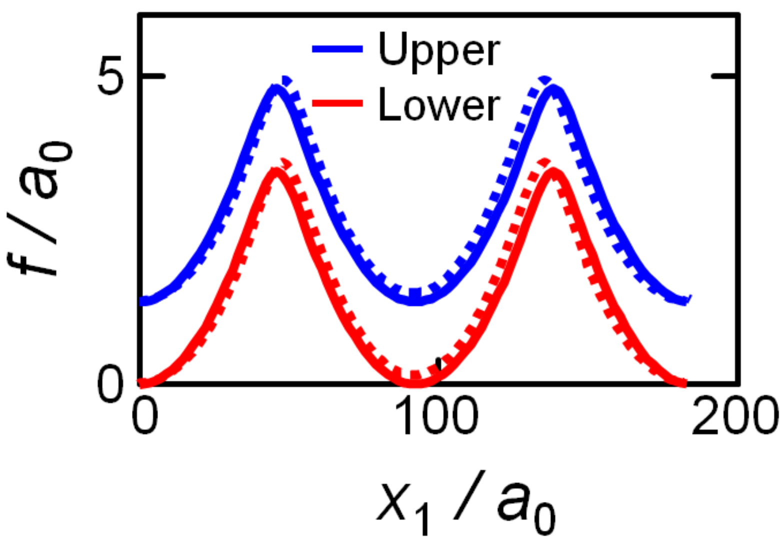
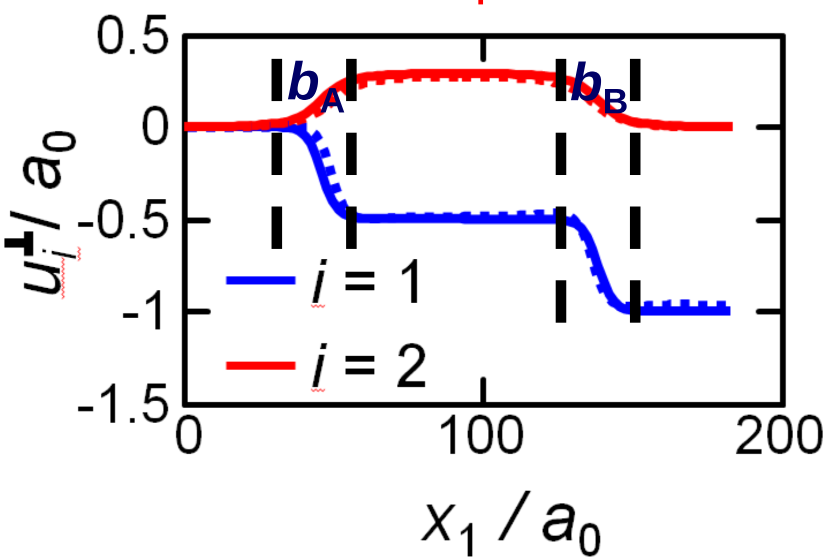
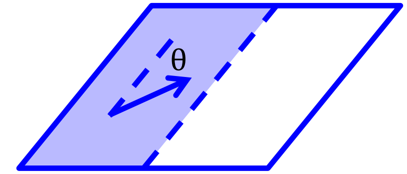


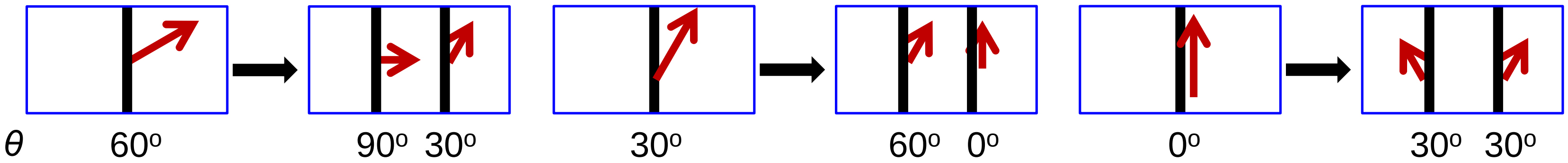
Relative displacements

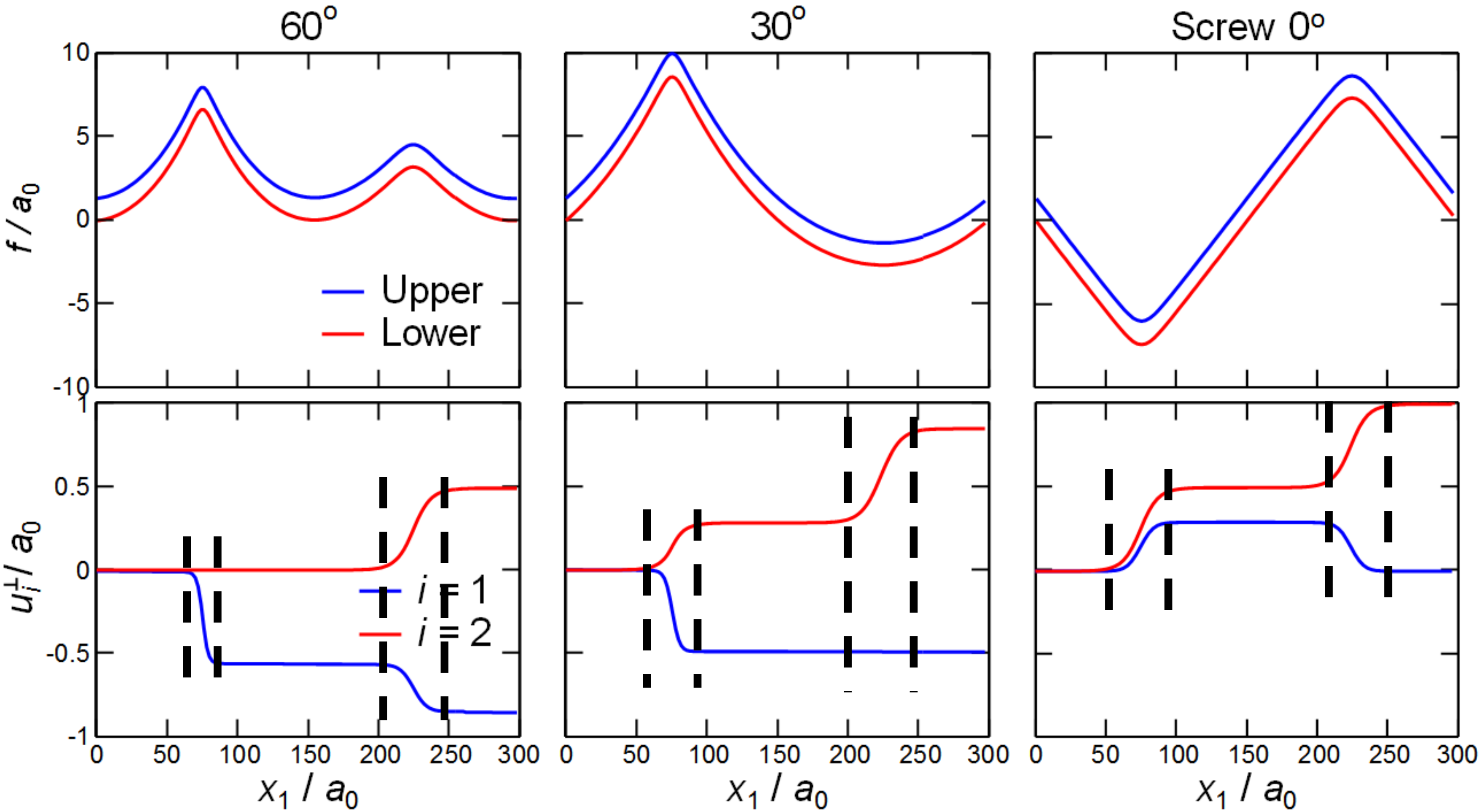


Interlayer dislocation in BLG



General dislocations: Structural features





Interlayer dislocation in Bilayer Graphene (BLG)

Core properties of partial dislocation:

Type	Edge 90^o	Mixed 60^o	Mixed 30^o	Screw 0^o
Width (nm)	1.5 (7.2)	2.4 (6.3)	3.7 (5.3)	4.5 (4.5)
Energy ($\times 10^{-10}$J)	0.318	0.508	0.905	1.081

Red: Core width in flat configuration ($f_+ = f_- = 0$)

- Buckled bilayer: Core width and energy ↑ as edge component ↓
- Flat bilayer: Core width ↓ as edge component ↓

Interlayer dislocation in Bilayer Graphene (BLG)

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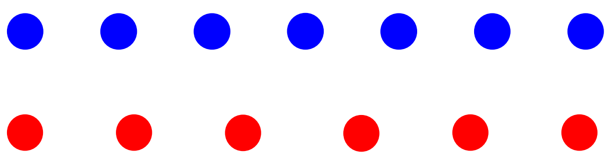
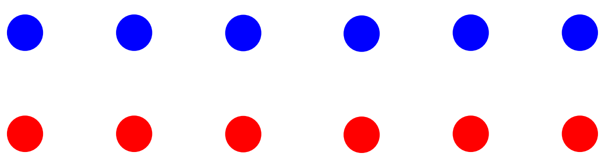
Edge partial (90^{o})



Screw partial (0^{o})



Interlayer dislocation in Bilayer Graphene (BLG)

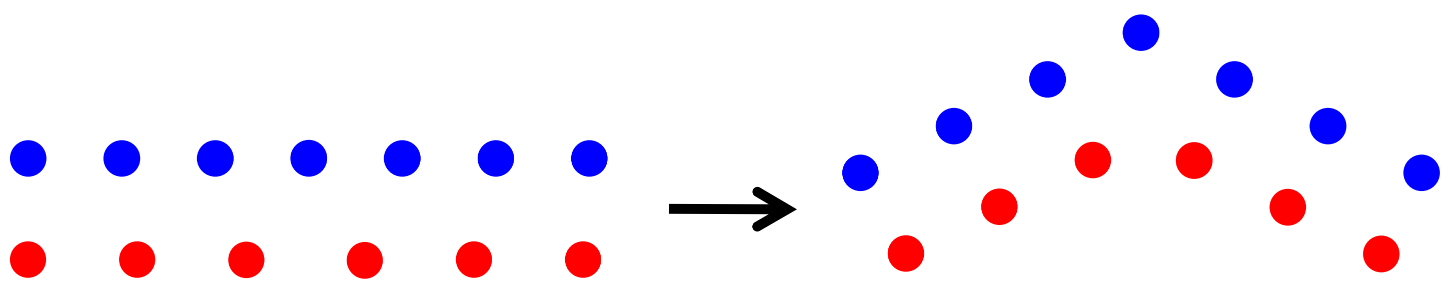
Core properties of partial dislocation:

Type	Edge 90º	Mixed 60º	Mixed 30º	Screw 0º
Width (nm)	1.5 (7.2)	2.4 (6.3)	3.7 (5.3)	4.5 (4.5)
Energy ($\times 10^{-10}$J)	0.318	0.508	0.905	1.081

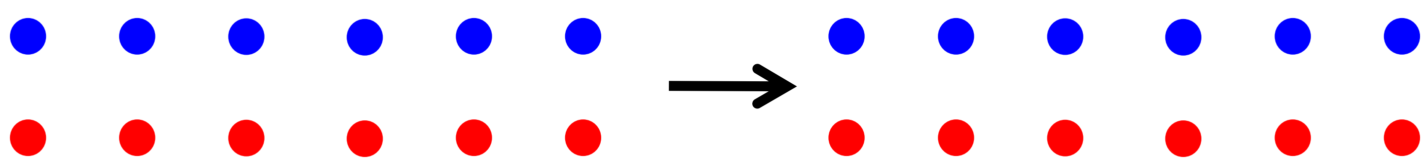
Red: Core width in flat configuration ($f_+ = f_- = 0$)

- Buckled bilayer: Core width and energy ↑ as edge component ↓
- Flat bilayer: Core width ↓ as edge component ↓

Edge partial (90º)

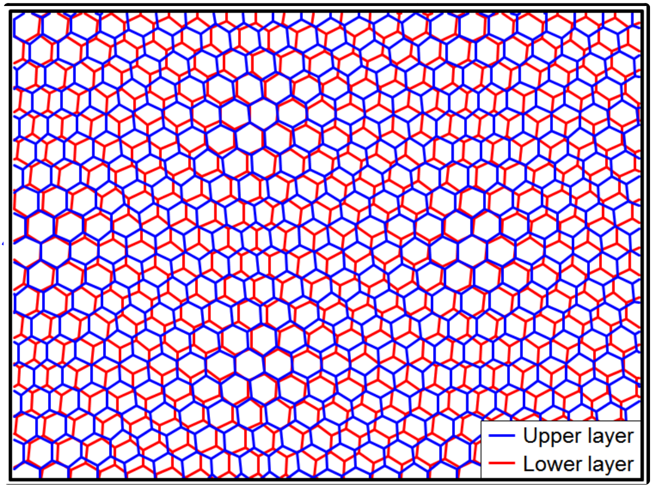


Screw partial (0º)



Interlayer twist in BLG

Counterclockwise twist



Substructures in twisted BLG:

- AB/AC stacking
- Partial dislocation
- AA stacking (intersection of dislocations)

Interlayer twist in BLG

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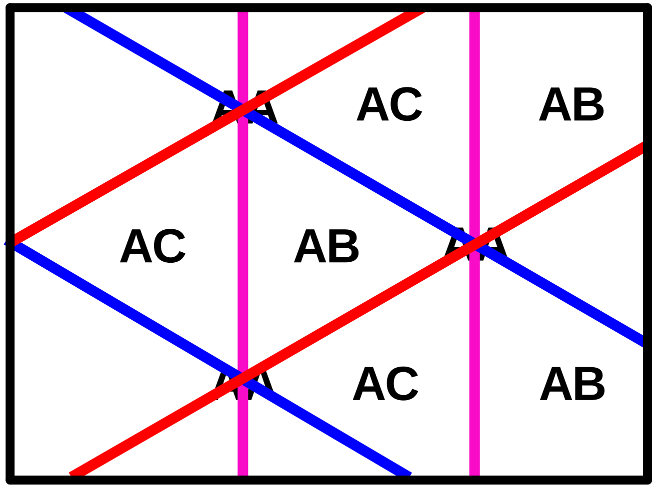

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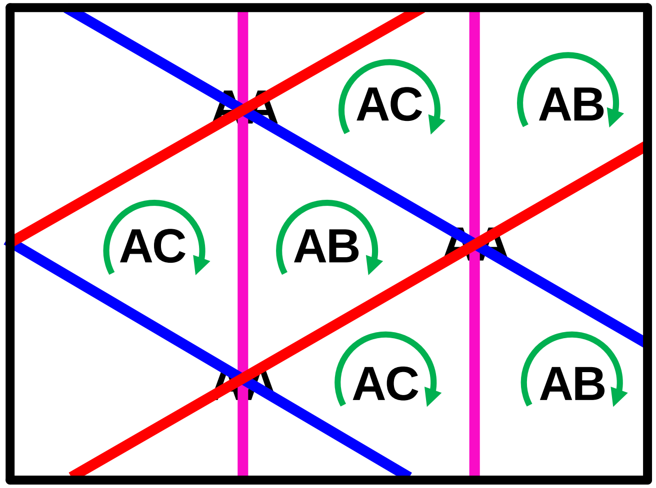

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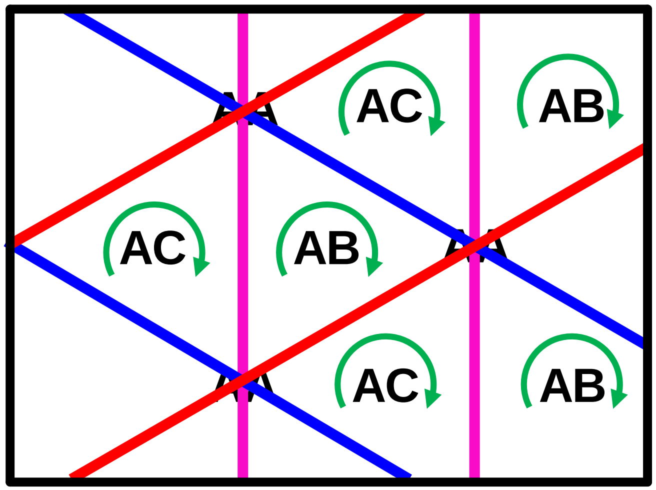

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Question: How AA stacking relax?

Interlayer twist in BLG

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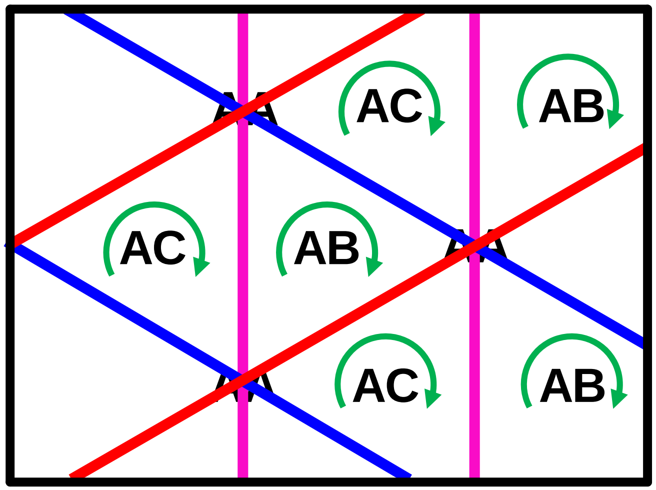

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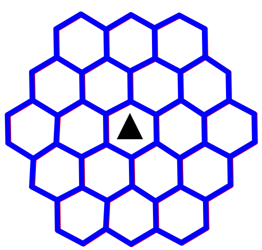
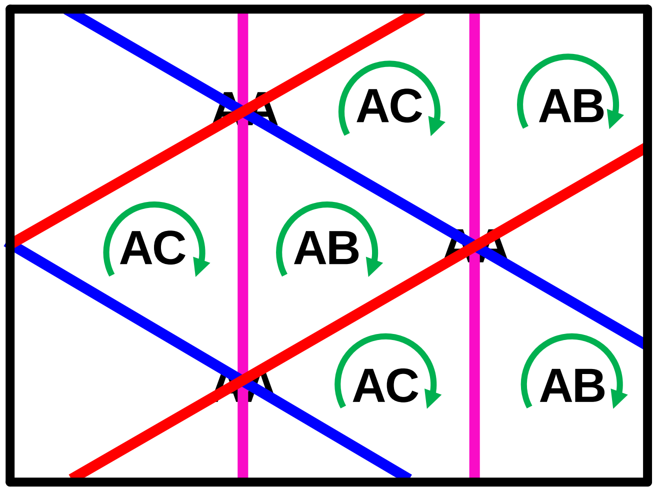


▲ Fixed to AA state

Interlayer twist in BLG

Counterclockwise twist



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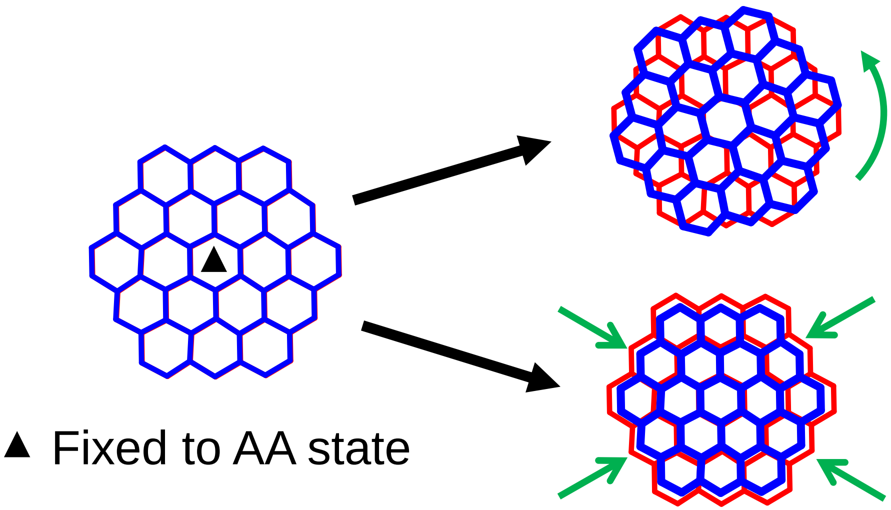

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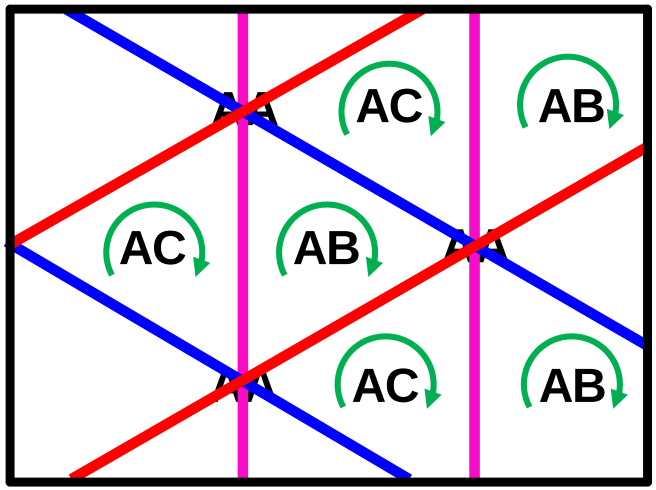

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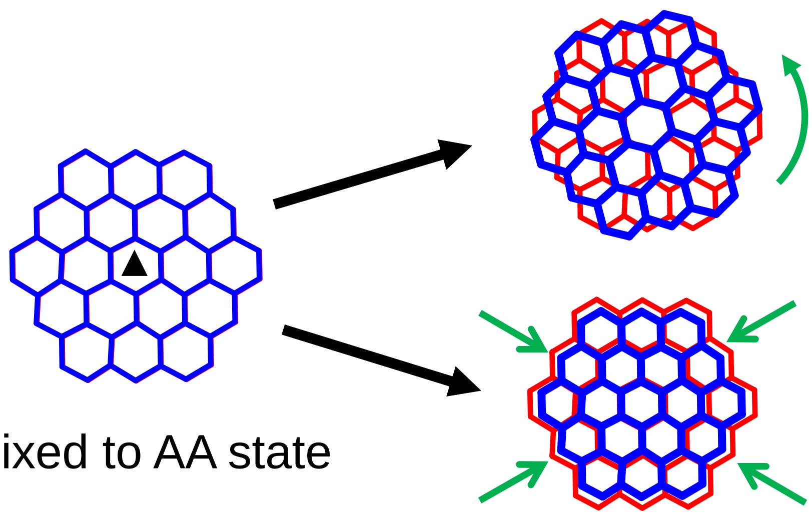
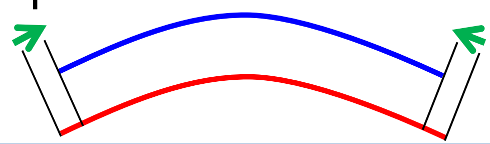


▲ Fixed to AA state

Not possible for flat bilayer

C_{11}(312.45J/m^2) > C_{44}(110.4J/m^2)

But possible in the deformed bilayer

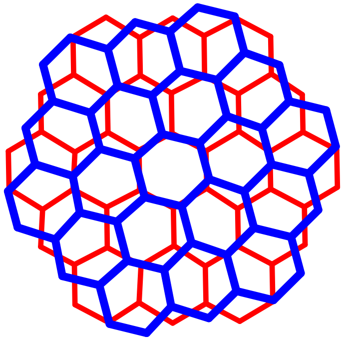


Interlayer twist in BLG

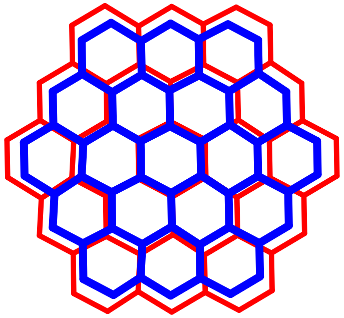
Initial guess: bilayer is flat → Case A

Initial guess: bilayer is buckled a little at AA stacking → Case B

Case A



Case B



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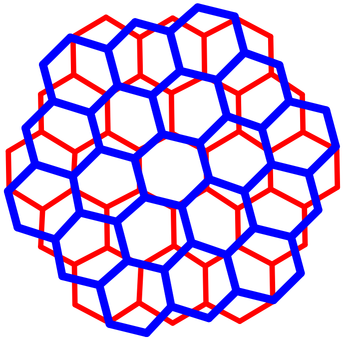
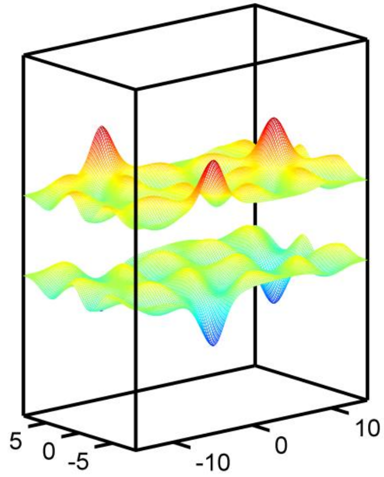
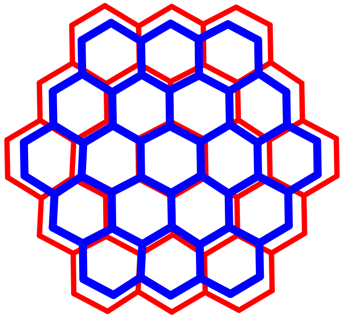
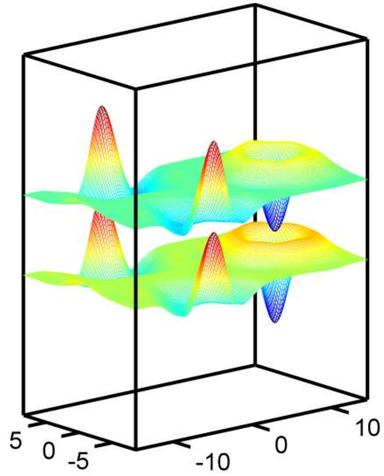




Case B





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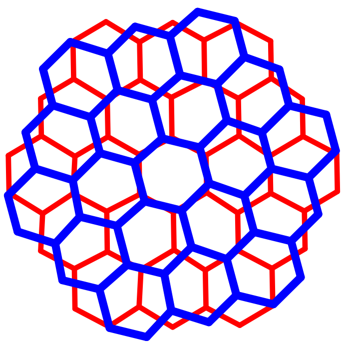
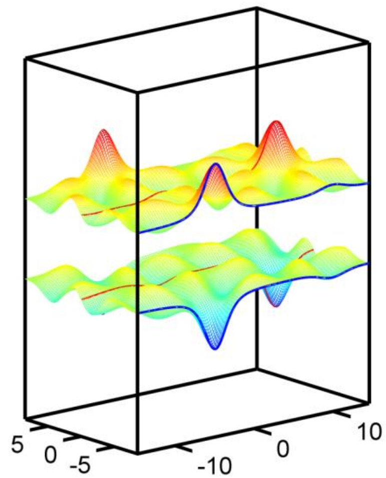
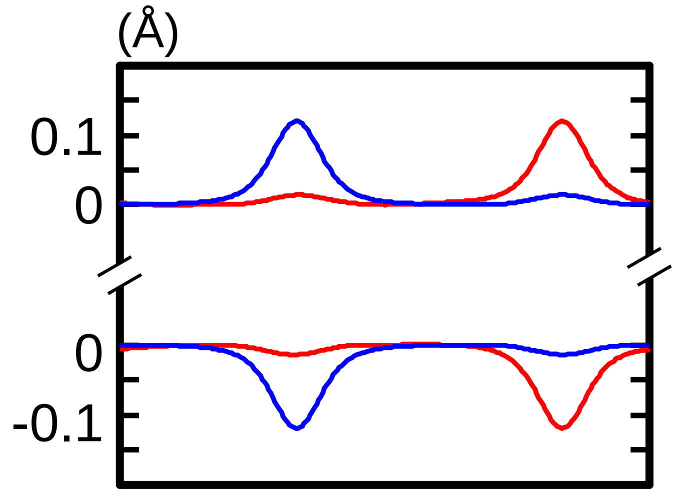
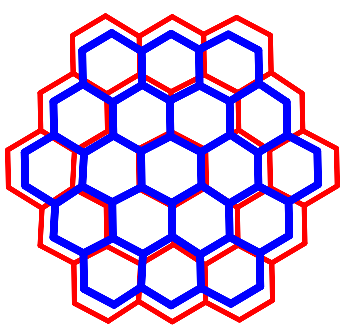
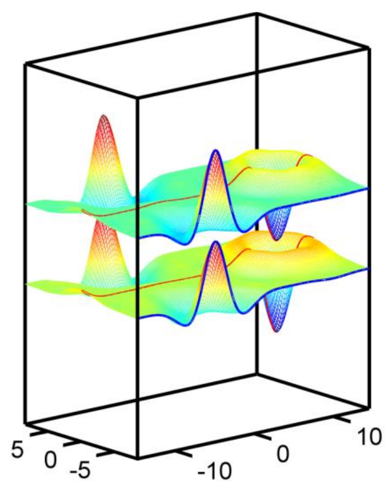


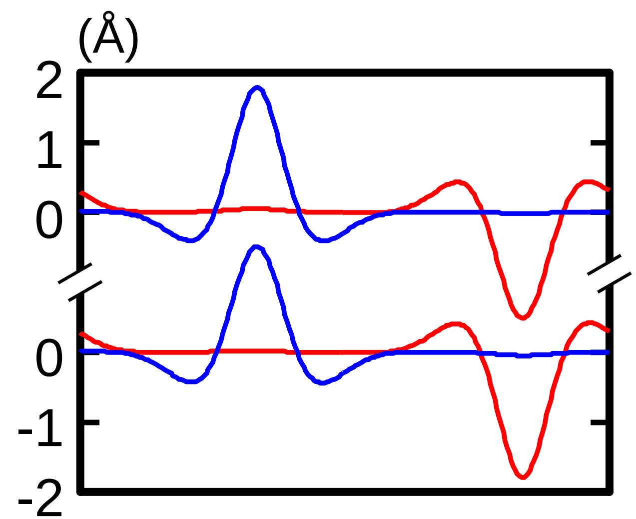




Case B







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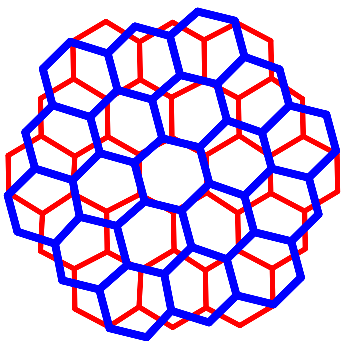
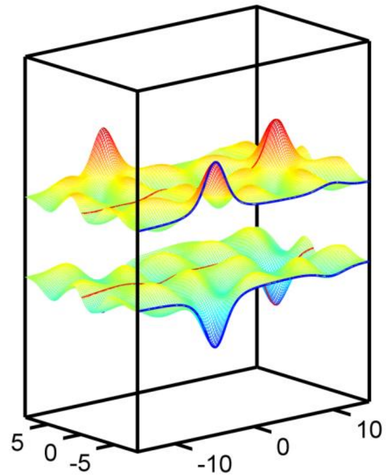
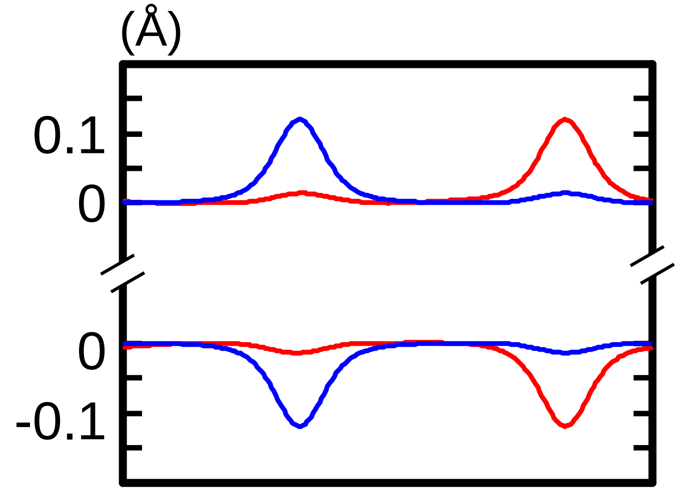
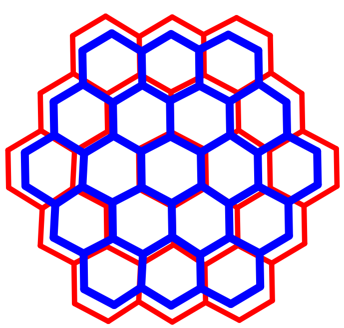


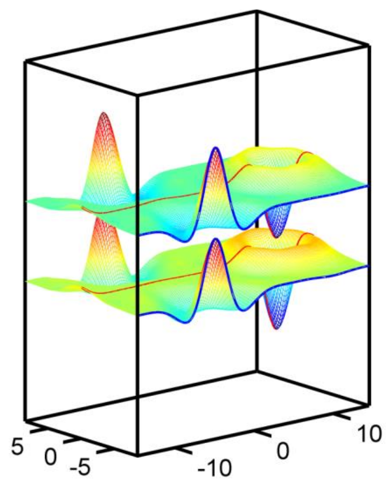


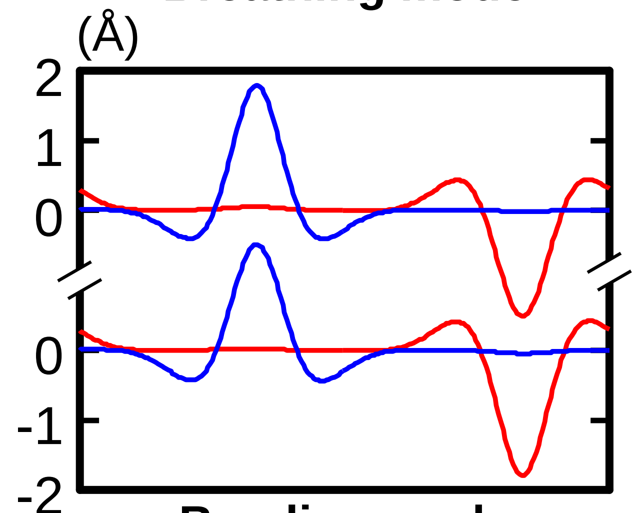


Breathing mode

Case B







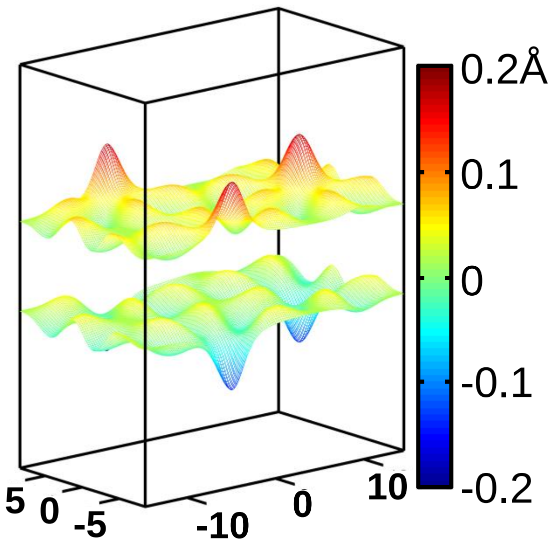
Bending mode

Interlayer twist in BLG

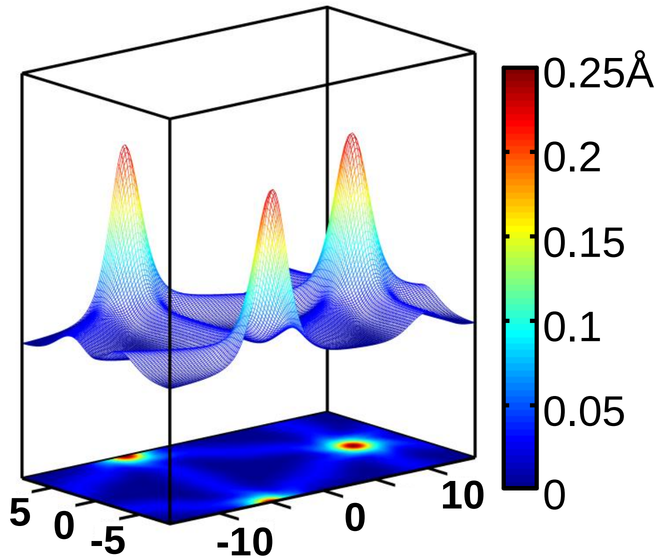
Breathing mode:

- At AA stacking, two layers buckles to different direction

Bilayer shape



Relative displacement
$f_+ - f_-$

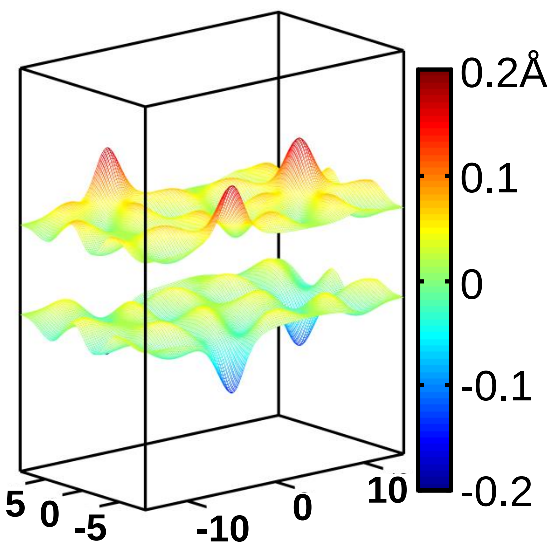


Interlayer twist in BLG

Breathing mode:

- At AA stacking, two layers buckles to different direction
- 3 sets of partial dislocations.
- Dislocations intersect at AA stacking with maximum buckling height.

Bilayer shape



Relative displacement
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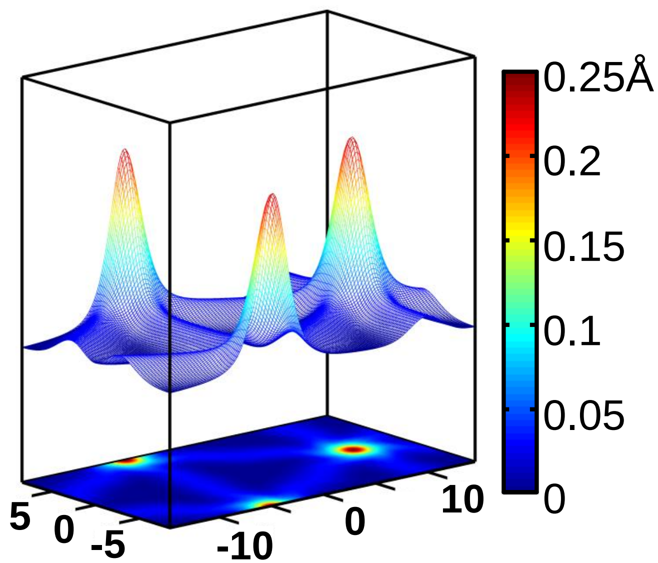
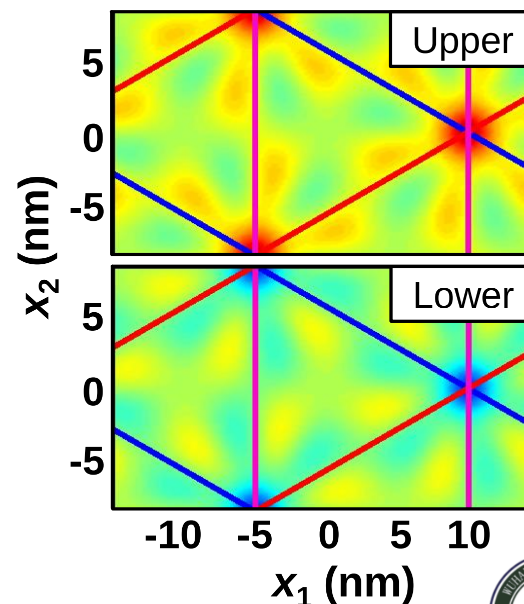
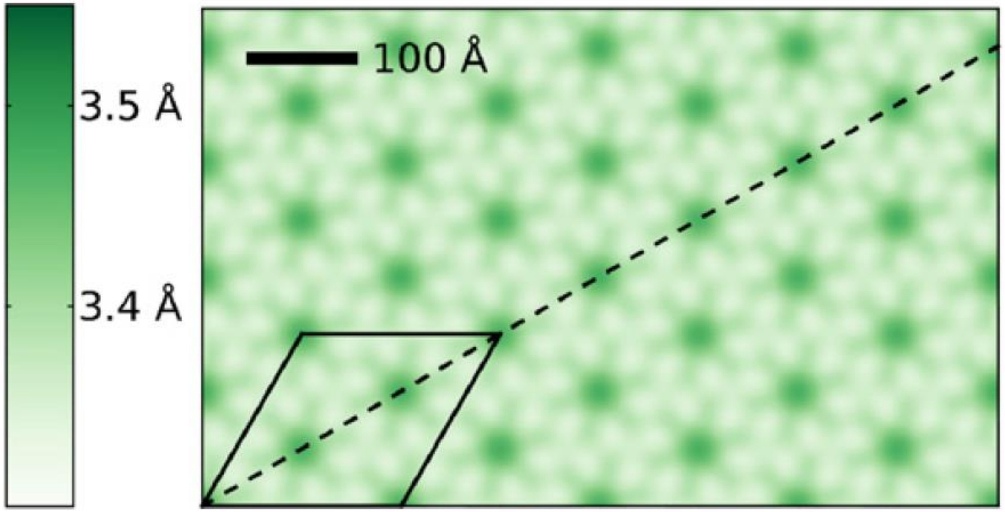


Dislocation network structure



Interlayer twist in BLG

Breathing mode: compare with MD (for free standing tBLG)



Upper layer out-of-plane displacement

- **MD:** [van Wijk *et al.* 2D Materials, 2015]
  - θ = 1.2^{o}
  - Intralayer: REBO
  - Interlayer: registry dependent potential

Interlayer twist in BLG

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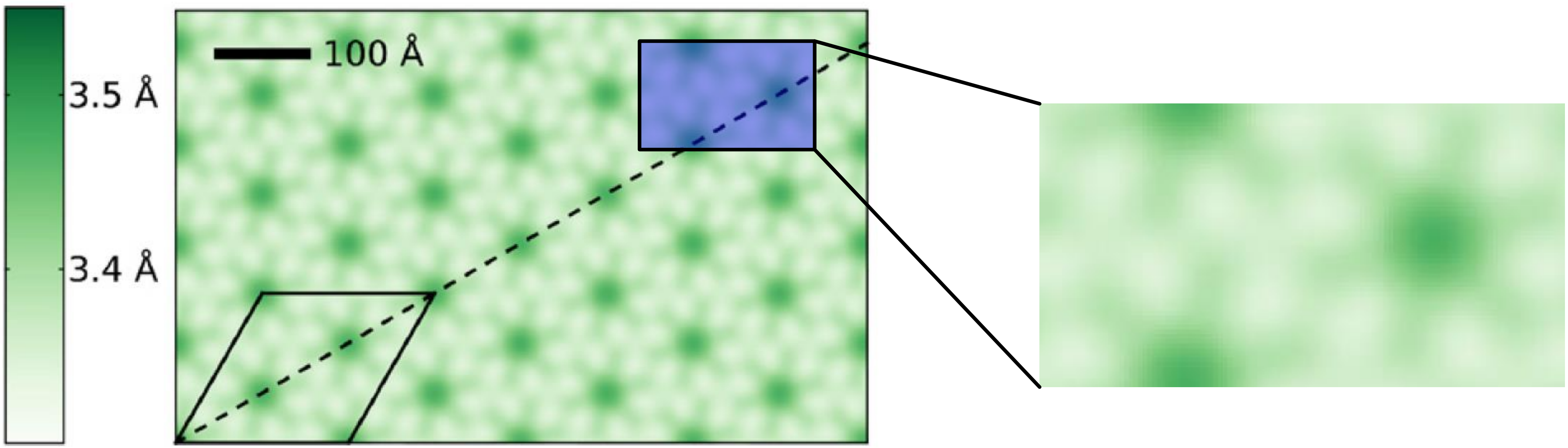

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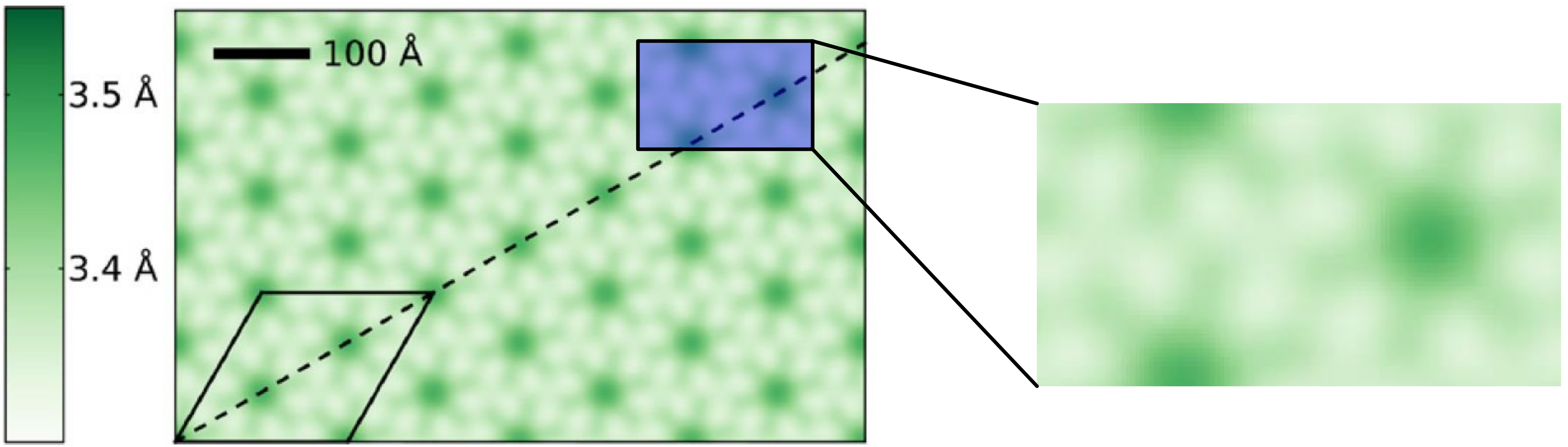

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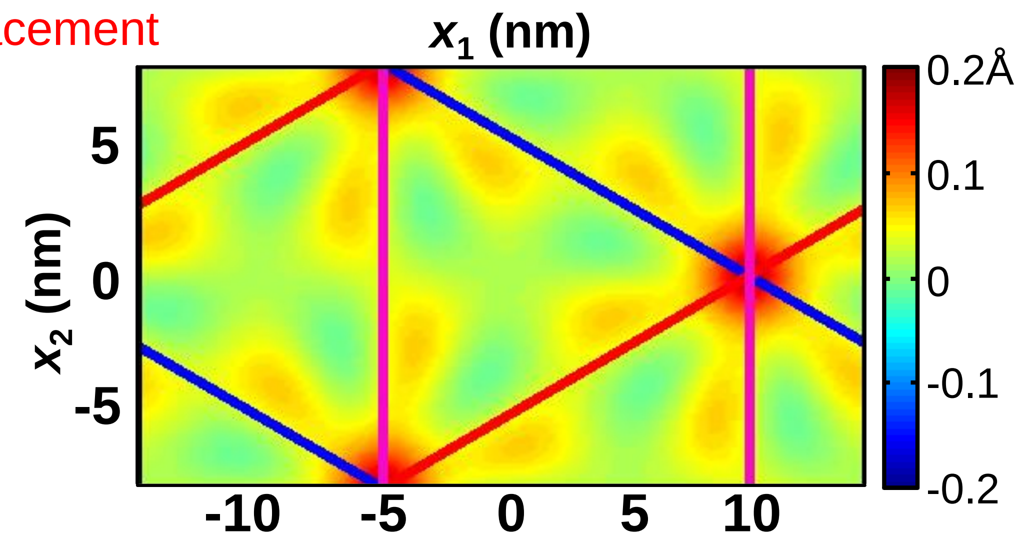


$\theta \approx 0.8°$

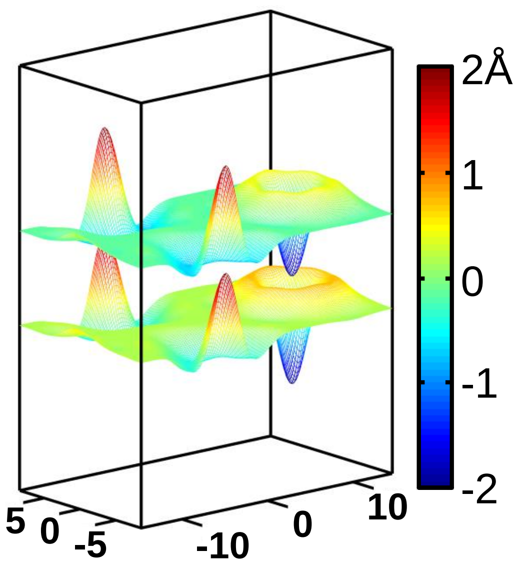
- **Similar micro-structure**
- **Qualitative agreement**

Interlayer twist in BLG

Bending mode:

- Two layers buckles to same direction → bulges

Bilayer shape



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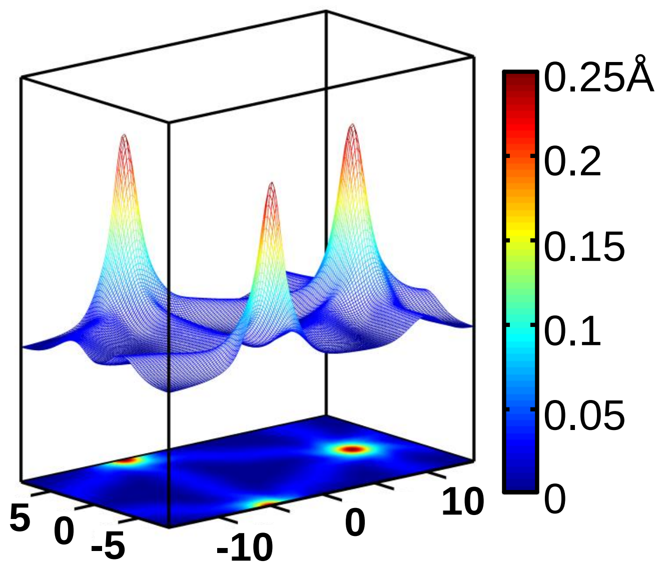

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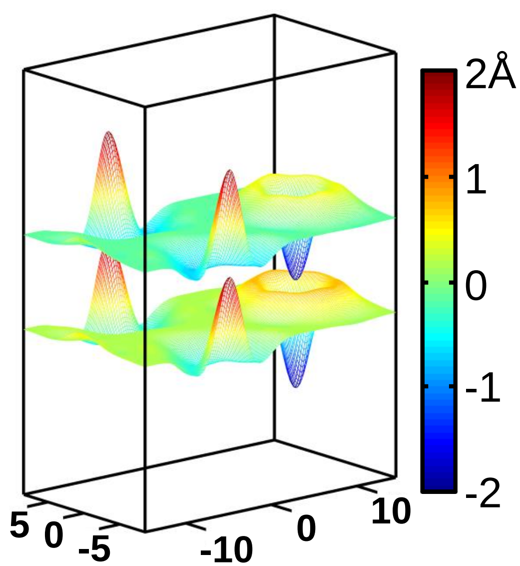
Bilayer shape



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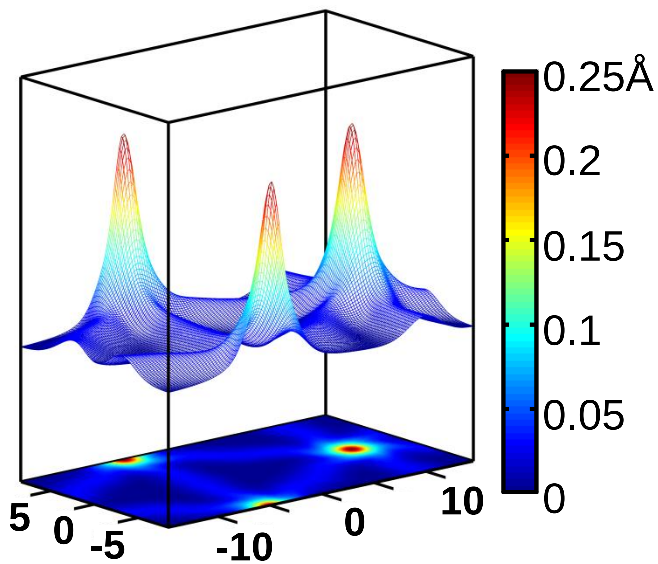

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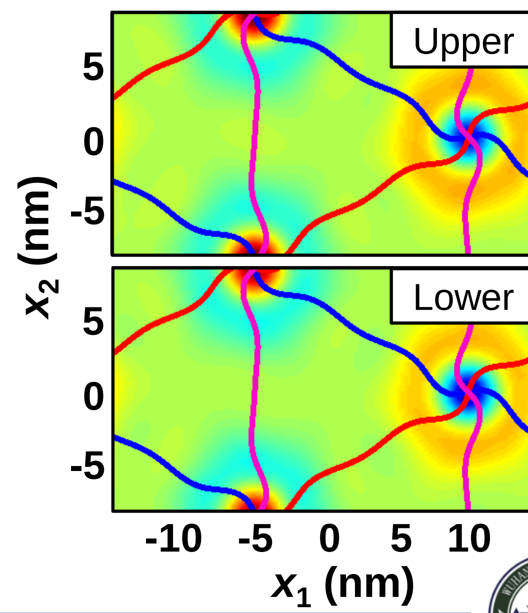

Interlayer twist in BLG

Bending mode:

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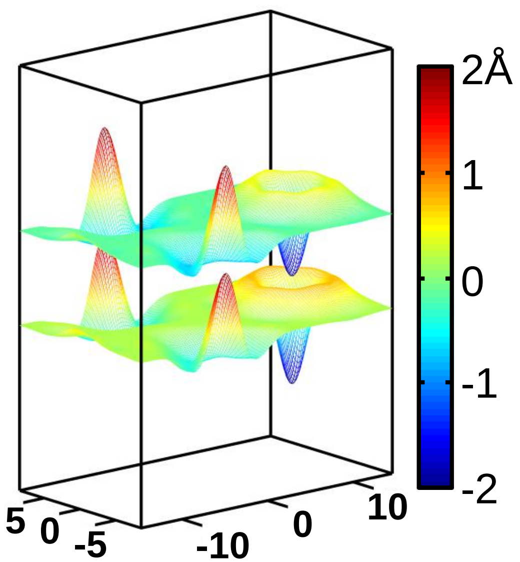
- 3 sets of partial dislocations.
- Dislocations intersect at AA stacking with maximum buckling height.
- Dislocation twists: clockwise/counterclockwise for upper/lower bulge

Bilayer shape



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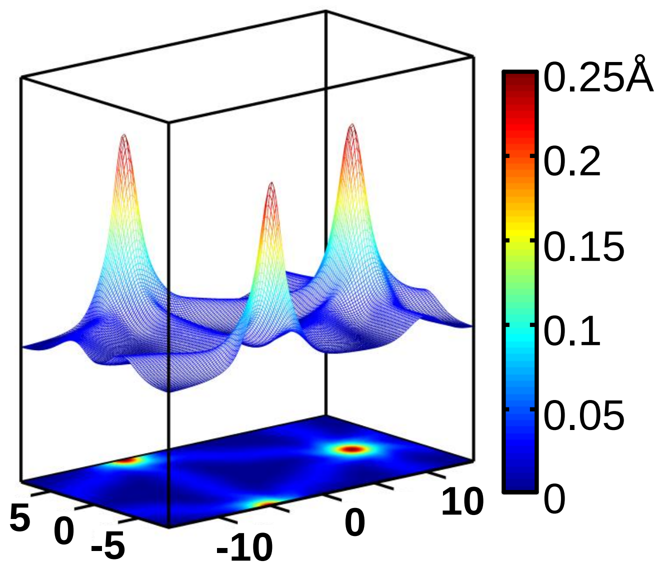

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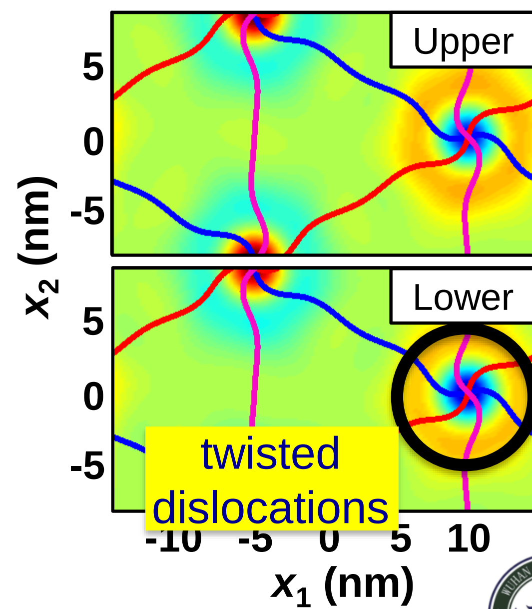
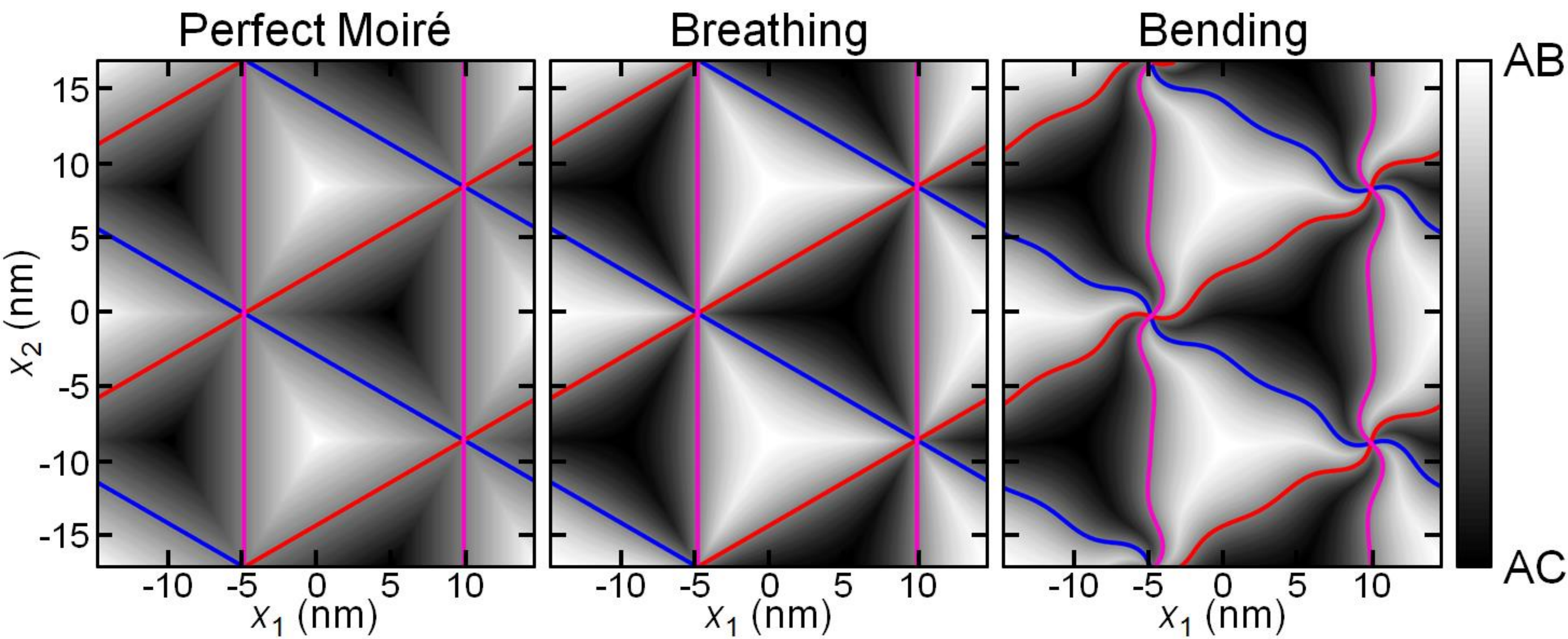


Interlayer twist in BLG

Perfect Moiré: small well-stacked domain, straight dislocations

Breathing mode: large well-stacked domain, straight dislocations

Bending mode: large well-stacked domain, spiral dislocations



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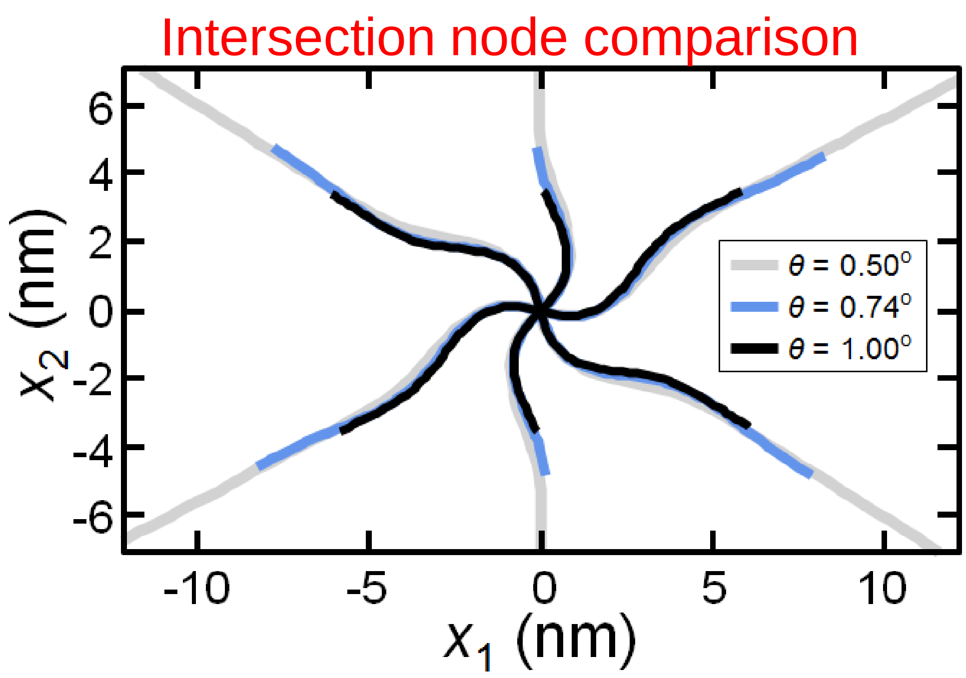

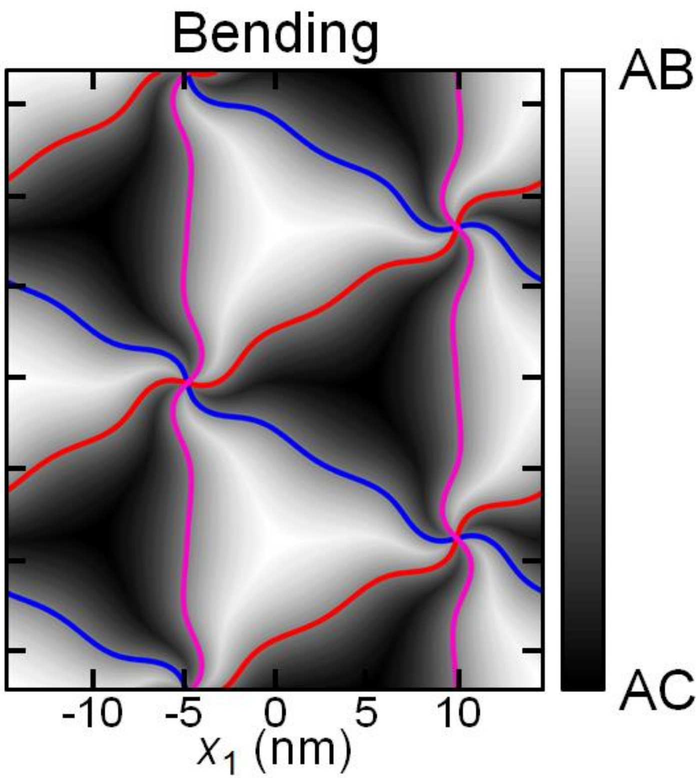

Interlayer twist in BLG

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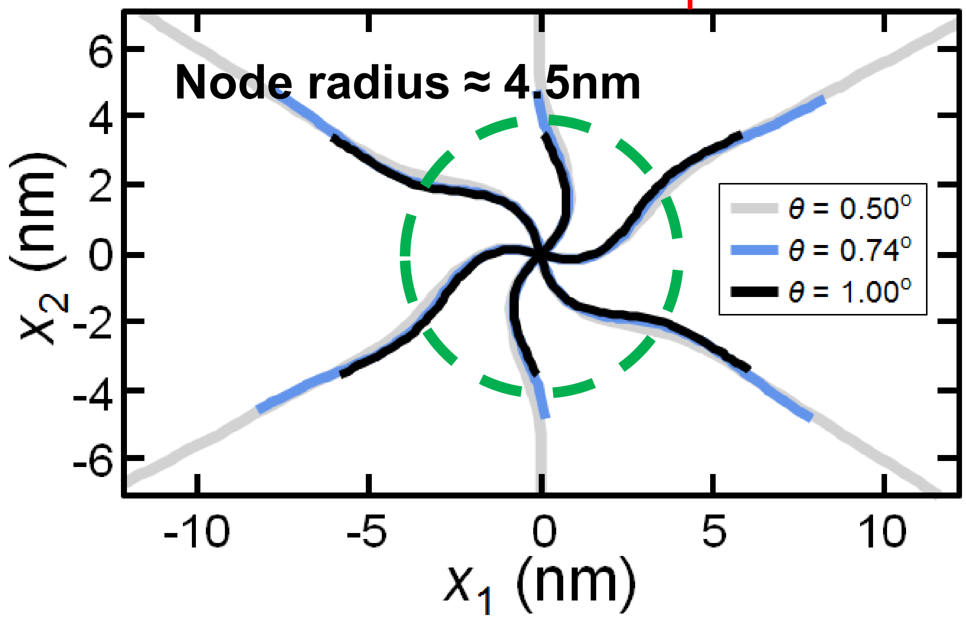
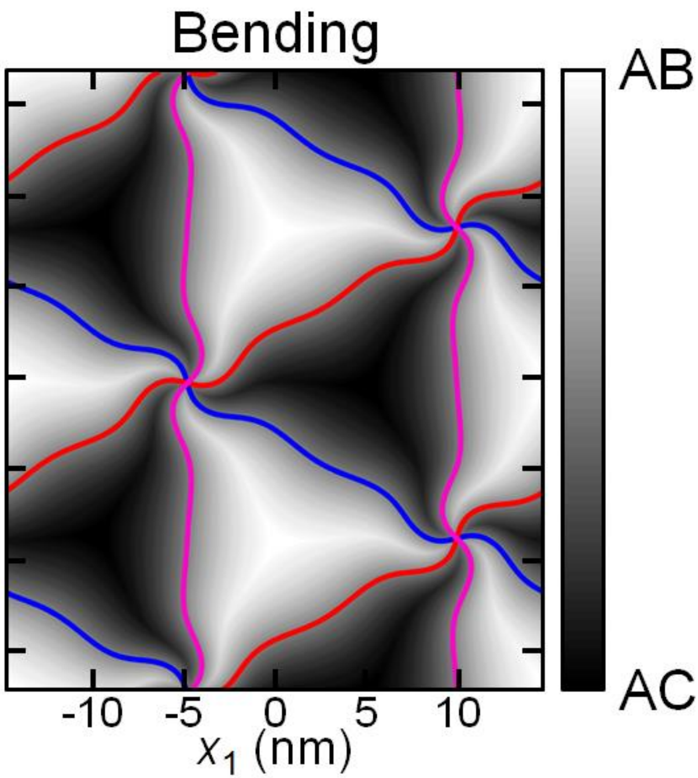
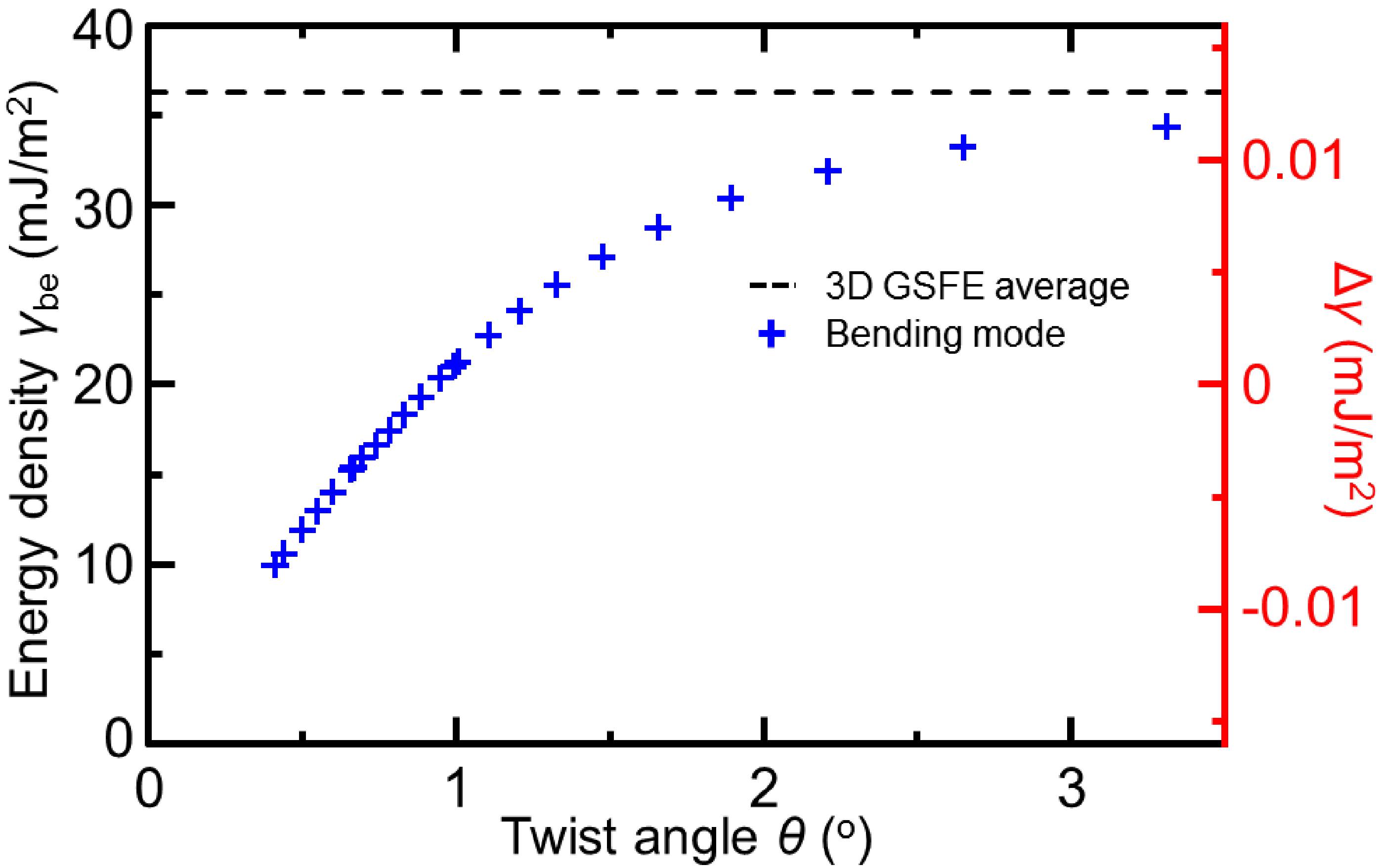
Node dislocation structure
weakly depends on θ

Intersection node comparison



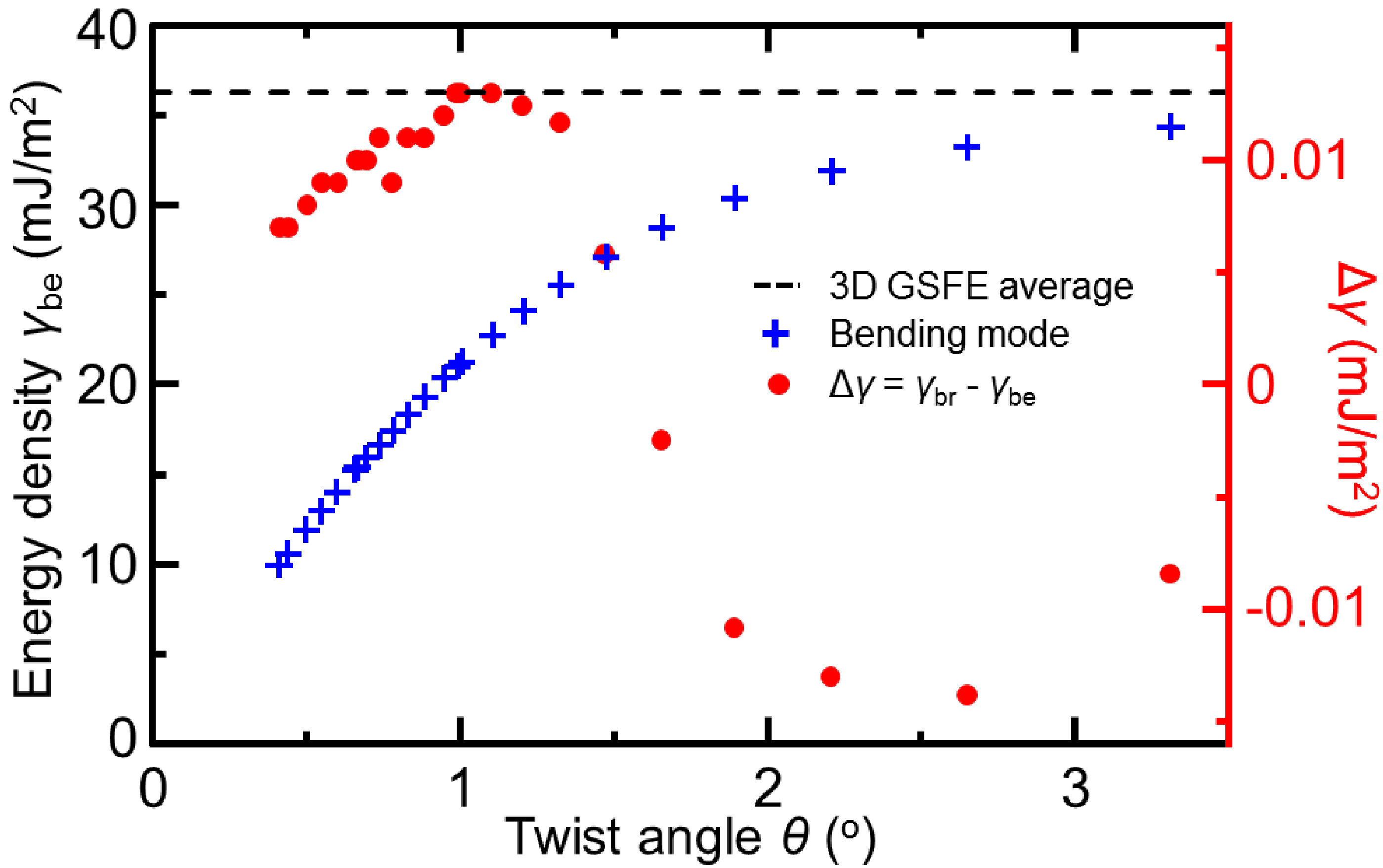


Energy of twisted BLG



- Energy approaches to a constant value (Perfect Moiré, no relaxation)

Energy of twisted BLG



- Energy approaches to a constant value (Perfect Moiré, no relaxation)
- Bending mode is stable for small θ
- Breathing mode is stable when θ gets larger.
- $\theta_c \approx 1.6^o \approx a_0/(2r)$, r is radius of node → Two nodes start to overlap

Conclusions

- **Multiscale model to describe the deformation of bilayer system**

- **Applied to bilayer graphene: accurate description of interlayer defects:**
  - Single Dislocation
    1. Edge component leads to buckling
    2. Buckling reduces the core size and the energy
  - Interlayer Twist

    Breathing mode vs. Bending mode (θ dependence)

- **General approach for defects in multilayer systems**