Poster Presentation : 재료세선 – 저차원 소재

2021년도 한국현미경학회 춘계학술대회

Anisotropic and top-down Cu intercalation in black phosphorus forming angstrom-wide conductive channels

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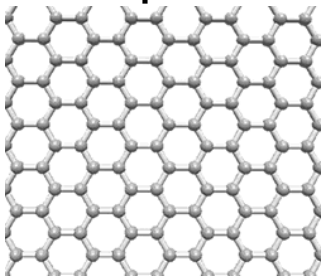
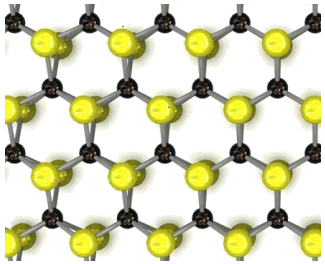
2D black phosphorus

Graphene



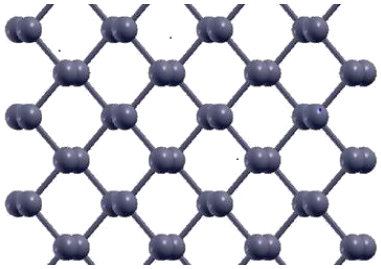
- High mobility (~200,000 $cm^2/V{\cdot}s$)
- Zero band-gap (negligible on/off ratio)

TMD



- Low mobility (~< 200$cm^2/V{\cdot}s$)
- Nonzero band-gap (good on/off ratio)

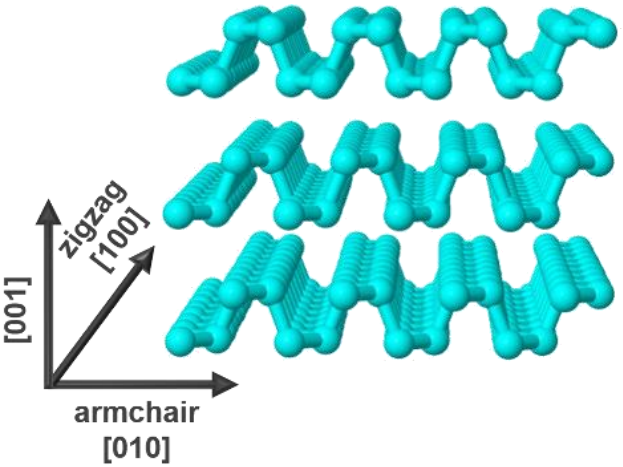
Black phosphorus



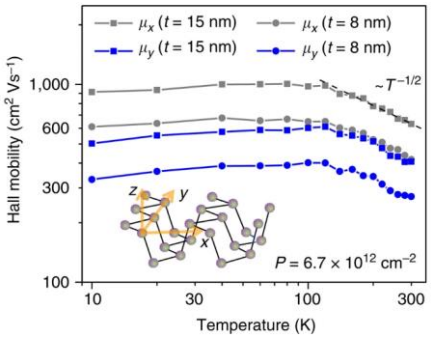
- **High mobility (> 1,000 $cm^2/V{\cdot}s$)**
- **Nonzero Band-gap : 0.3 ~2.0 eV (> 10^4 on/off ratio)**

Anisotropy of black phosphorus

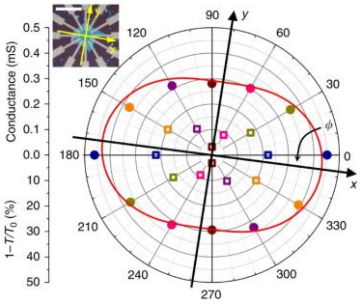
Structure



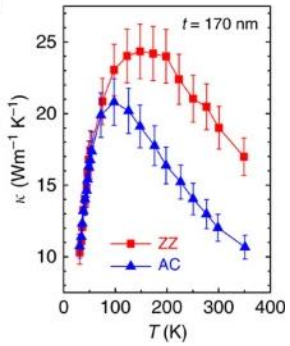
Electronic property



Optical property



Thermal property



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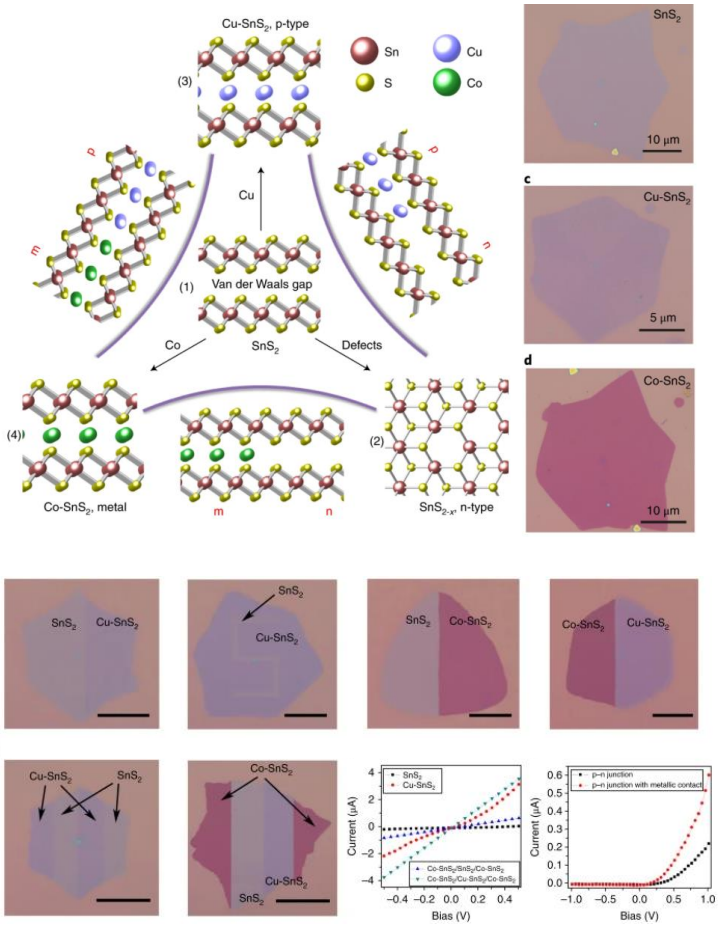
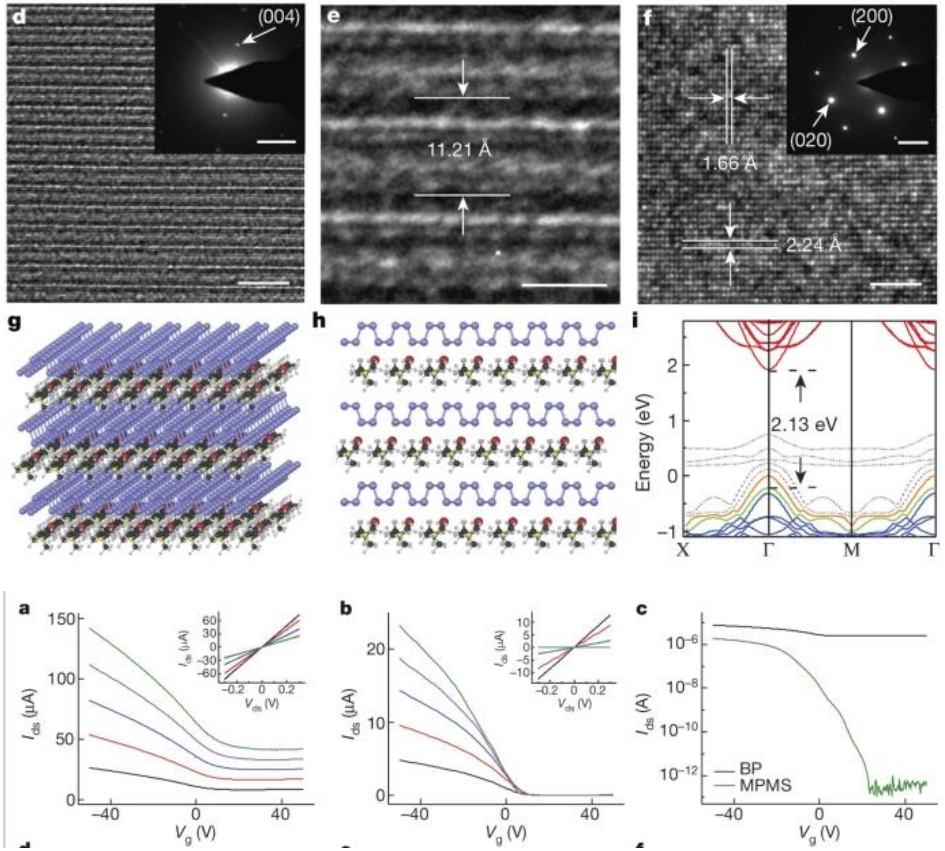
Intercalation in 2D materials





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C. Wang et al. *Nature* **2018**, 555, 231-236

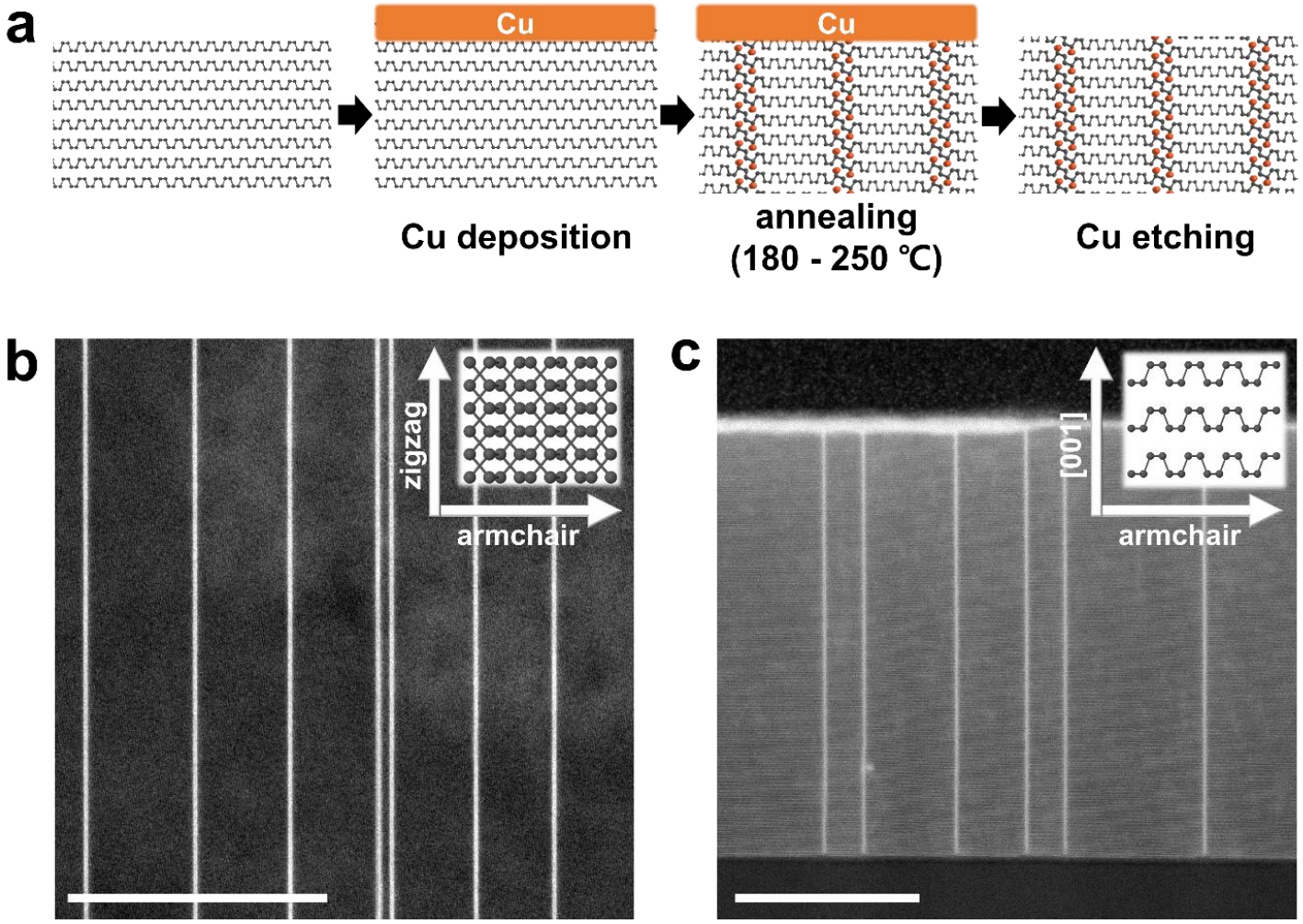


Figure 1. (a) Schematic diagram of the method for Cu intercalation in BP. (b,c) High-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) images in plan-view (b) and cross-sectional view (c) of BP after Cu intercalation. Scale bars are 50 nm.

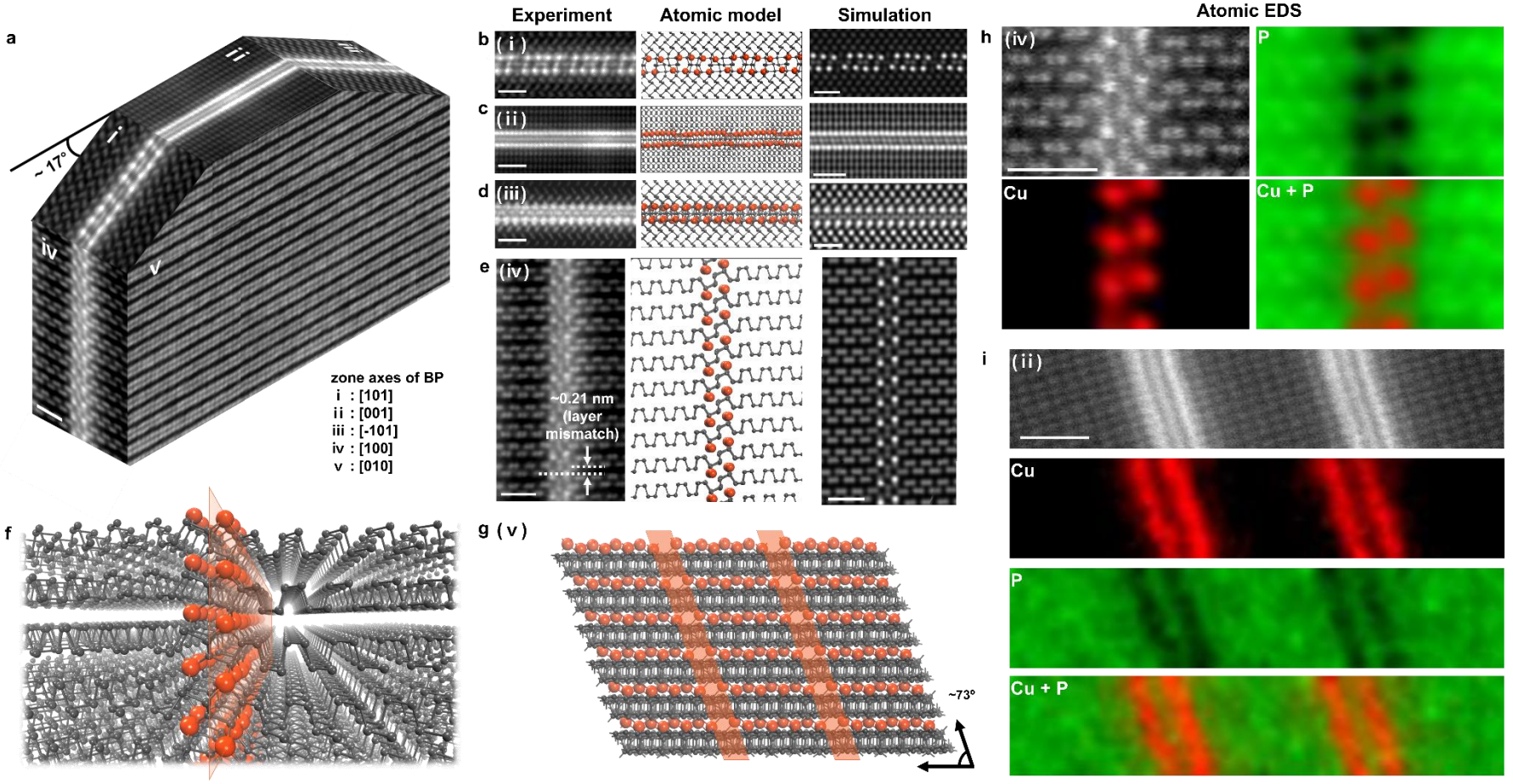


Figure 2. (a) Three-dimensional image constructed from atomic resolution HAADF-STEM images of Cu intercalated BP at five different zone axes of BP. (b-e) HAADF-STEM images (left) with the corresponding atomic models (right) calculated from density functional theory (DFT) at the four zone axes of BP ((c) [101], (d) [001], (e) [$\bar{1}$01], (f) [100]). Scale bars are 1 nm. (f) Perspective atomic model of Cu intercalated BP. (g) Atomic model of Cu intercalated BP at [010] zone axis of BP. (h,i) Atomic resolution energy dispersive X-ray spectroscopy (EDS) mappings at [100] (h) and [001] (i) zone axes of BP. Scale bars are 1 nm.

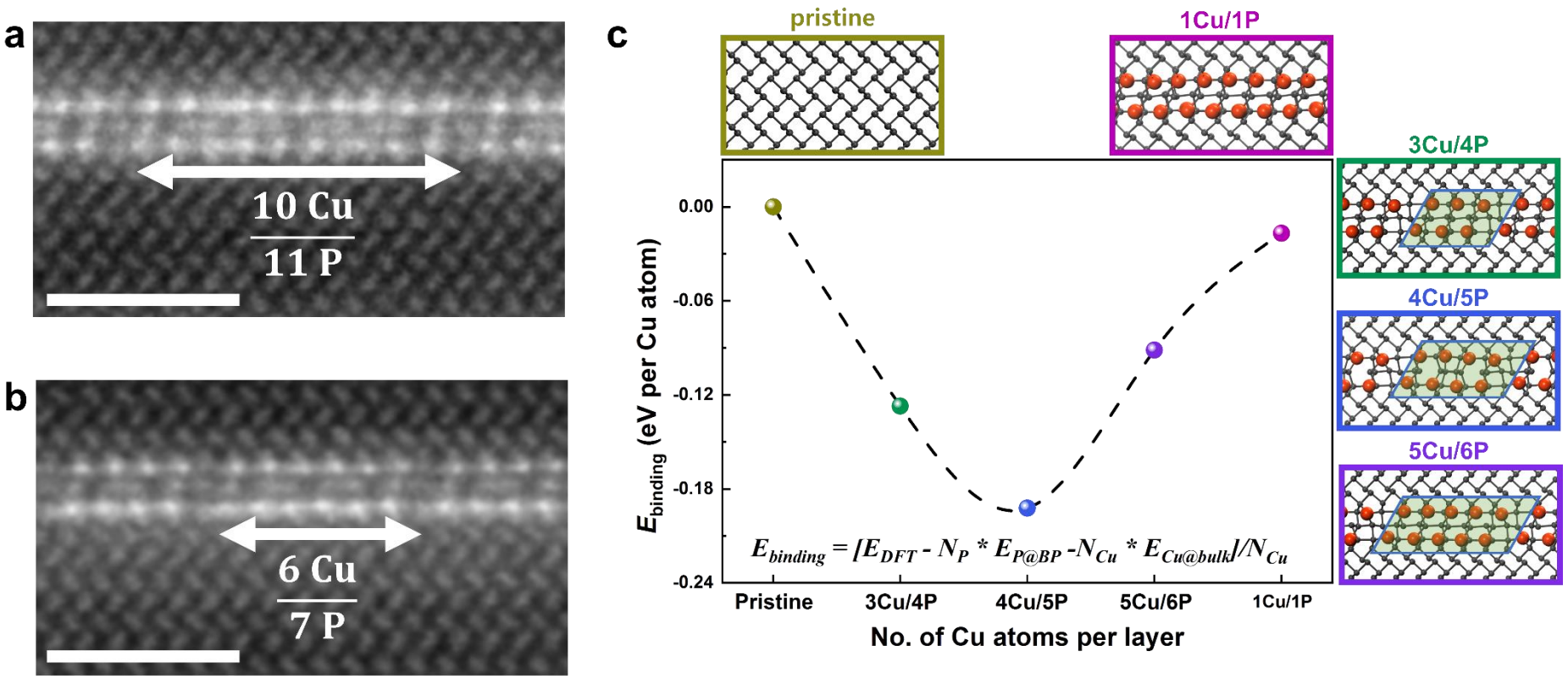
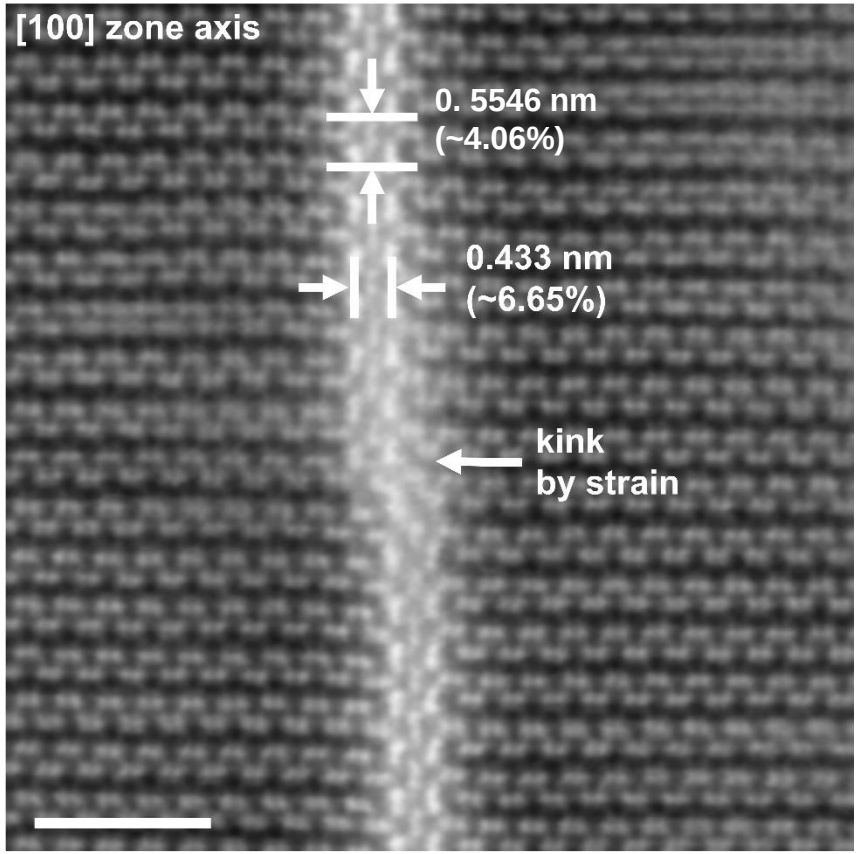
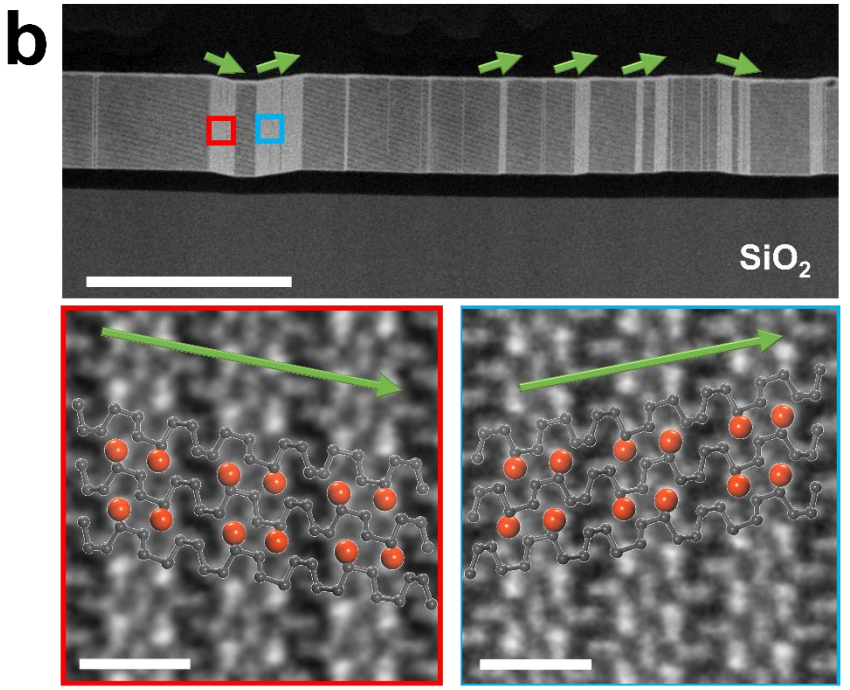


Figure 3. (a,b) HAADF-STEM images of Cu intercalated samples with periodicities where 11th (a) and 7th (b) copper atoms are missing. Scale bars are 2 nm. (c) Calculated Cu binding energies for different periodicities of missing Cu atoms.

Strain



Deformation



$$D \cong 0.21 \cdot |n_{mirror\ A} - n_{mirror\ B}|\ nm$$

D is the height difference caused by deformation resulting from Cu intercalation at the two end surfaces of the region of interest, and $n_{mirror\ A\ (B)}$ is the number of Cu intercalated structures;

Figure 4. (a) Atomic resolution HAADF-STEM image of strain-induced kink formation in a Cu intercalated structure ([100] zone axis). Scale bar is 2 nm. (b) Low magnification (top) and atomic resolution (bottom) HAADF-STEM images of densely Cu intercalated BP in cross-sectional view ([100] zone axis). Scale bars are 200 nm (top) and 1 nm (bottom).

Four different atomic configurations in single crystalline BP

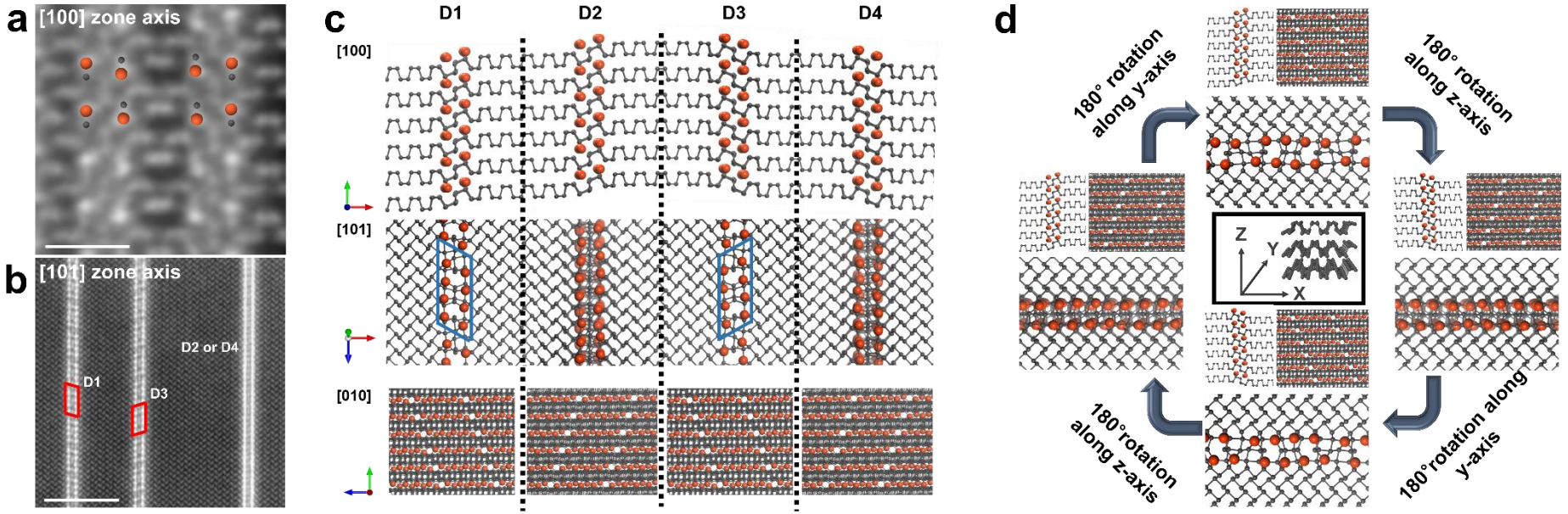


Figure 5. (a) Atomic resolution HAADF-STEM image of two different atomic configurations of the Cu intercalated structure at the [100] zone axis. Scale bar is 1 nm. (b) Atomic resolution HAADF-STEM image showing the three different atomic configurations of the Cu intercalated structure at the [101] zone axis. Scale bar is 5 nm. (c) Atomic models of the four possible atomic configurations of Cu intercalated BP in single crystal of BP. (d) Illustration showing that the four atomic configurations are superimposable through rotation.

Top-down intercalation: rate-limiting process

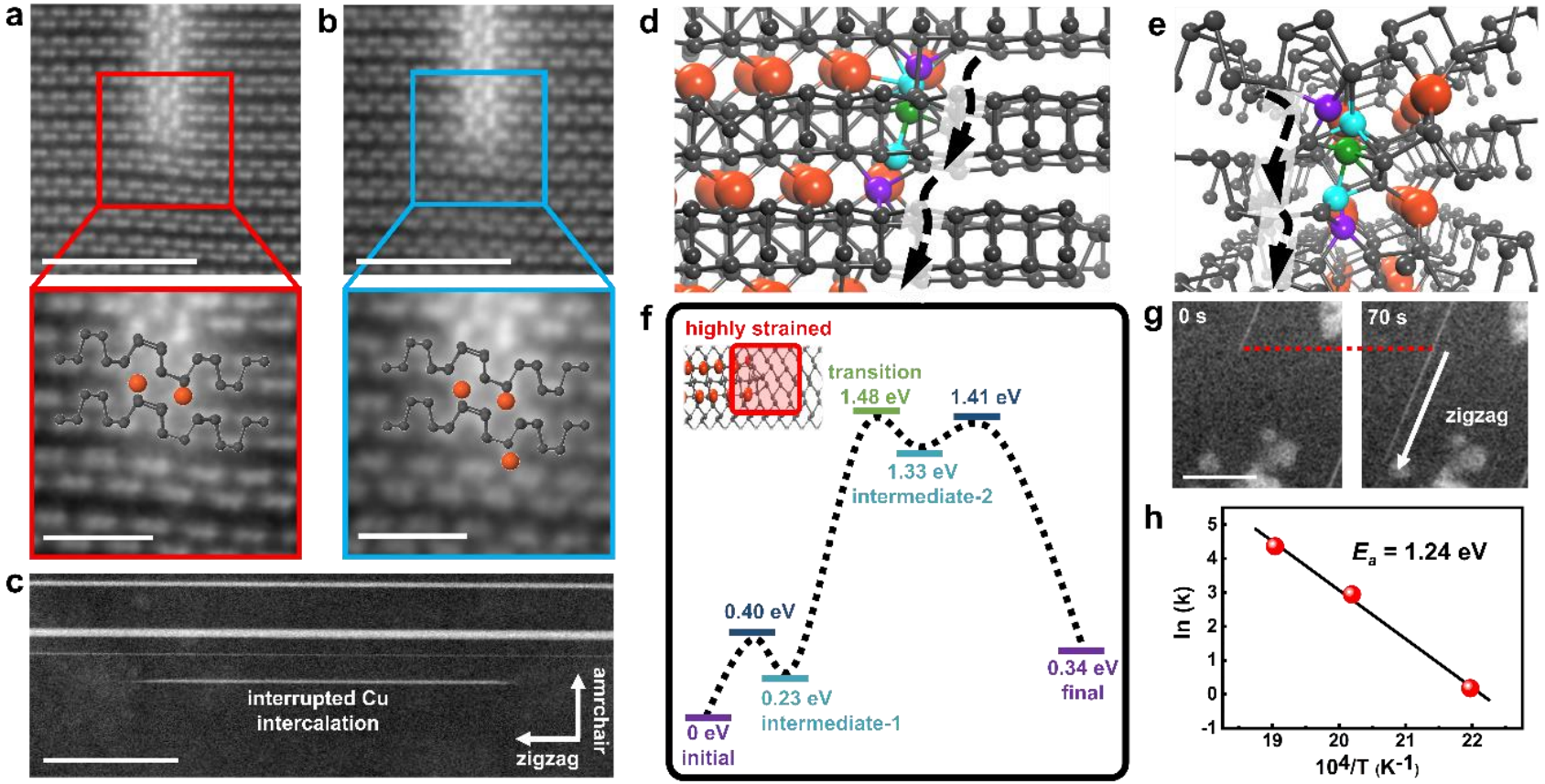


Figure 6. (a-c) HAADF-STEM images of interrupted Cu intercalated structures in cross-sectional view (a,b) and plan-view (c). Scale bars are 3 nm (upper figures of a, b), 1 nm (lower figures of a,b), and 100 nm (c). (d-f) Illustrations (d,e) and corresponding energy barriers (f) of top-down Cu intercalation of strained BP determined from DFT calculations. (g) HAADF-STEM images of Cu intercalation taken during *in situ* heating at 180 ºC. Scale bar is 50 nm. (h) Diffusion rate (log-scale) as a function of inverse of temperature obtained from *in situ* heating experiments.

Angstrom wide conductive channels

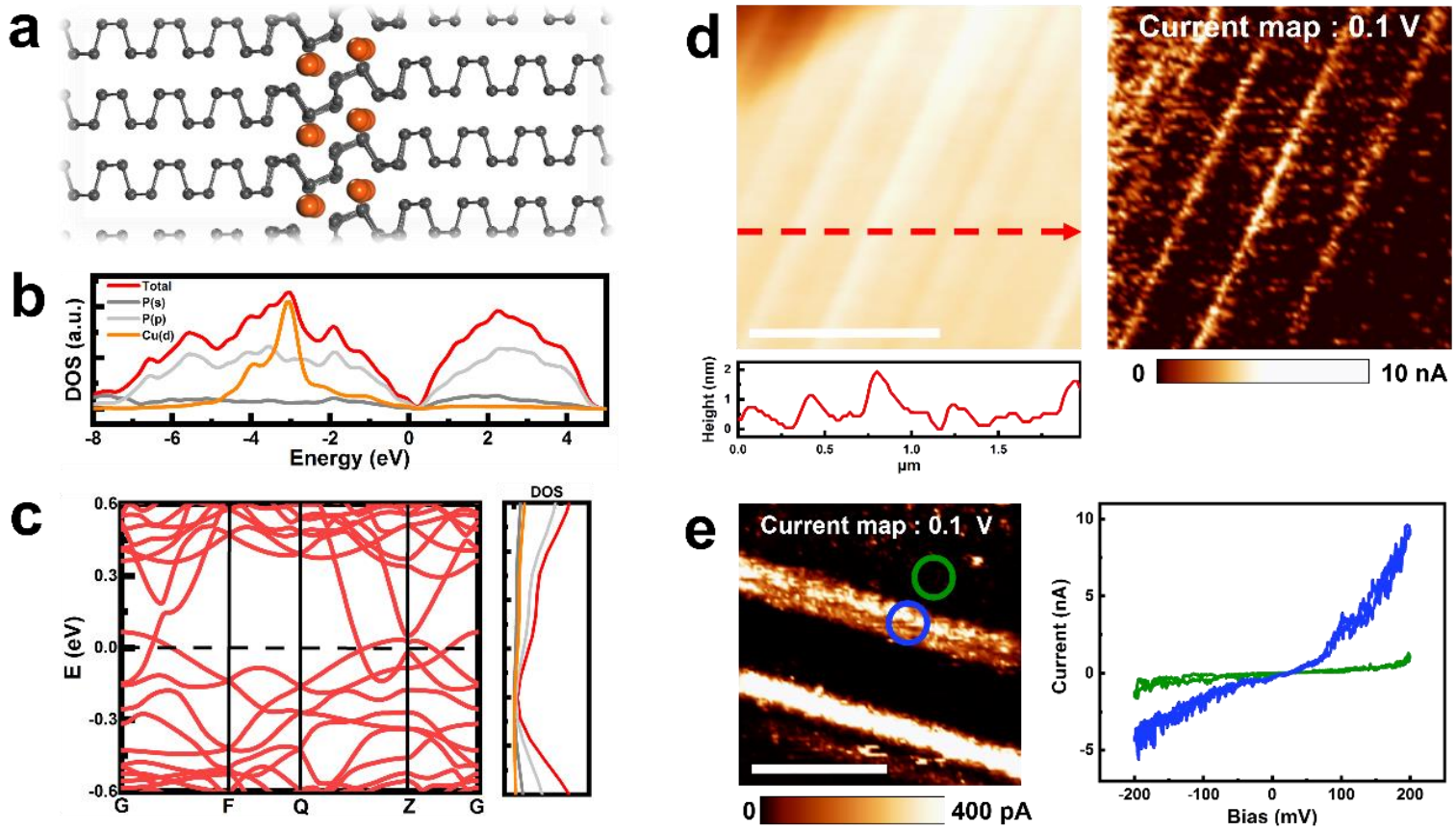


Figure 7. (a) Atomic model used for computational calculation of the density of states (DOS) and the electronic band structure. (b,c) calculated DOS (b) and electronic band structure (c) with the atomic model. (d) Topography and current maps of Cu intercalated BP. Scale bar is 1 μm. (e) a magnified current map (left). Scale bar is 100 nm. *I-V* curves at the location of Cu intercalated region (blue) and BP region (green).

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