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Slip Transmission and Voiding during Slip Band Intersections in $Fe_{70}Ni_{10}Cr_{20}$ Stainless Steels

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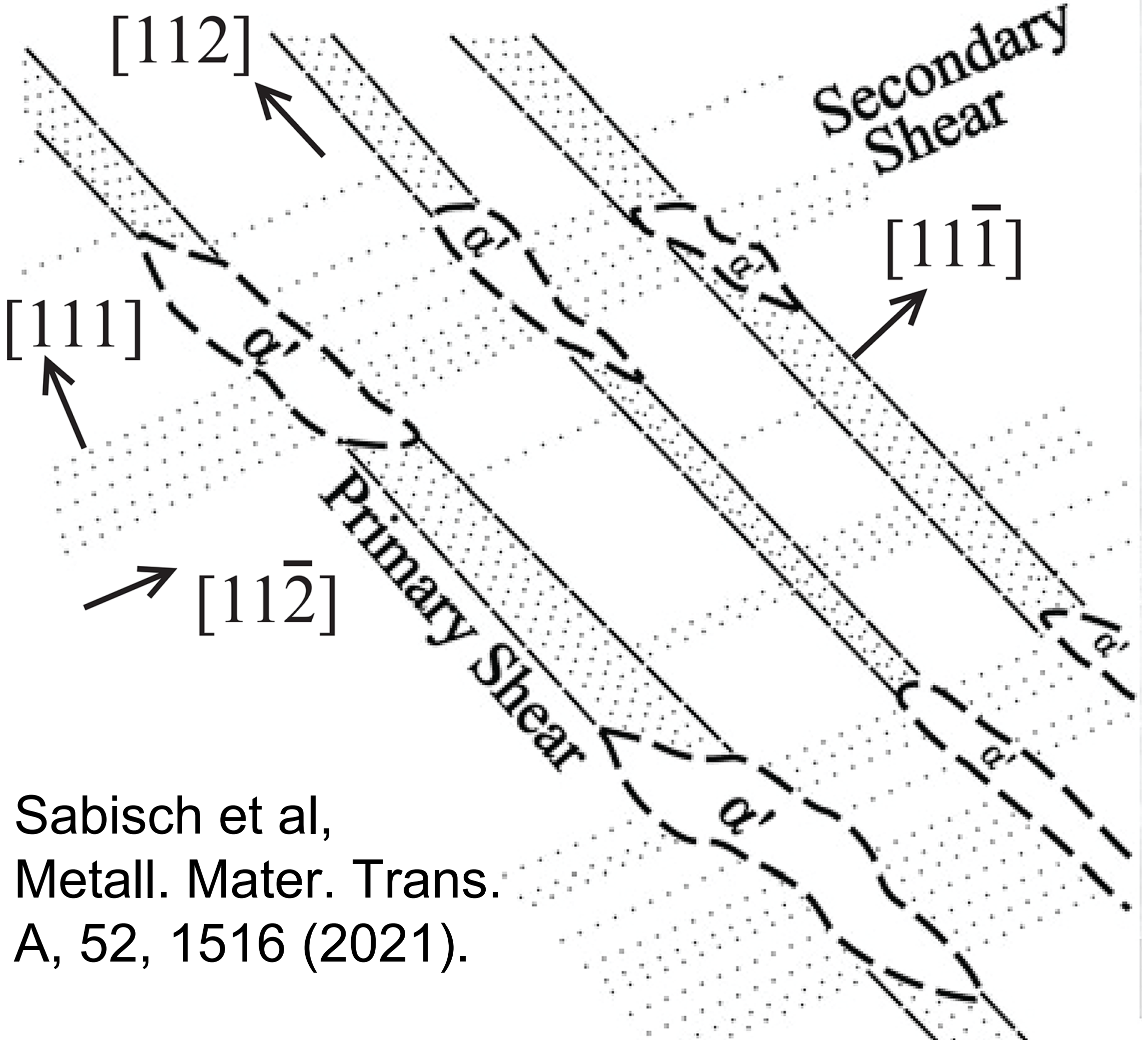
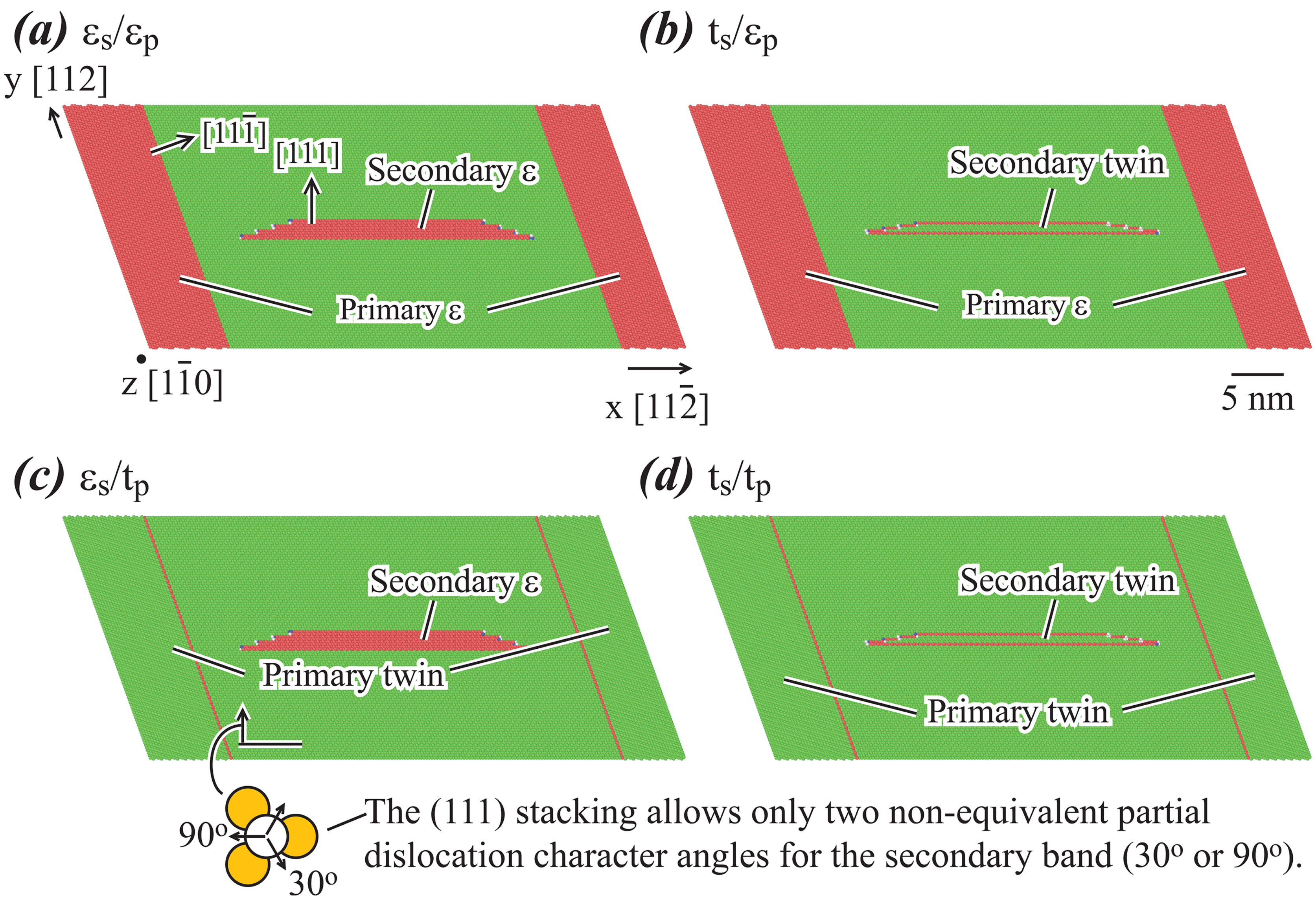
Experimental Observations in Fe-Ni-Cr Stainless Steels



Sabisch et al, Metall. Mater. Trans. A, 52, 1516 (2021).

- ❑ Deformation features slip bands;
- ❑ Hydrogen promotes ε-
- ❑ Slip bands contain twins / ε-martensite;
- ❑ ε → α' martensite at band

Eight Possible Band Intersections



- ❑ Four band combinations $\varepsilon_s/\varepsilon_p$, t_s/ε_p, ε_s/t_p, and t_s/t_p exist, where α_s/β_p represents secondary band α_s hitting primary band β_p (α, β = ε or t for twin);
- ❑ Each secondary band has 30º and 90º dislocation character angles;

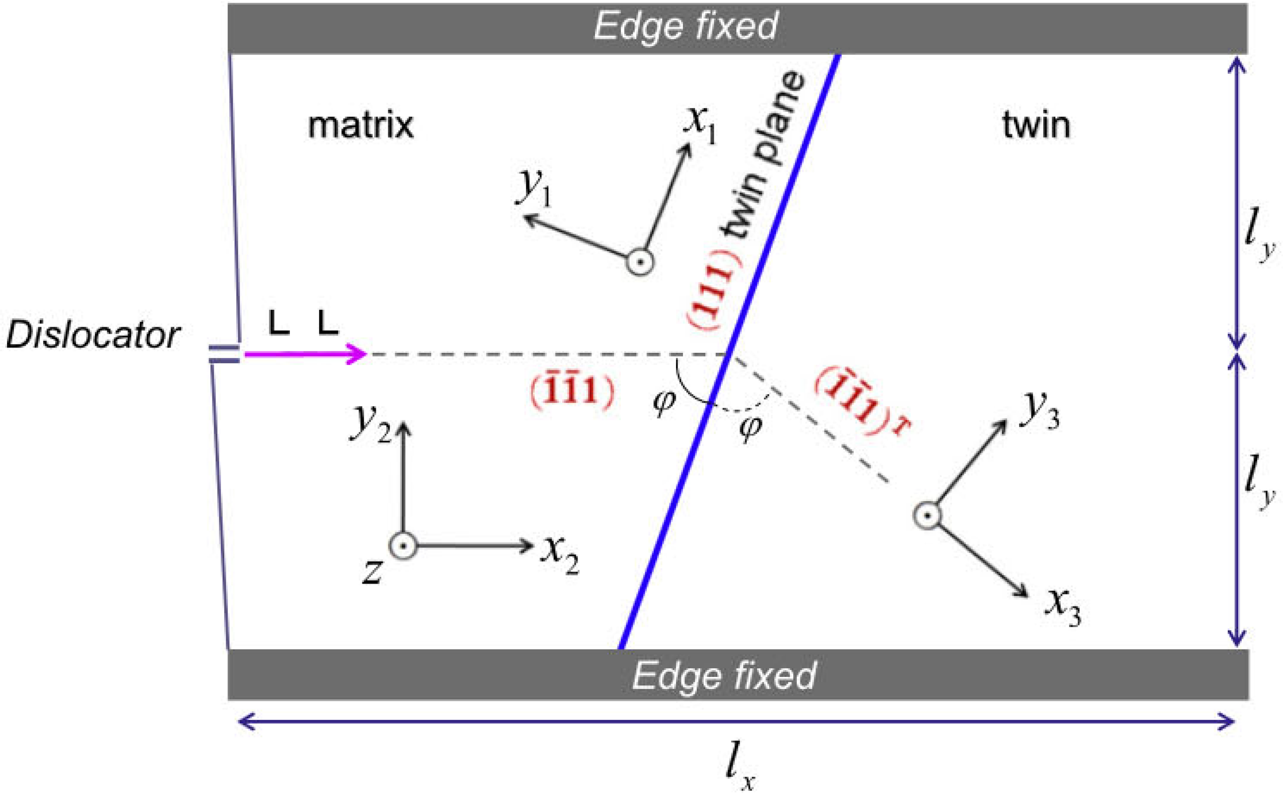
Questions

- ❑ What is the slip transmission propensity order for the eight band intersection processes?
- ❑ What is the voiding propensity order for the eight band intersection processes?
- ❑ Why the ε-martensite becomes α'-martensite when a secondary band penetrates an ε-band?
- ❑ We perform molecular dynamics (MD) simulations to answer these questions.

Literature MD Simulations

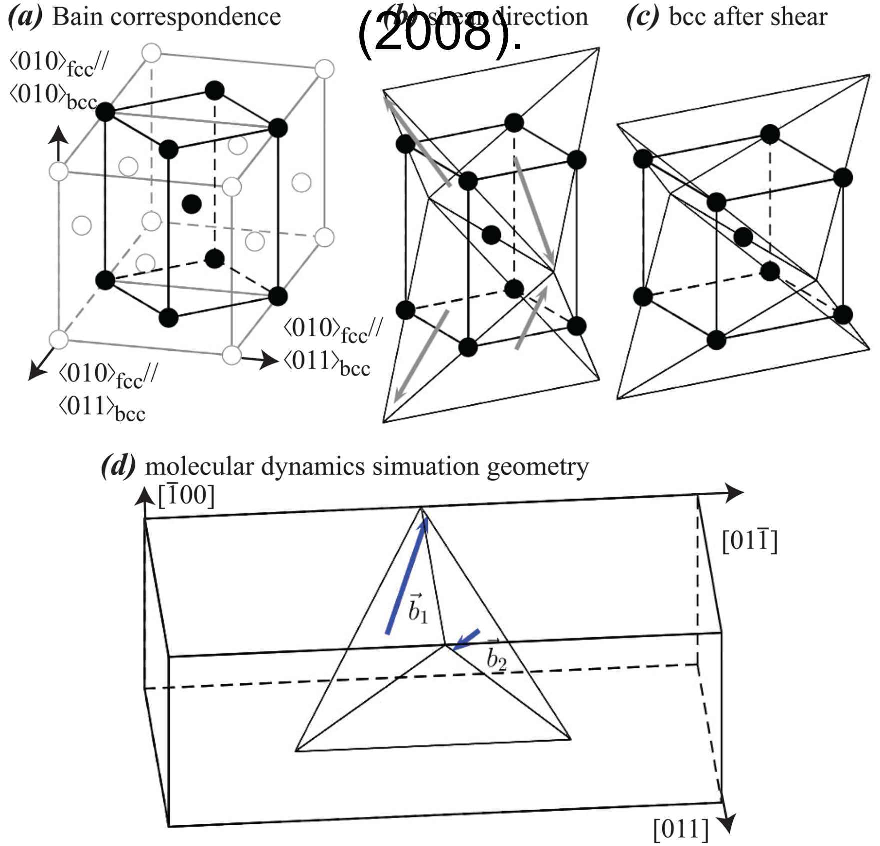
Single Dislocation / Twin Interaction

Jin et al, Acta Mater. 56, 1126 (2008).



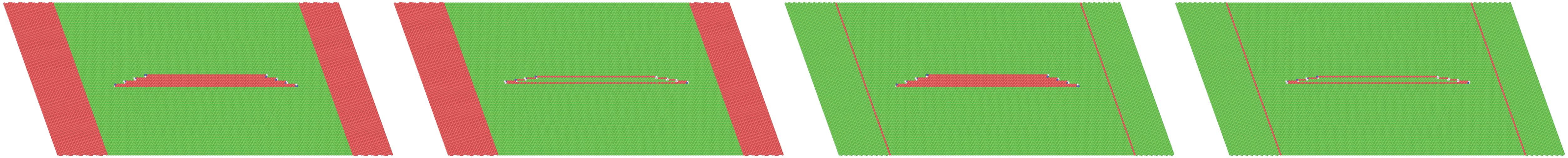
α' (bcc) Formation

Sinclair et al, Acta Mater. 56, 4160 (2008).



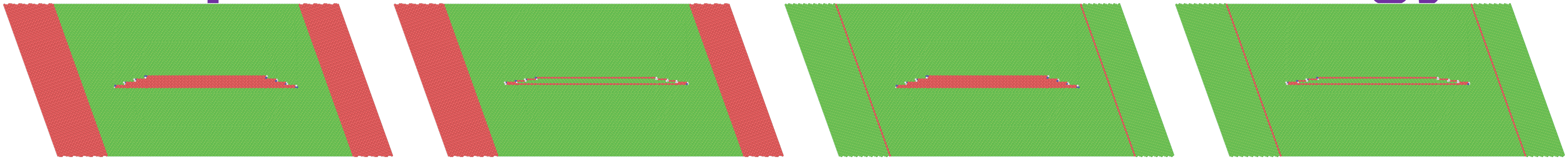
- ❑ Do not study slip band intersections;
- ❑ Enforce artificial shear;
- ❑ Predict wrong orientation

Unique Features of Our MD Simulations



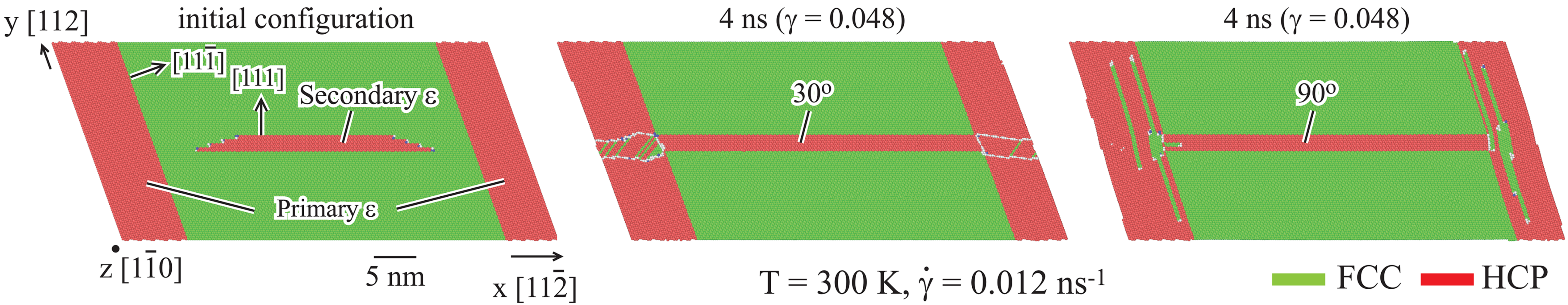
- Use non-orthogonal cells to enforce fully periodic boundary conditions to eliminate artificial surface effects that are present in previous studies;
- Explore all eight possible slip band intersections;
- Identify propensity of both slip transmission and interfacial voiding;
- Predict α’ formation without manual constraints.

Slip Transmission MD Methodology



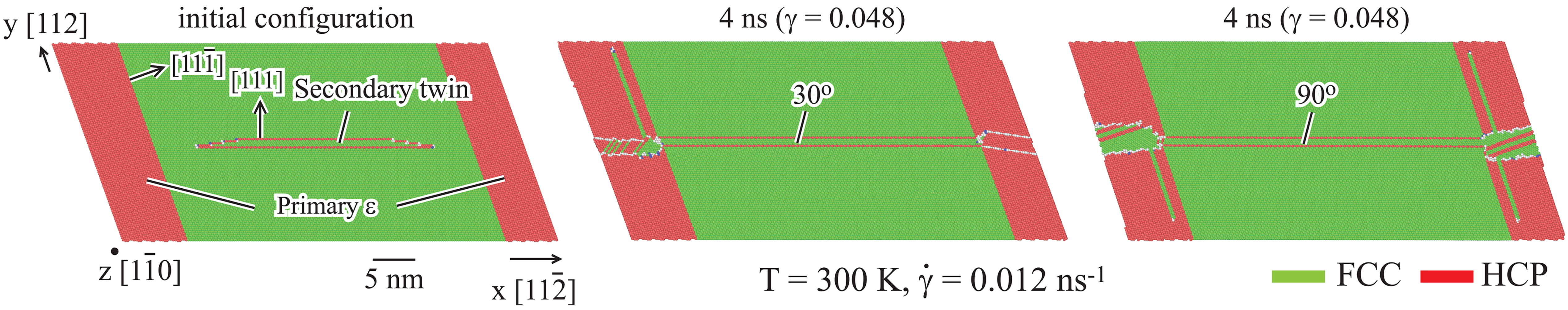
- ❑ Use NVT (constant volume) ensemble;
- ❑ Perform simulations at 300 K for 8 ns;
- ❑ Apply shear strain-controlled method at a shear strain rate of 0.012 /ns with the shear direction parallel to the Burgers vector;
- ❑ The shear strain rate is modeled in segments: a 0.00192 instantaneous shear strain is applied every 0.16 ns to enable time-averaged shear stress to be calculated for each segment;

ε-to-ε Transmission



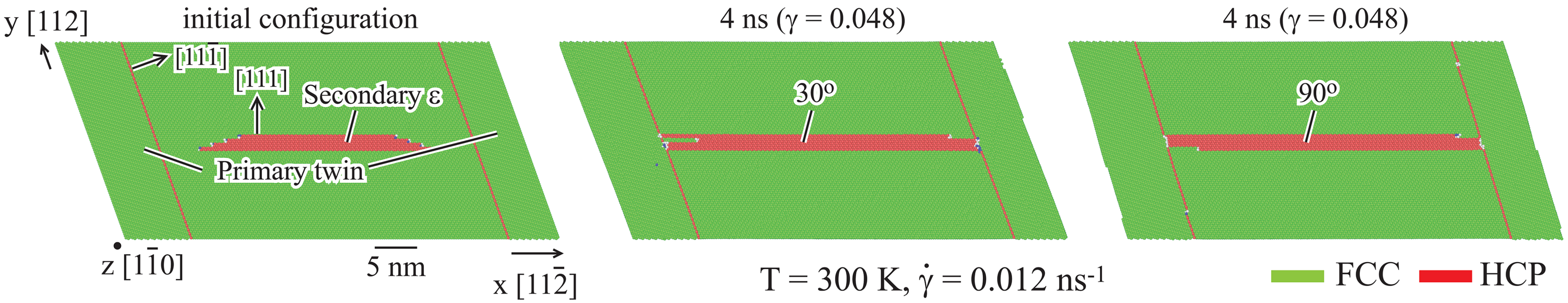
- ❑ Our MD algorithm is able to capture the expansion of the secondary ε-band and its collision with the primary ε-band;
- ❑ Regardless of the character angle (30°, 90°), the secondary ε-band is seen to transmit into the primary ε-band at a shear strain of 0.048;
- ❑ The transmission mode depends on the character angle

Twin-to-ε Transmission



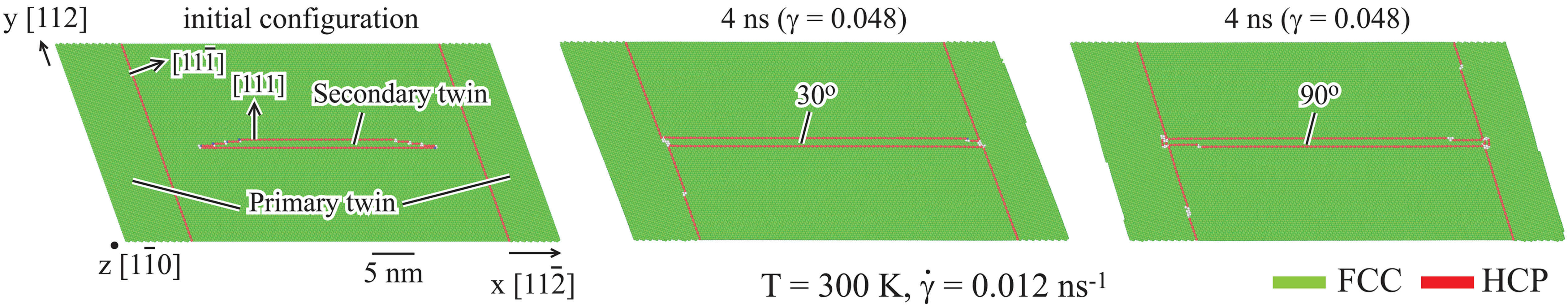
- ❑ Our MD algorithm is able to capture the expansion of the secondary twin-band and its collision with the primary ε-band;
- ❑ Regardless of the character angle (30°, 90°), the secondary twin -band is seen to transmit into the primary ε-band at a shear strain of 0.048;
- ❑ The transmission mode depends on the character angle

ε-to-Twin Transmission



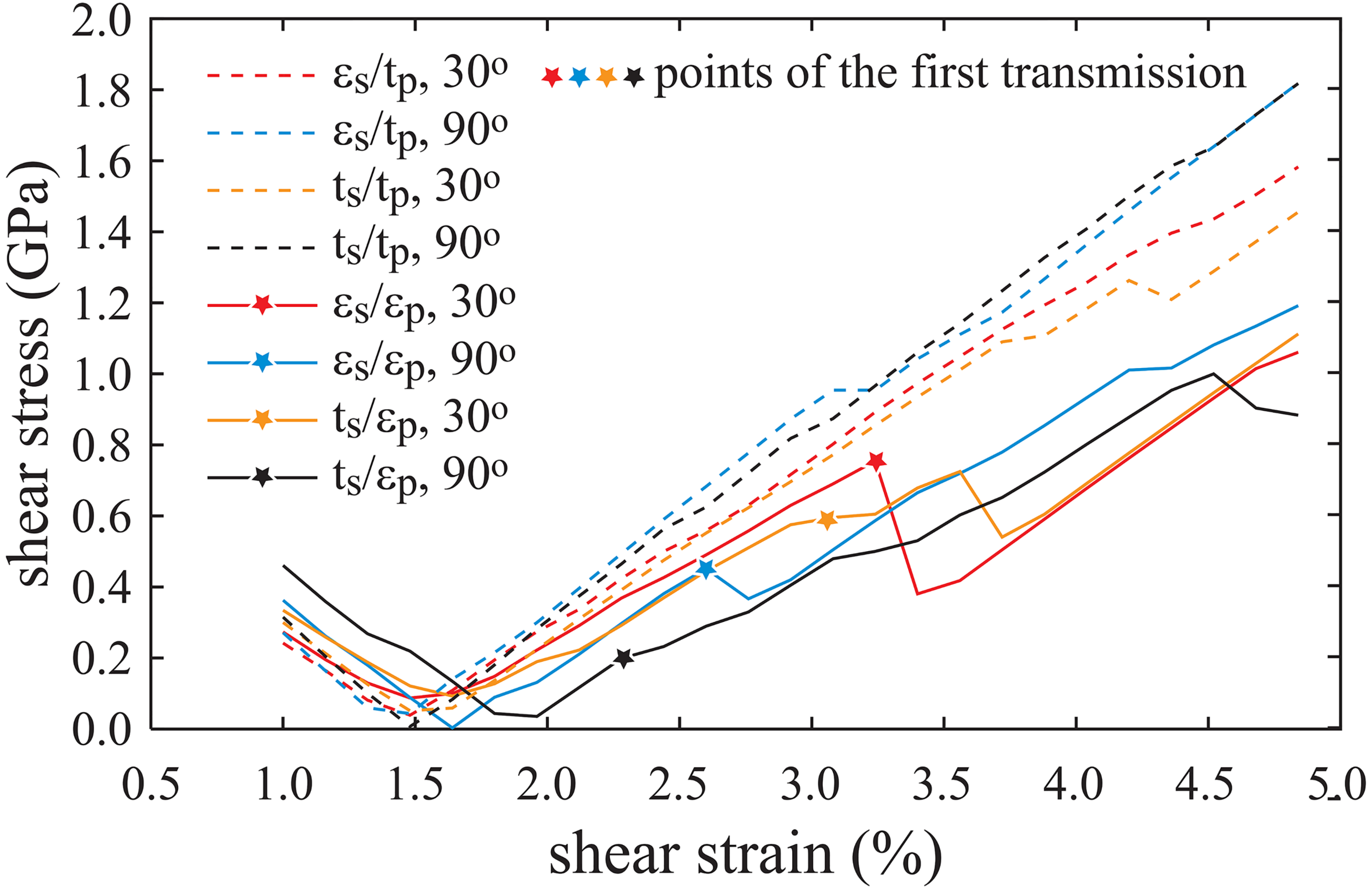
- ❑ Our MD algorithm is able to capture the expansion of the secondary ε-band and its collision with the primary twin-band;
- ❑ Regardless of the character angle (30º, 90º), the secondary ε-band is seen to unable to transmit into the primary twin-band at the shear strain of 0.048.

Twin-to-Twin Transmission



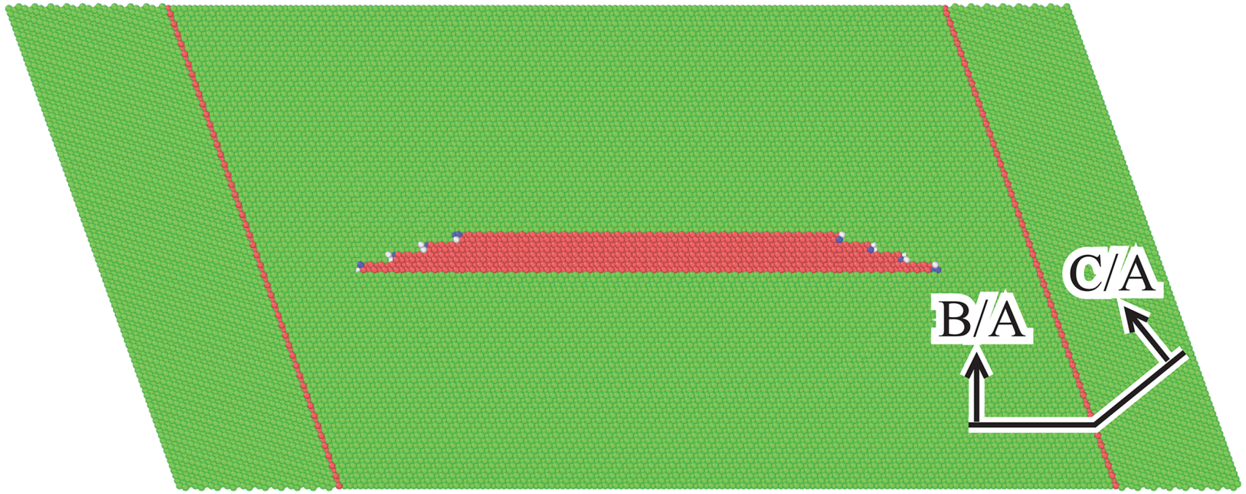
- Our MD algorithm is able to capture the expansion of the secondary twin-band and its collision with the primary twin-band;
- Regardless of the character angle (30º, 90º), the secondary twin -band is seen to unable to transmit into the primary twin-band at the shear strain of 0.048.

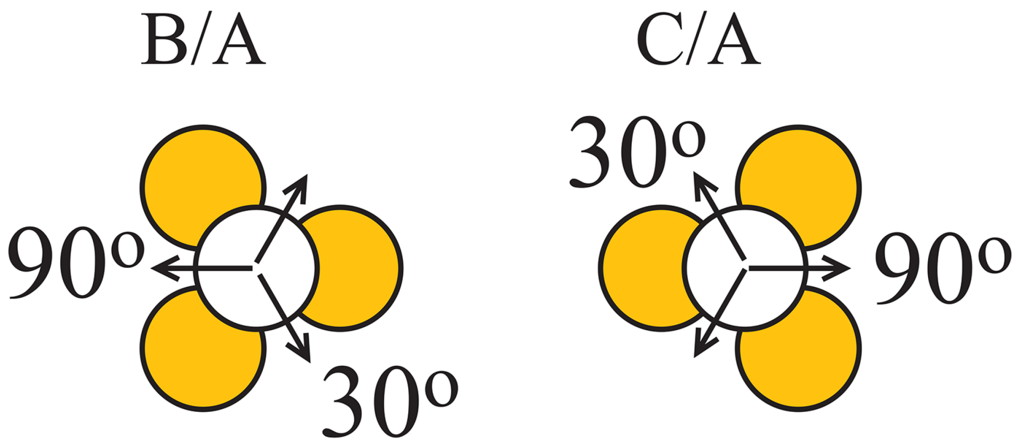
Stress-Strain Curves for all 8 Intersections



- ❑ Regardless of the secondary band type, intersection with ε-band produces lower stresses;
- ❑ The stress drops correlate well with transmission events;
- ❑ Transmission into ε-band is easier than into

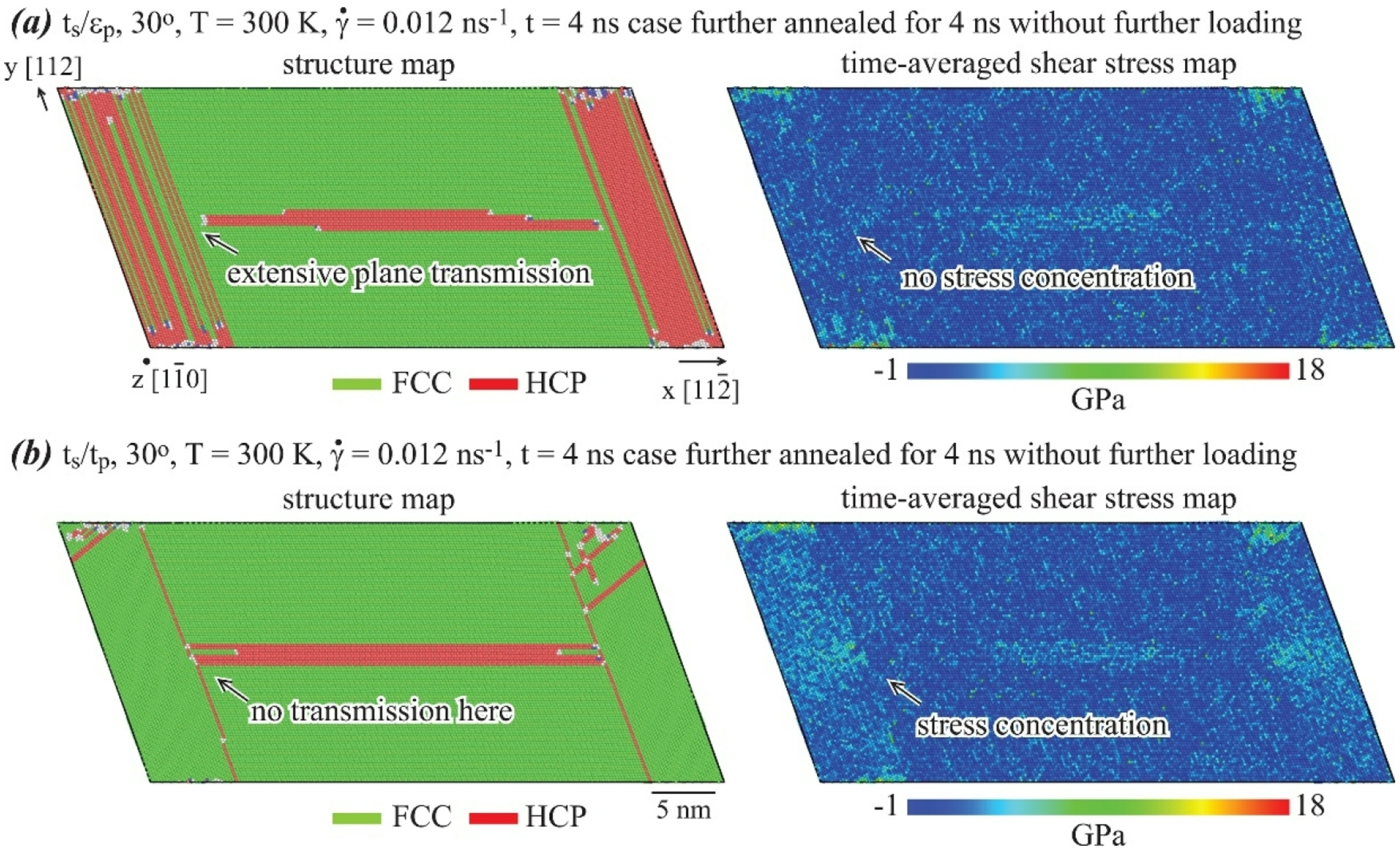
Transmission Pathways into twin





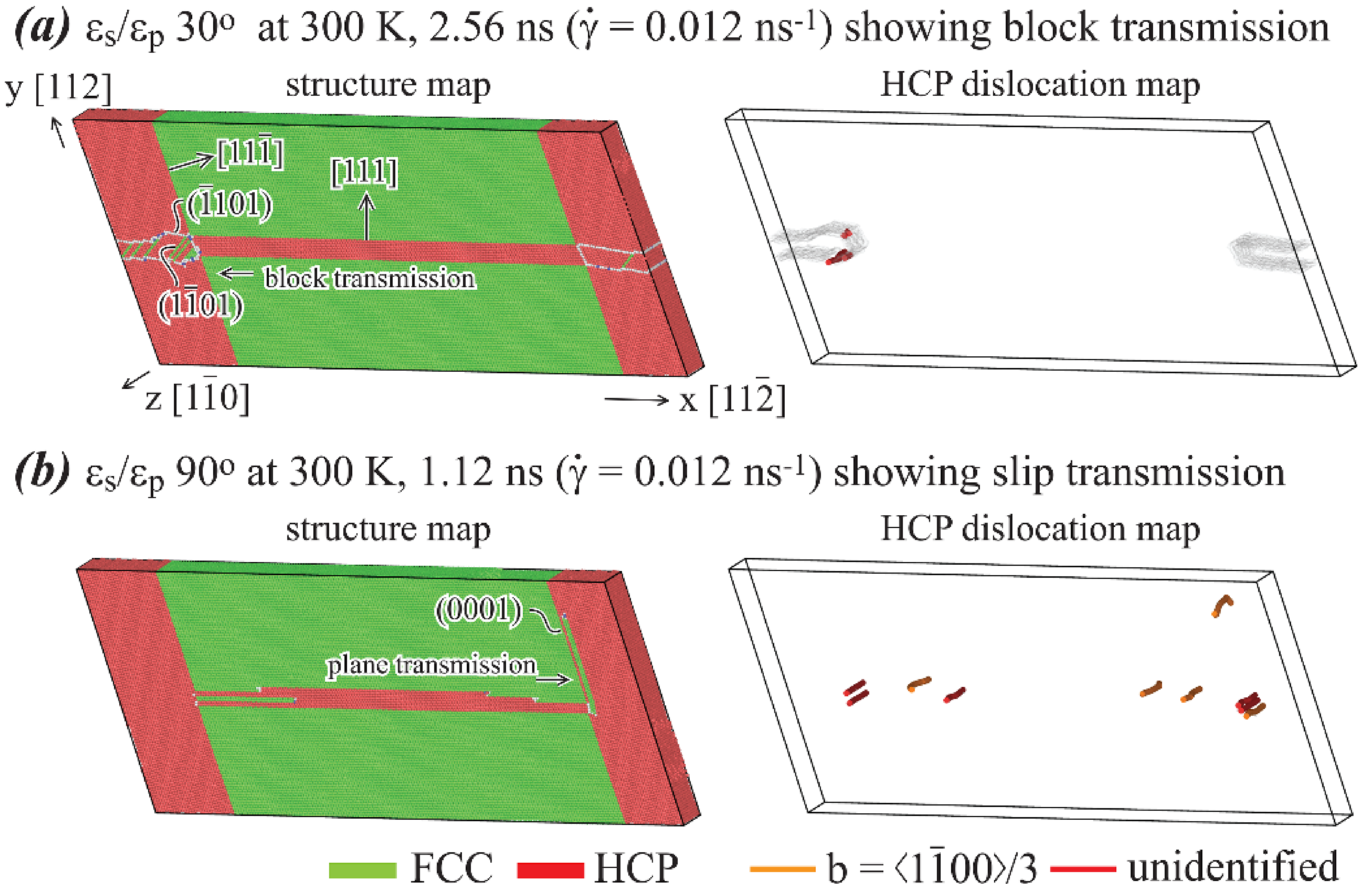
- The {111} stacking in matrix and twin regions is B-on-A (B/A) or C-on-A (C/A) respectively;
- Top-views of stackings indicate that the Burgers vectors of partial dislocations in B/A and C/A stackings are anti-aligned;
- The lack of more aligned slip pathways accounts for the difficulties to transmit into twin-bands.

Stress Concentration



- ❑ Hitting ε bands causes no stress concentration;
- ❑ Hitting twin bands causes stress concentration;
- ❑ These agree with slip pile-ups and transmission.

Transmission Mechanisms

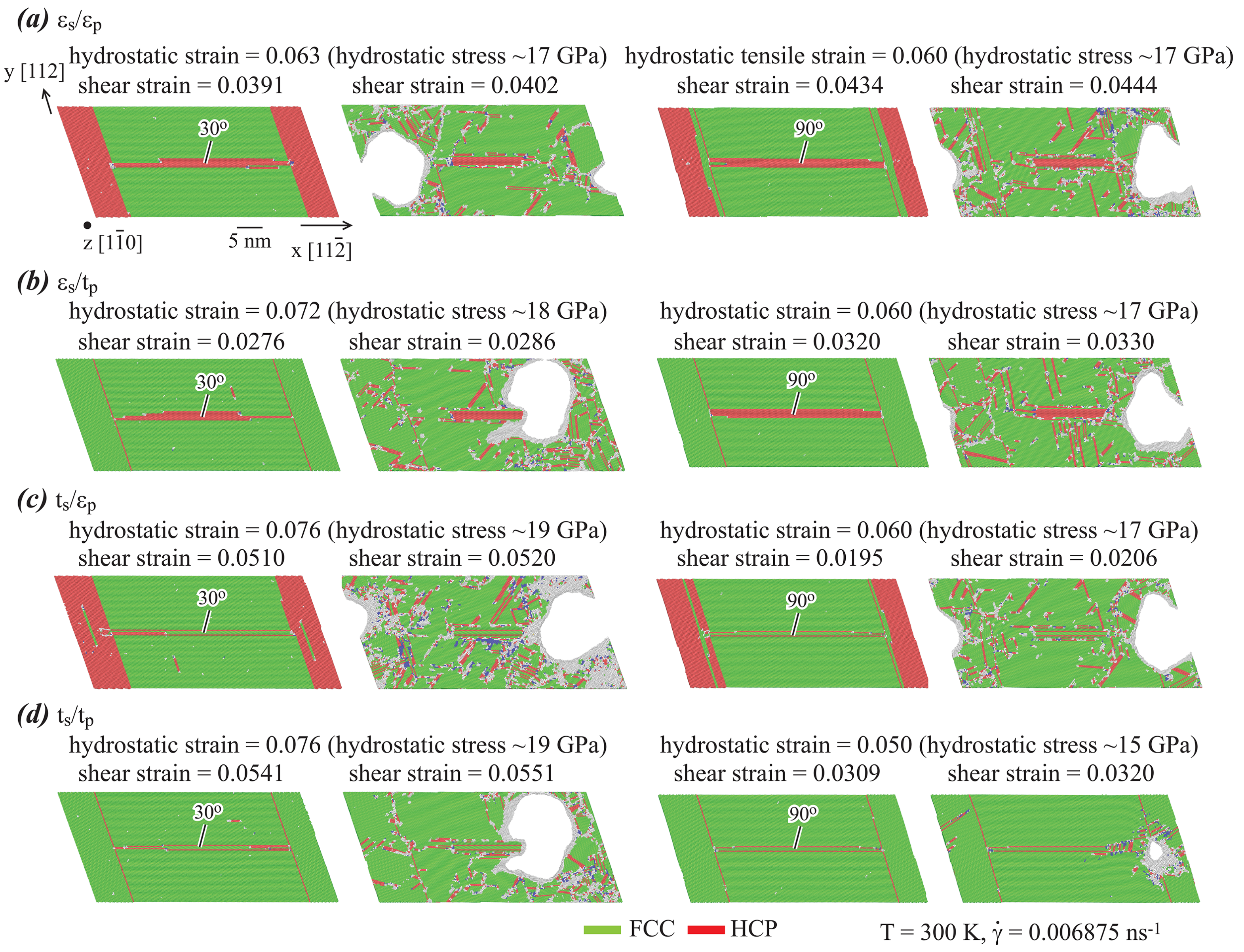


- ❑ Slip transmission occurs through plane and block mechanisms;
- ❑ Both mechanisms involve migration of dislocation;

Voiding MD Methodology

- MD time/length scales do not allow simulation of voiding under realistic conditions;
- Instead, we focus on identifying relative voiding propensities for the eight slip band intersection processes;
- The same shear straining simulations as used in transmission studies are used here except at a reduced strain rate of 0.006875 /ns;
- A constant hydrostatic tensile strain is added during the shear simulations to help voiding. If voiding does not occur, the tensile strain is progressively increased in small increments;
- The combination of tensile / shear strains for the onset of voiding is used to rank the relative voiding propensities.

Voiding MD Results

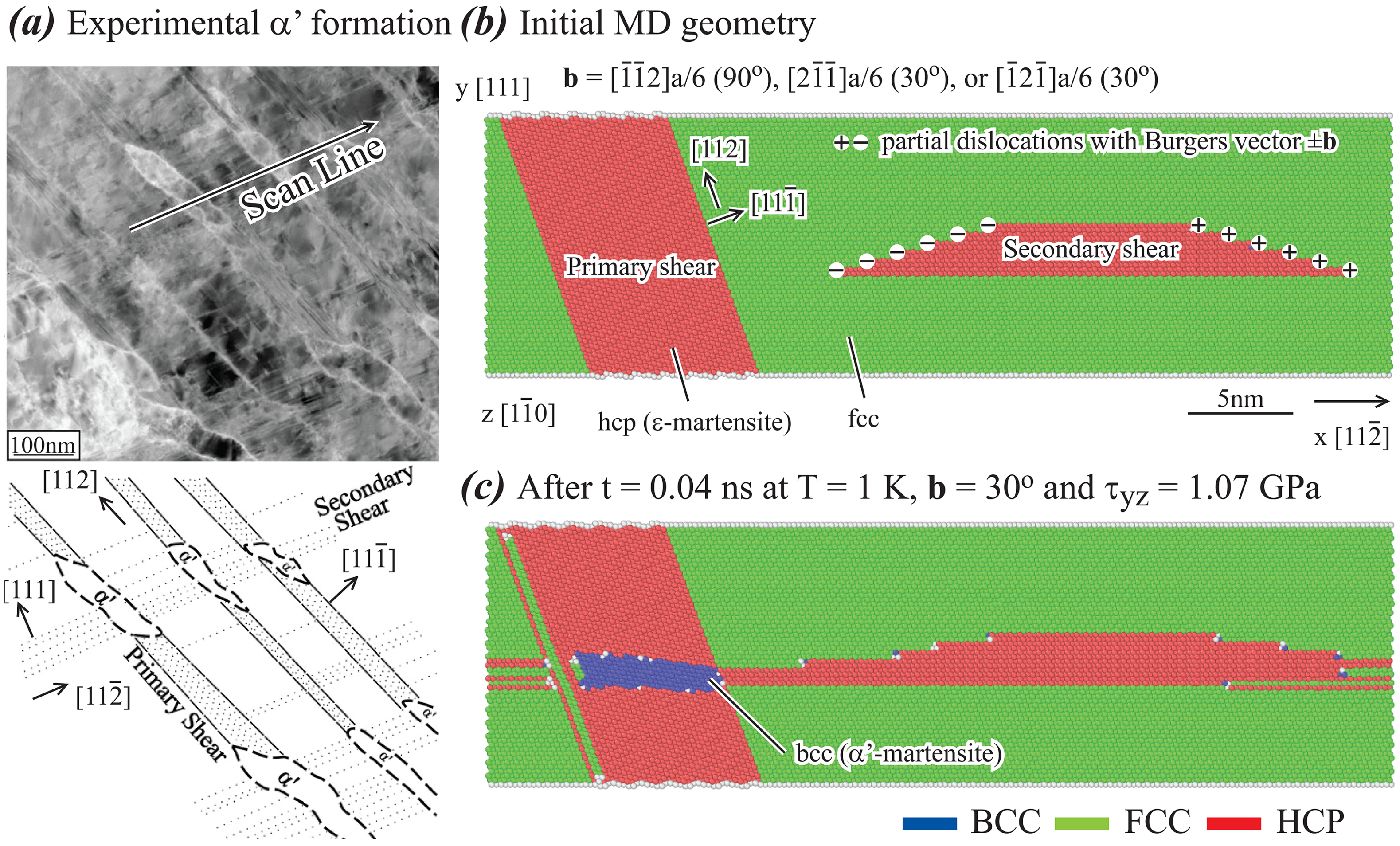


less difficult ↔ more difficult

t_s/t_p-90°, t_s/ε_p-90°, ε_s/t_p-90°, $\varepsilon_s/\varepsilon_p$-90°, $\varepsilon_s/\varepsilon_p$-30°, ε_s/t_p-30°, t_s/ε_p-30°, t_s/t_p-30°

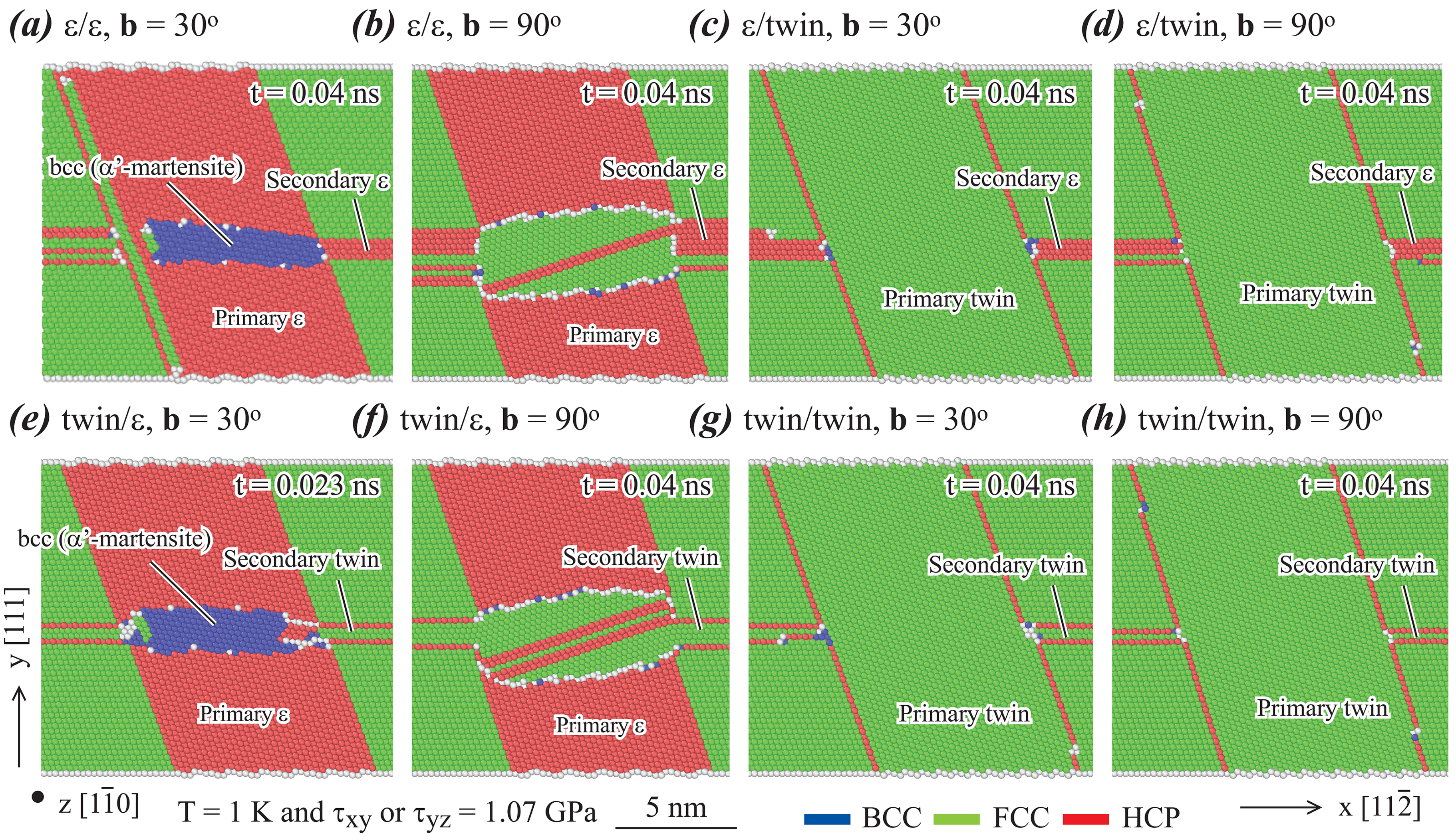
- ❑ All voiding occurs at the band intersection interfaces;
- ❑ Voiding more easily occurs when the secondary band has edge dislocations.

MD Prediction of α' Formation in ε-primary band



- ❑ Other than the two slip bands inserted, our simulations do not have any constrains;
- ❑ We predict the formation of α' at $\varepsilon_s/\varepsilon_p$ intersections;
- ❑ We find $[11\bar{1}]_\gamma$ // $[0001]_\epsilon$ // $[1\bar{1}0]_{\alpha'}$, $[1\bar{1}0]_\gamma$ // $[11\bar{2}0]_\epsilon$ // $[111]_{\alpha'}$, in agreement with experiments.

MD Prediction of α' Formation in All Eight Band Intersections



- ❑ α' always forms if the primary band is ε;
- ❑ α' does not form if the primary band is not ε;
- ❑ We are studying the reason for this phenomenon

SUMMARY

1. MD simulations have been used to study all eight slip band intersections in $Fe_{90}Ni_{10}Cr_{20}$ stainless steels;
2. Slip is found to transmit into ε-bands more easily than twin-bands. This is because twin bands do not provide transmission pathways;
3. Voiding always occurs at the slip intersection regions;
4. Voiding more easily occurs when the impinging (secondary) band is associated with edge dislocations rather than the 30^o dislocations;
5. MD predicts α' formation when slip penetrates ε-bands. No α' formation is observed when slip penetrates twin-bands;
6. The predicted orientation relations between α', γ, and ε agree with experiments.