# Helium bubble growth in tungsten nanotendril

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# Outline

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I. Background of tungsten fuzz formation and nano-tendril structures

II. Computational model

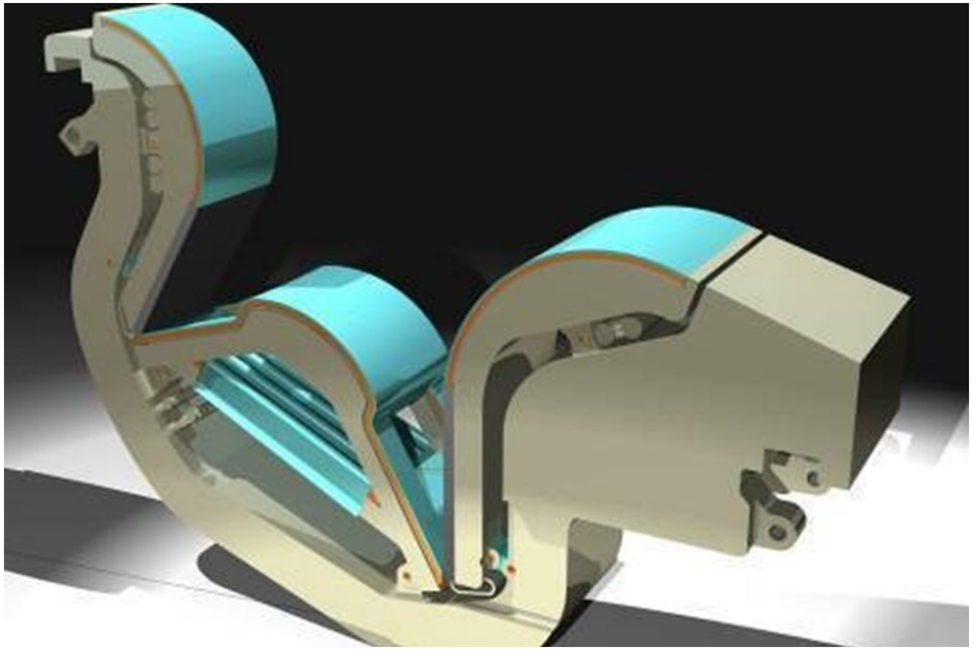
III. Results and discussions

III. Summary

# Tungsten: a promising PFM

## Extremely harsh environment

- H/He plasma (0-100 eV)
- Neutron: 14 MeV
- High heat flux (10 $MW/m^2$)



ITER divertor cassettes

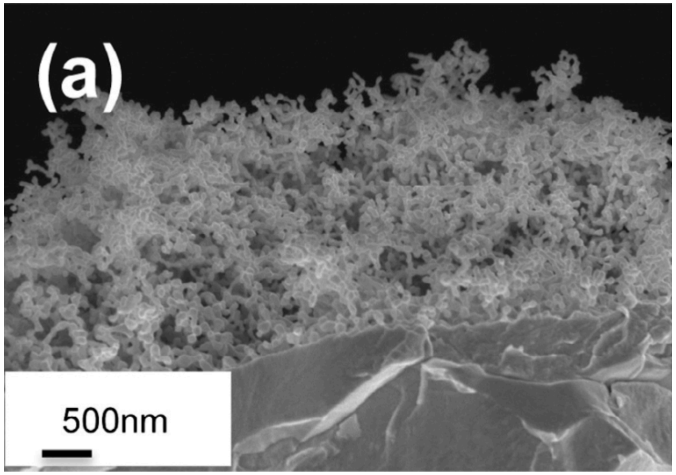
## Issues

- Surface damage: hydrogen induced blistering; helium induced fuzz formation
- Degradation of mechanical properties
- Melting

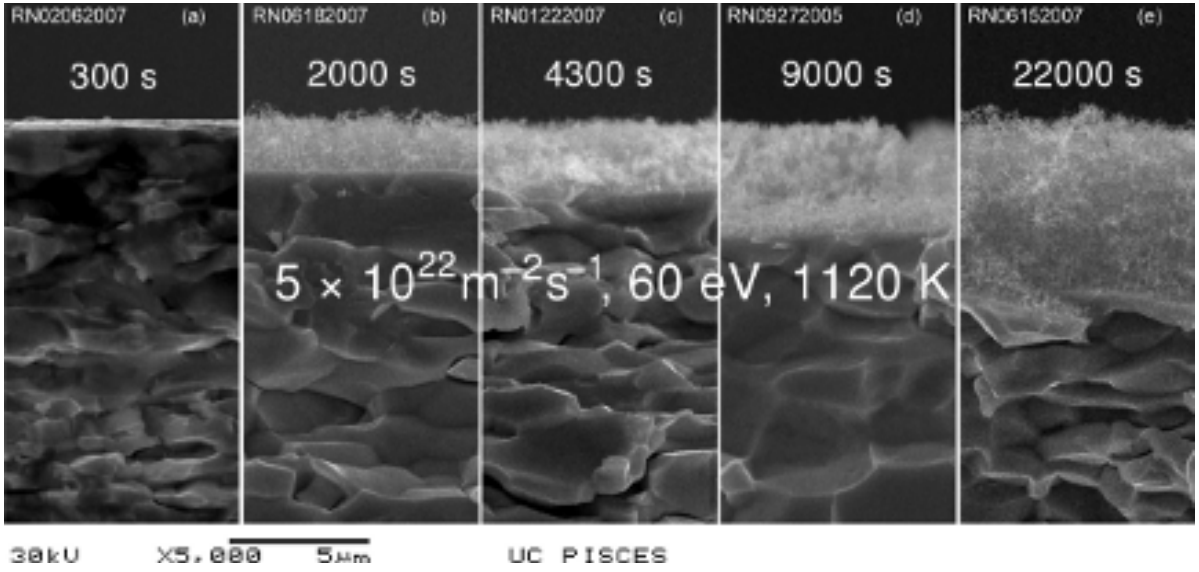
# Fuzz formation by low-energy He irradiation

## Formation conditions

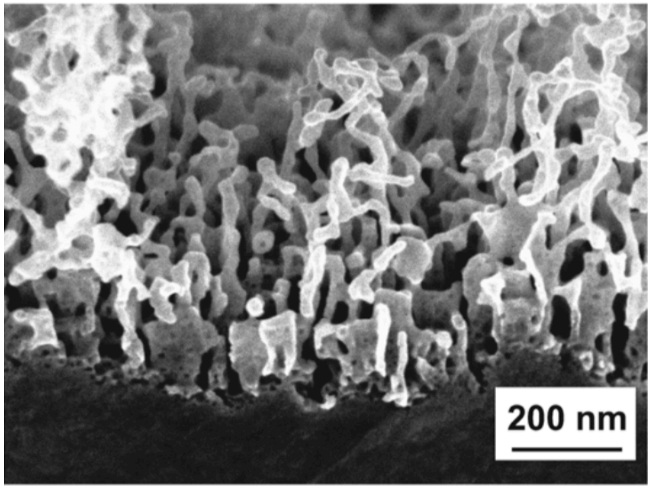
- Temperature: 900 – 2000 K
- He energy threshold: ~ 30 eV
- Fluence > $10^{24}$ $m^{-2}$ when $E_{He}$=50-80eV
- Thickness: up to several micrometers
- Fuzz layer growth dynamics: $\propto \sqrt{t}$




De Temmerman, et al.
*J. Nucl. Mater.* 438: S78–S83 (2013).



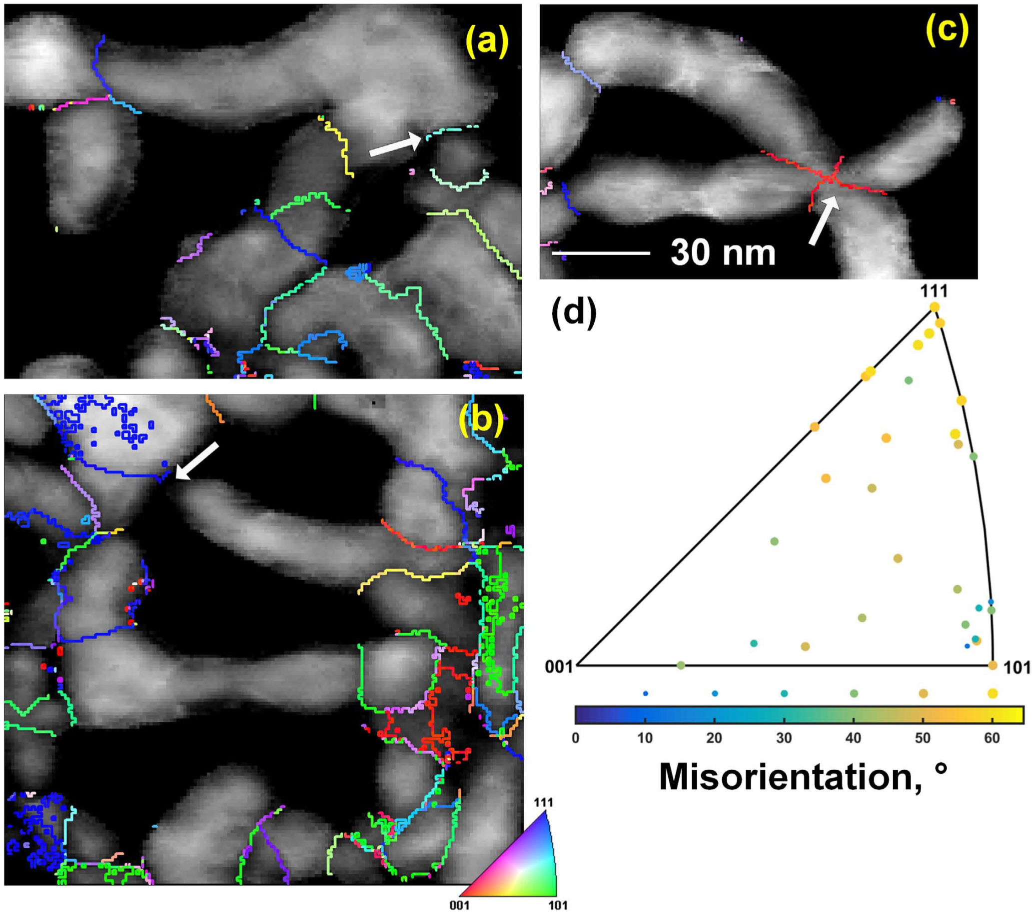

M. J. Baldwin, et al. J. Nucl. Mater. 390–391: 886 (2009)

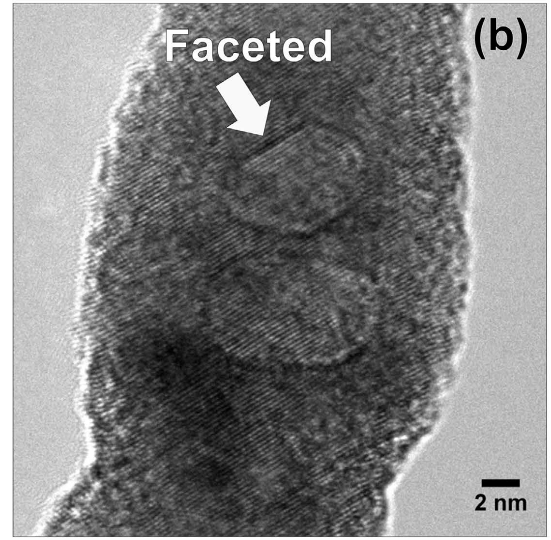



Kajita, Nucl. Fusion, 49 (2009) 095005

# ➢ Microstructures of nanotendrils





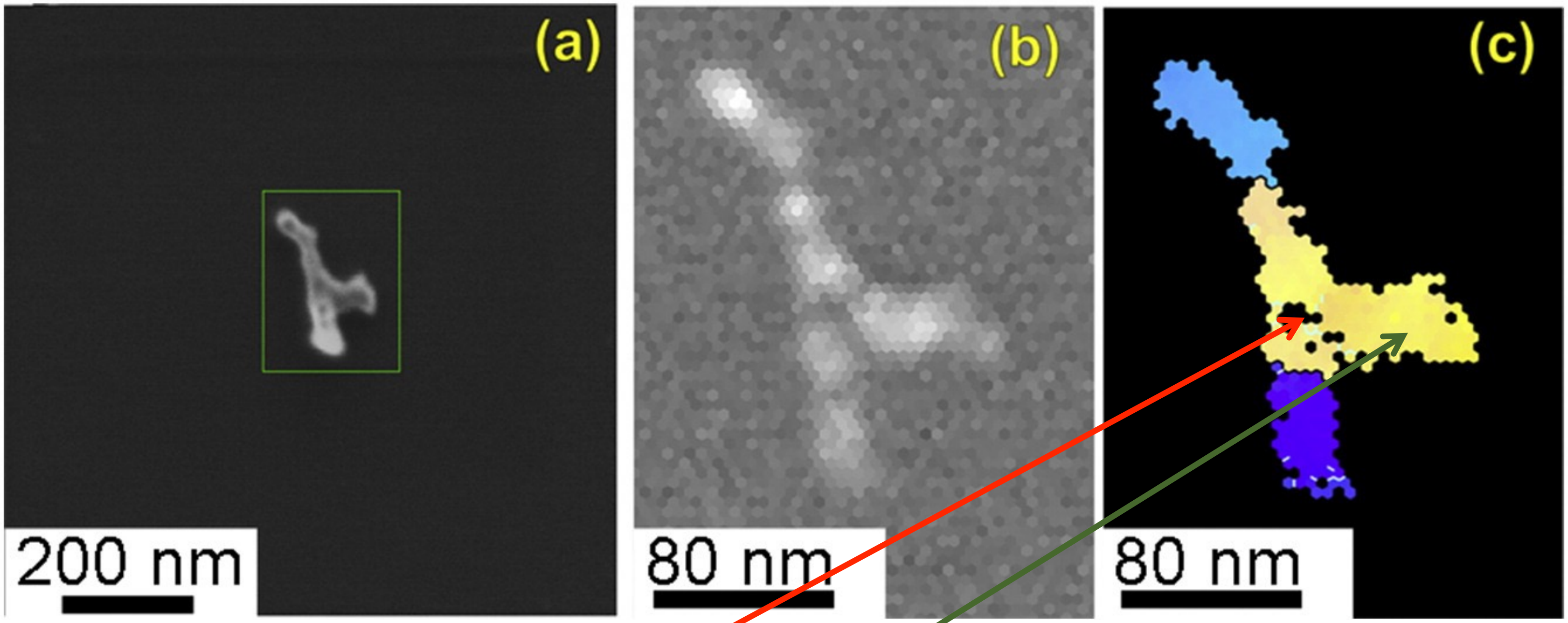




**Take a look at the nanotendrils:**

- ➢ Grain boundaries
- ➢ Faceted and rounded bubbles

*Wang et al. Scientific reports 7 (2017): 42315.*

# Introduction




**Take a closer look :**

- Branch structure near the GB
- He bubbles near GB

**Qestions:**

- How He bubble grows near GB?
- How surface morphology changes?

*C.M. Parish, Scr. Mater. 127 (2017) 132–135.*

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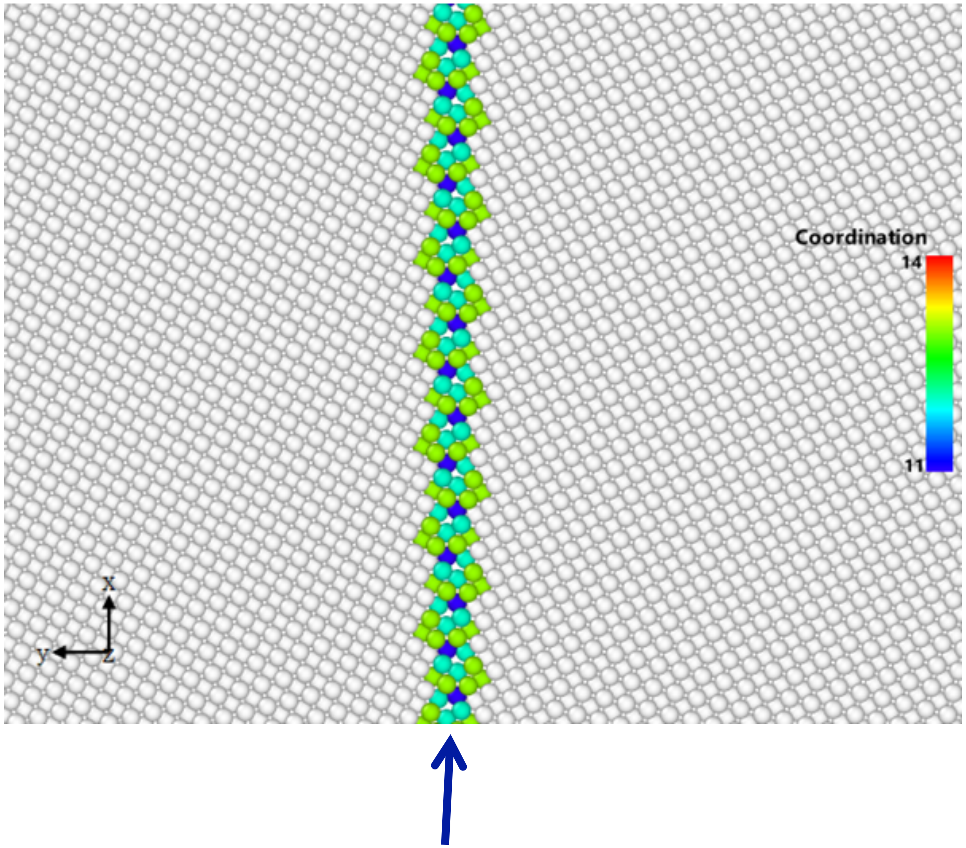
# ➢ Modeling – MD simulations



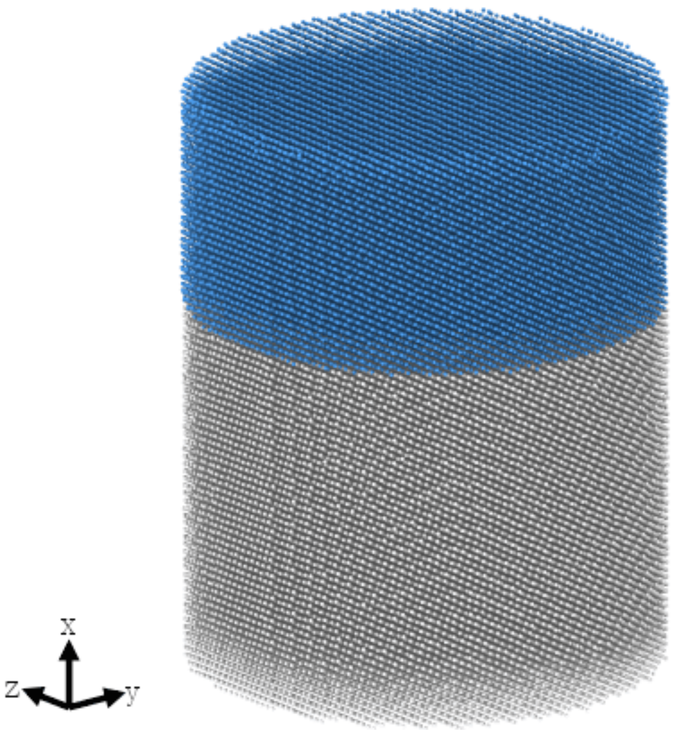



Σ17<100>{410} symmetric tilt grain boundary (STGB).

**Create tilt grain boundary structure:**

1. Rotate two grains by the opposite angles;
2. Optimize the GB structure and use the minimum energy structure as the model.
3. Four common types of GB are studied: Σ3, Σ5, Σ7 and Σ17;

# Modeling




Σ3 GB structure

**Create nanotendrils:**

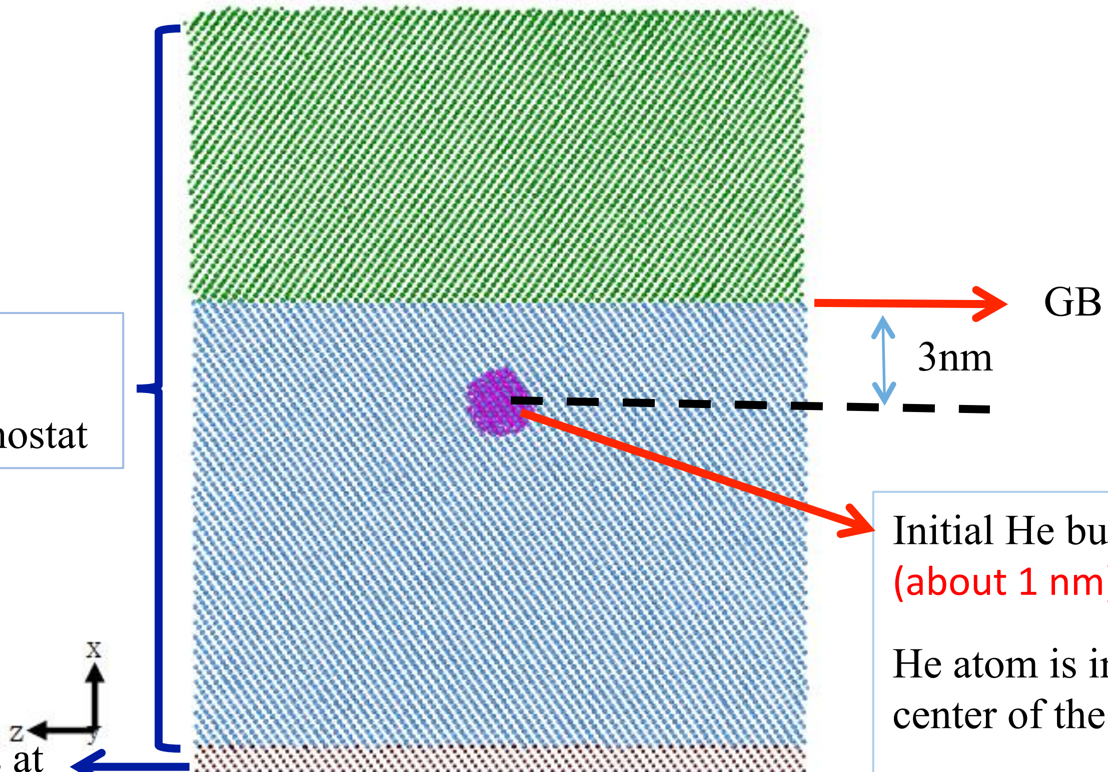
1. Delete the atoms to create a cylindrical nano-column
2. Radius:~8nm, Height:~20nm
3. Total atoms: 250000~300000
4. The grain boundary is located in the middle of the tendril.

# Simulation Settings

Free to move

Nose-Hoover thermostat

T = 1000 K




Several layers of atoms at bottom are fixed

**Side picture of tendril**

Initial He bubble: radius = $3a_0$ (about 1 nm);

He atom is introduced into the center of the bubble every 10 ps;

He bubbles rupture after around 6000 He insertion.

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# ➢ Σ3 GB tendril: morphology

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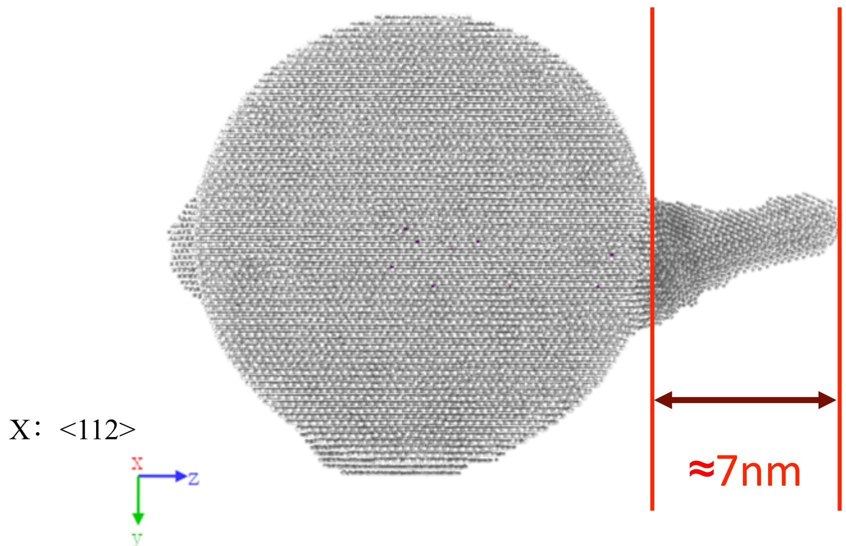


- Protruding ≈ 7nm
- Most of dislocations are [11-1] dislocations, leading to the interstitials stacking in the [11-1] direction
- A few <100> dislocations

| <100> Dislocations |
|---|
| 5.1%(2) |

- Σ7 GB structure shows similar behaviors.

| [111] dislocations | [-1-1-1] dislocations | [-111] dislocations | [1-1-1] dislocations | [1-11] dislocations | [-11-1] dislocations | [11-1] dislocations | [-1-11] dislocations |
|---|---|---|---|---|---|---|---|
| 5.1%(2) | 0%(0) | 2.6%(1) | 12.8%(5) | 0%(0) | 0%(0) | 41.1%(16) | 33.3%(13) |

# ➢ Σ5 GB tendril: morphology

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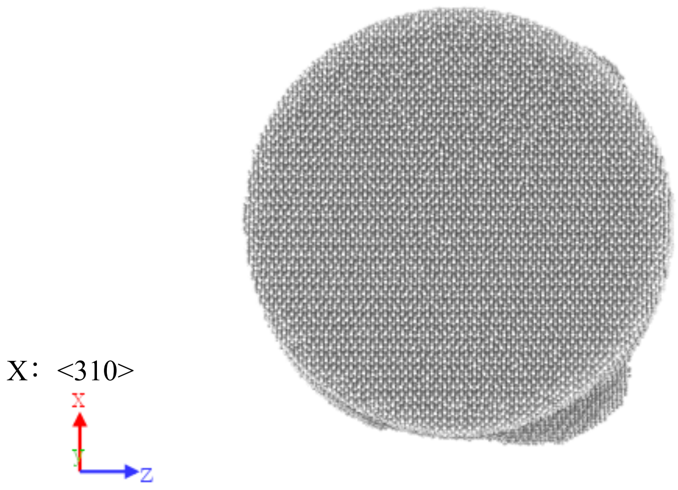
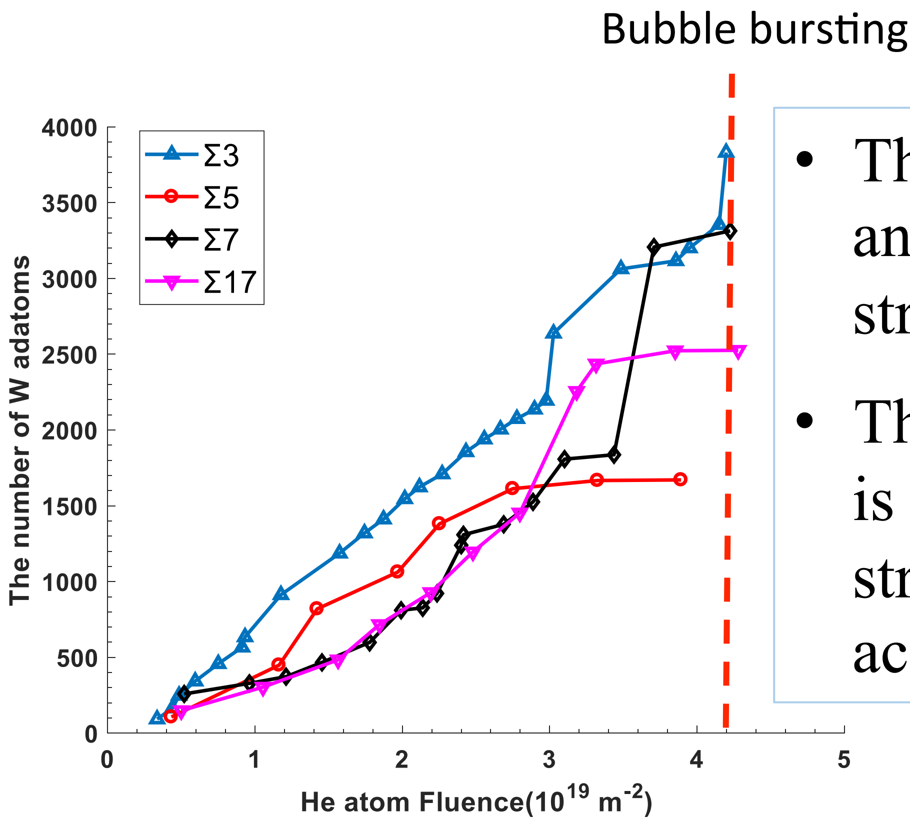



- Much fewer dislocations before bubble rupture, resulting in fewer adatoms at the surface and smaller protruding part.
- Adatoms spread on the surface rather than stacking
- No <100> dislocations

| [111] dislocations | [-1-1-1] dislocations | [-111] dislocations | [1-1-1] dislocations | [1-11] dislocations | [-11-1] dislocations | [11-1] dislocations | [-1-11] dislocations |
|---|---|---|---|---|---|---|---|
| 0%(0) | 11.8%(2) | 17.6%(3) | 17.6%(3) | 5.9%(1) | 5.9%(1) | 35.3%(6) | 5.9%(1) |

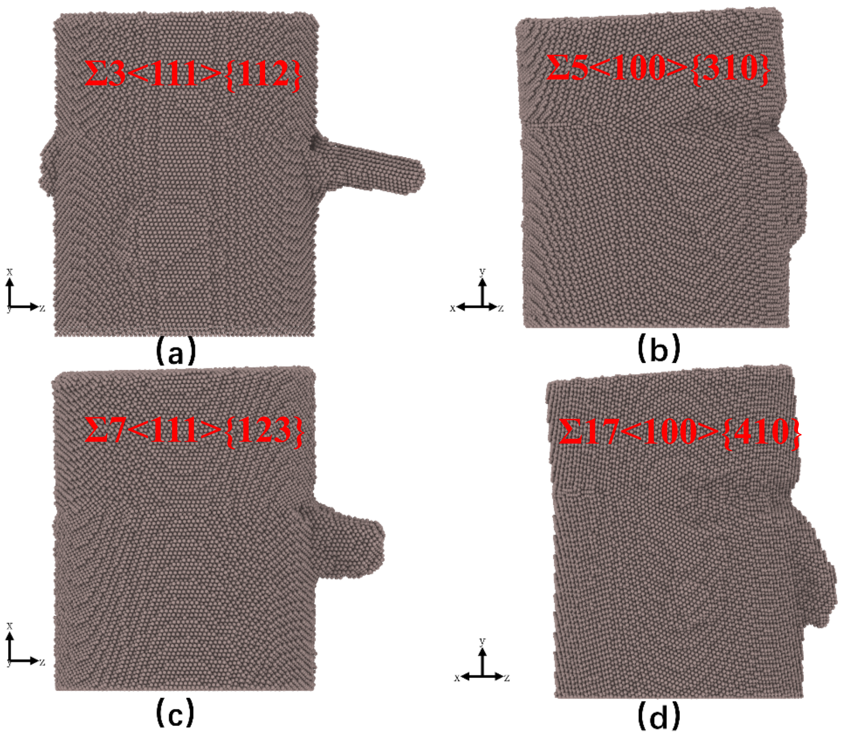
# Surface adatoms




- There are much more adatoms in Σ3 and Σ7 structures than the other two structures when bubbles rupture.
- The rupture time of the four structures is similar, which means that these four structure have equivalent ability to accommodate He atoms.

# Summary of surface morphology



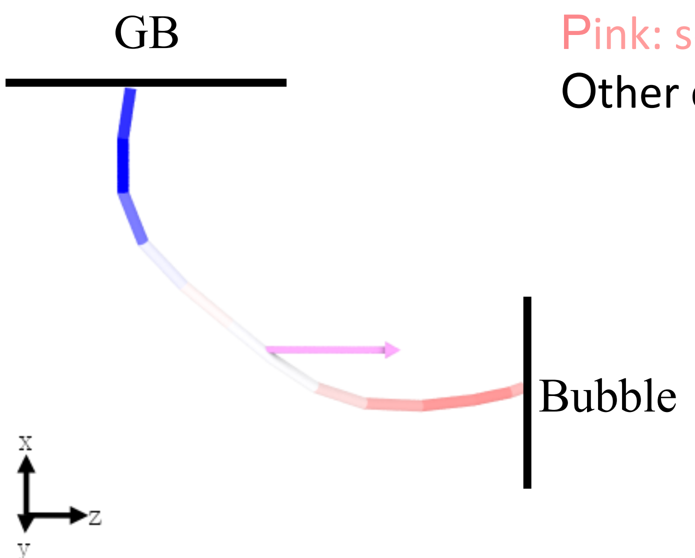



- Σ3 and Σ7 structures have a more obvious protruding part caused by the interstitial atoms stacking.
- In the Σ5 and Σ17 structures, the interstitial atoms spread on the surface so that smaller protruding part forms.
- The number and direction of dislocations determine the shape and size of the protruding part.

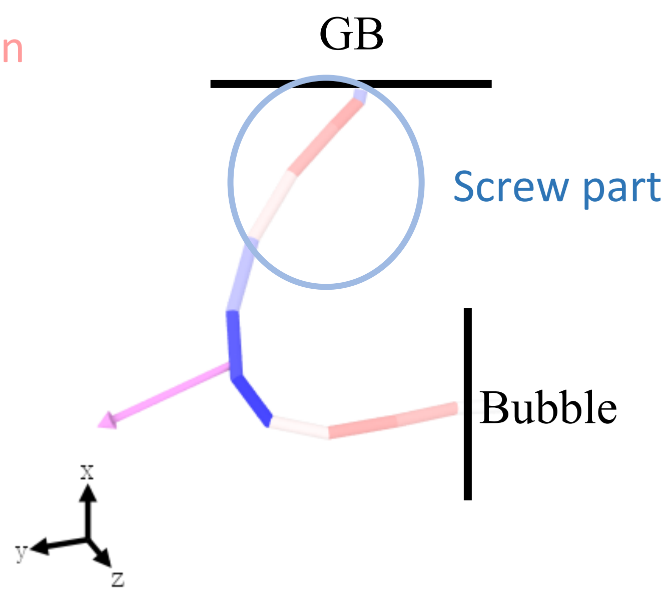
# ➢ Dislocation motion: analysis

- Most of the dislocations in the simulations are hybrid dislocations. Very few integrated prismatic dislocation loops exist.
- There are two type of hybrid dislocations.

Blue: edge dislocation
Pink: screw dislocation
Other color: hybrid




Type (a)
Exists in Σ3 and Σ7 structures




Type (b)
Exists in Σ5 and Σ17 structures

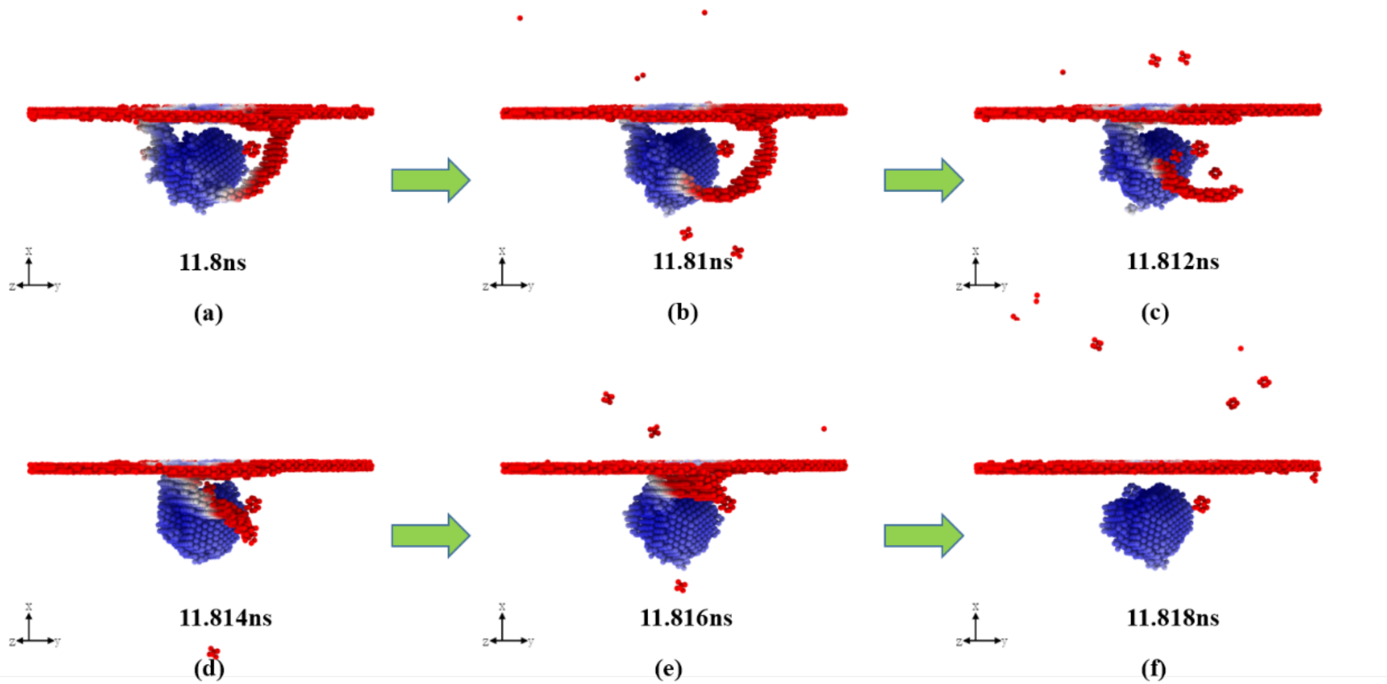
# Dislocation motion: animation



Σ7 structures (type a)

# ➢ Dislocation motion: type (a)






- Above: the snapshots of the type (a) dislocation in a Σ3 structure.
- The color from blue to red designates the distance from the present atomic site to the center of the He bubble.
- As can be seen from the figure, the grain boundary is an important medium for the sliding of dislocations.

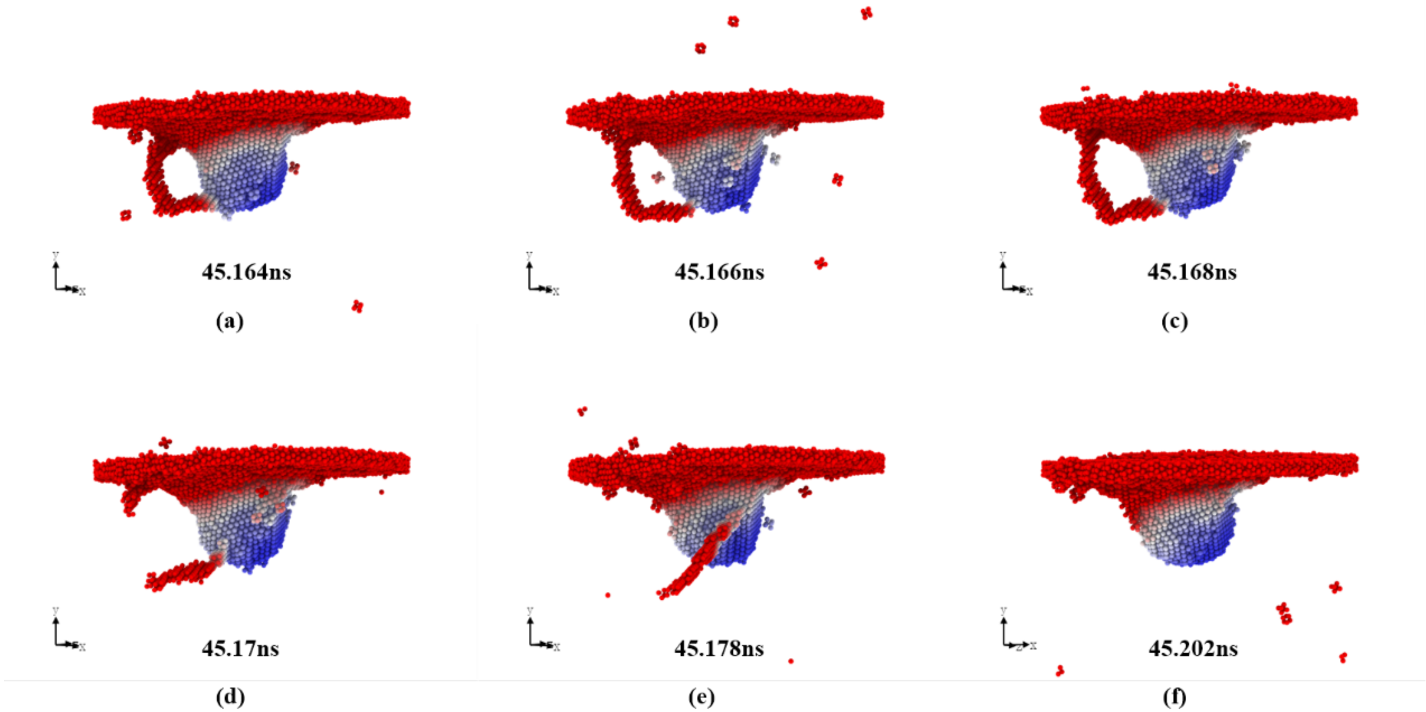
# Dislocation motion: animation



Σ5 structures

# ➢ Dislocation motion: type(b)



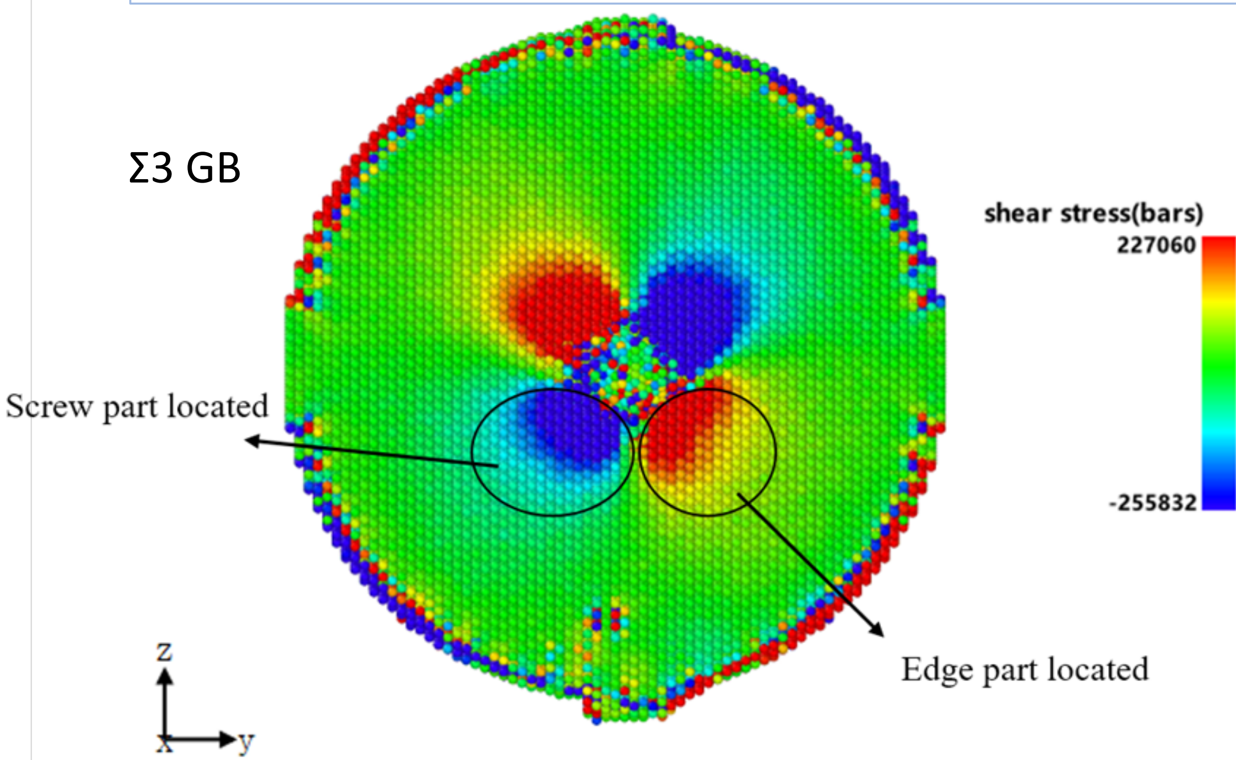


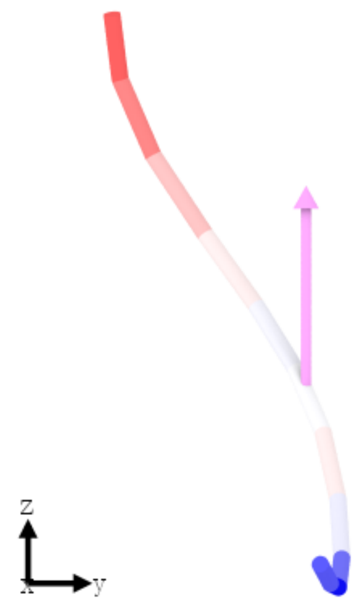

- Above: the snapshots of the type (b) dislocation in a Σ5 structure.
- The edge part dislocation plays a key role in the movement of hybrid dislocations.

# ➢ Dislocation motion: driving force

Below:

- The shear stress-field nephogram around the He bubble.
- The edge part dislocation and screw part dislocation have opposite shear stress direction.



# ➢ Dislocation motion explanation

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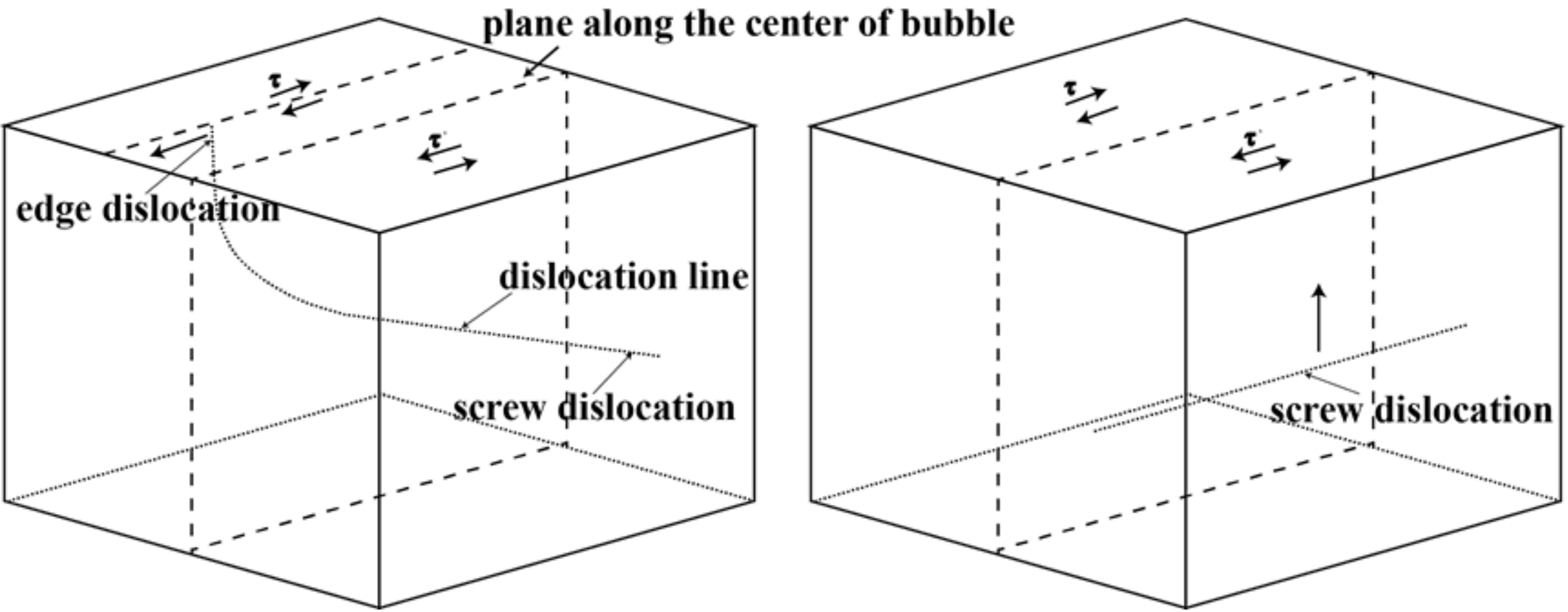


- A sketch of the movement process of the type (a) hybrid dislocation under shear stress.
- Firstly, the edge part glides toward the surface and then annihilates at surface leaving a pure screw dislocation;
- Subsequently the remaining screw part moves toward the GB driven by shear stress and then annihilates at the GB

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# ➢ Summary

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- He bubble growth in the vicinity of 4 types of GBs in W nanotendril has distinct features compared to bubble growth in the bulk or near surface.
  - ➢ He bubbles are attracted by GBs;
  - ➢ Generation of hybrid dislocations;
  - ➢ Rapid evolution of surface morphology.
- The formation of large protruding part in Σ3 and Σ7 structures could probably explain the formation of branch structures in the fuzz tendrils.
- For both two types of hybrid dislocations, the edge part dislocation moves first to drive the motion of the entire dislocation and then annihilates at the surface leaving the screw dislocation part. The remaining screw dislocation will either move to GBs or move to the surface.

# Thanks for your attention!