AMPMI 2024 @ Metsätalo, University of Helsinki, Finland

Bulk, surfaces, and grain boundaries

in the lifetime of cascades in W

Byeongchan Lee Kyung Hee University, Korea, July 18, 2024

경희대학교 KYUNG HEE UNIVERSITY

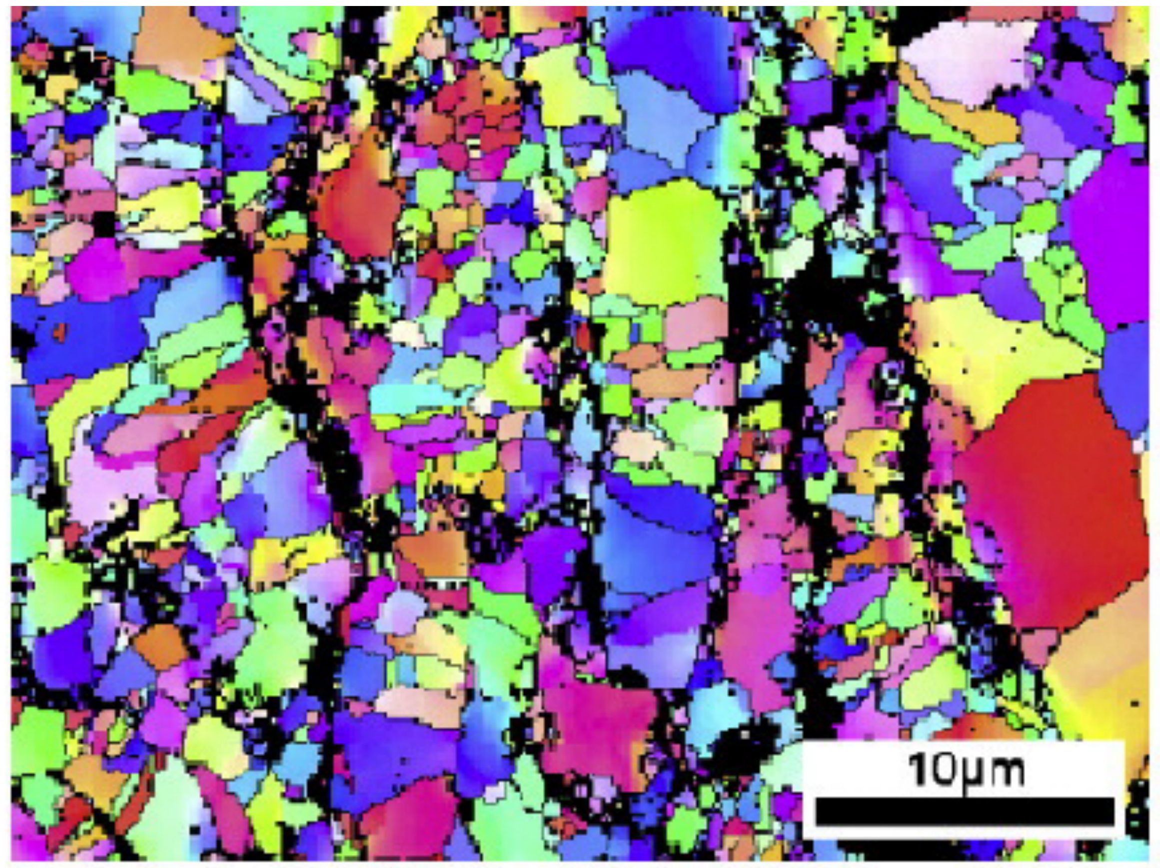
Acknowledgments

- PhD students: **Younggak Shin, Vichhika Moul** (Kyung Hee University)
- Collaborator: **Keonwook Kang** (Yonsei University)

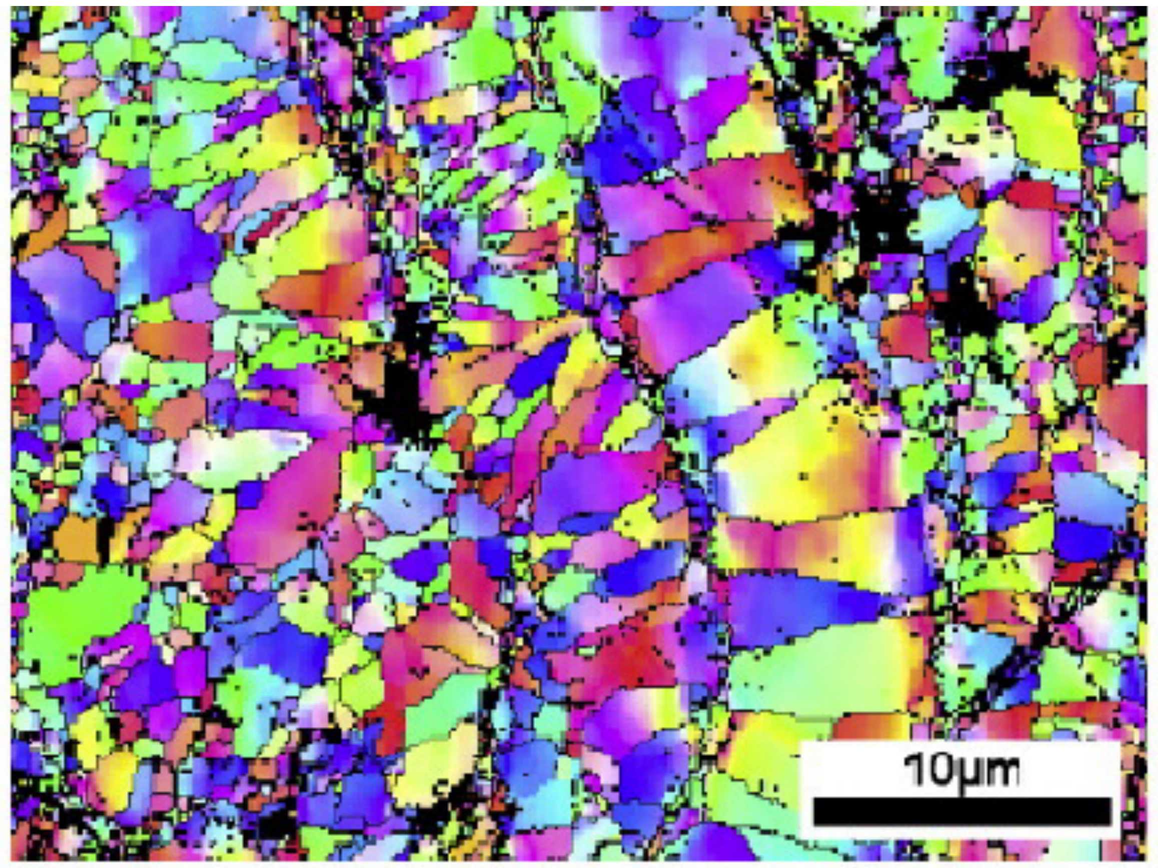
- Funding
- National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2020R1A2C201510913)
- Korea Hydro & Nuclear Power Co., LTD (No. 2022-Tech-11).

Mechanical properties

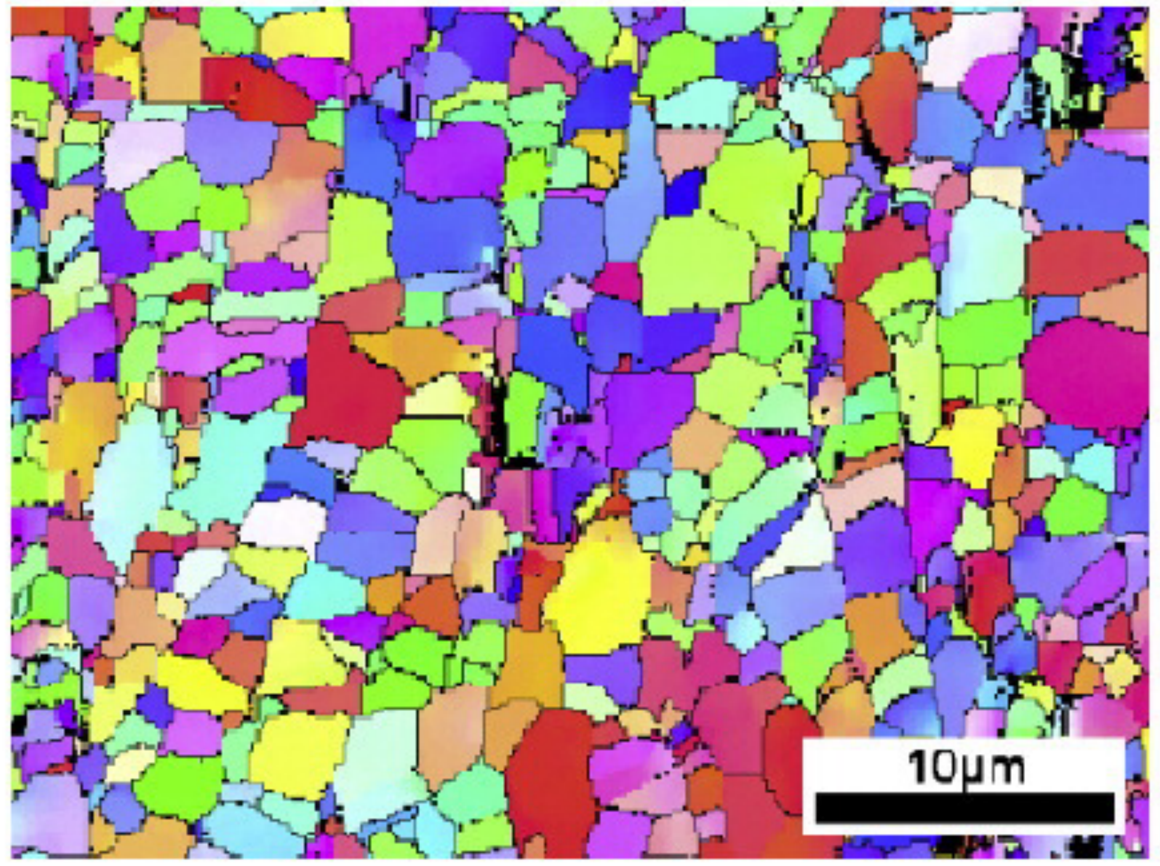
depend on grain uniformity (let alone H-P)



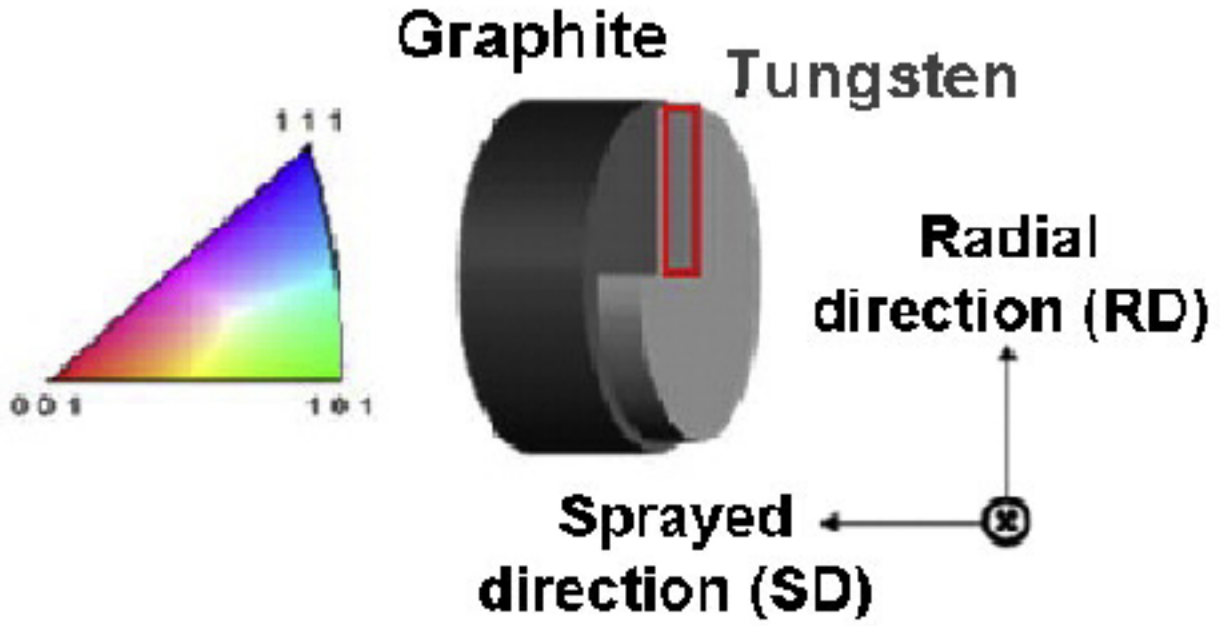
As-sprayed



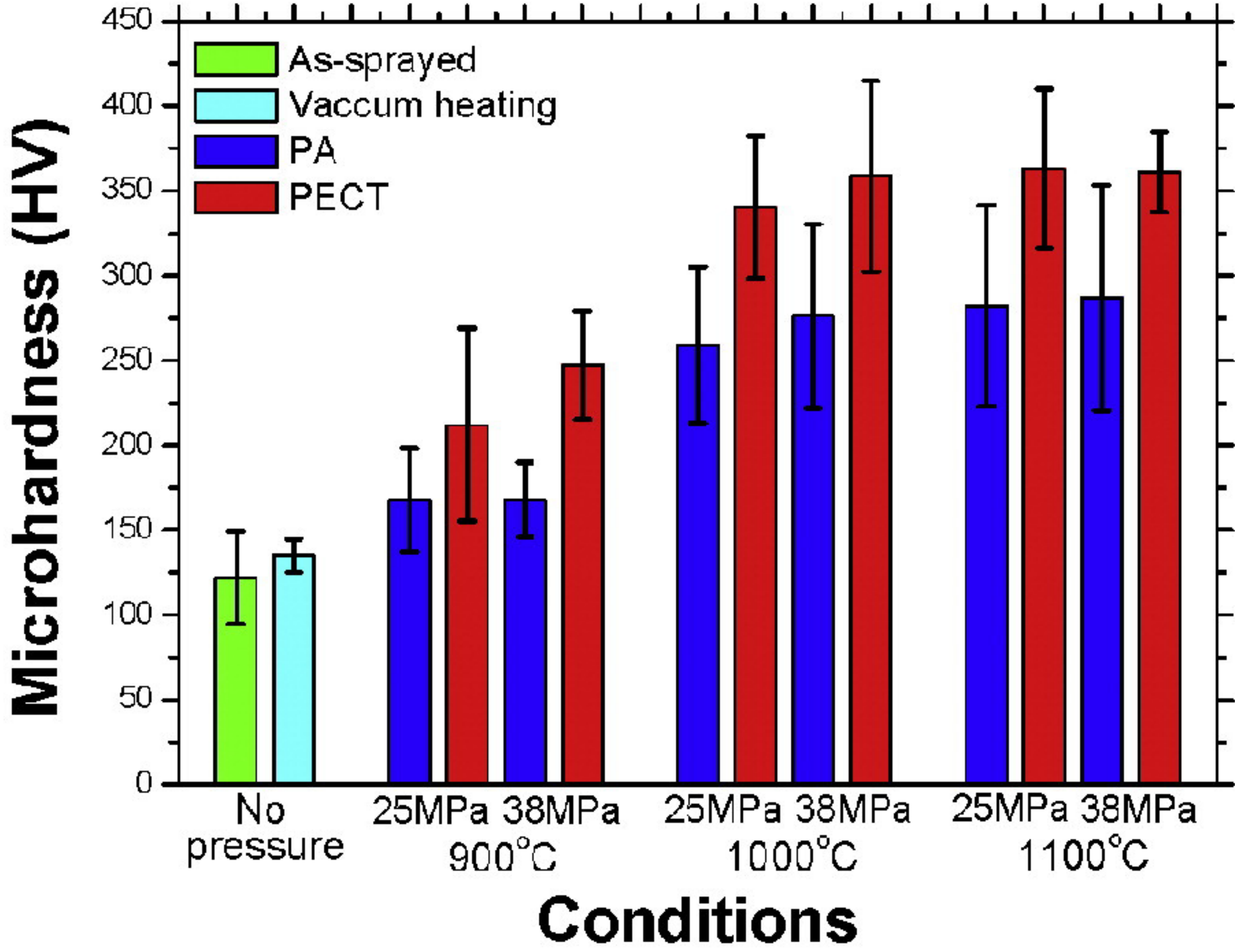
Press-annealing (PA)



Pulsed electric current treatment (PECT)



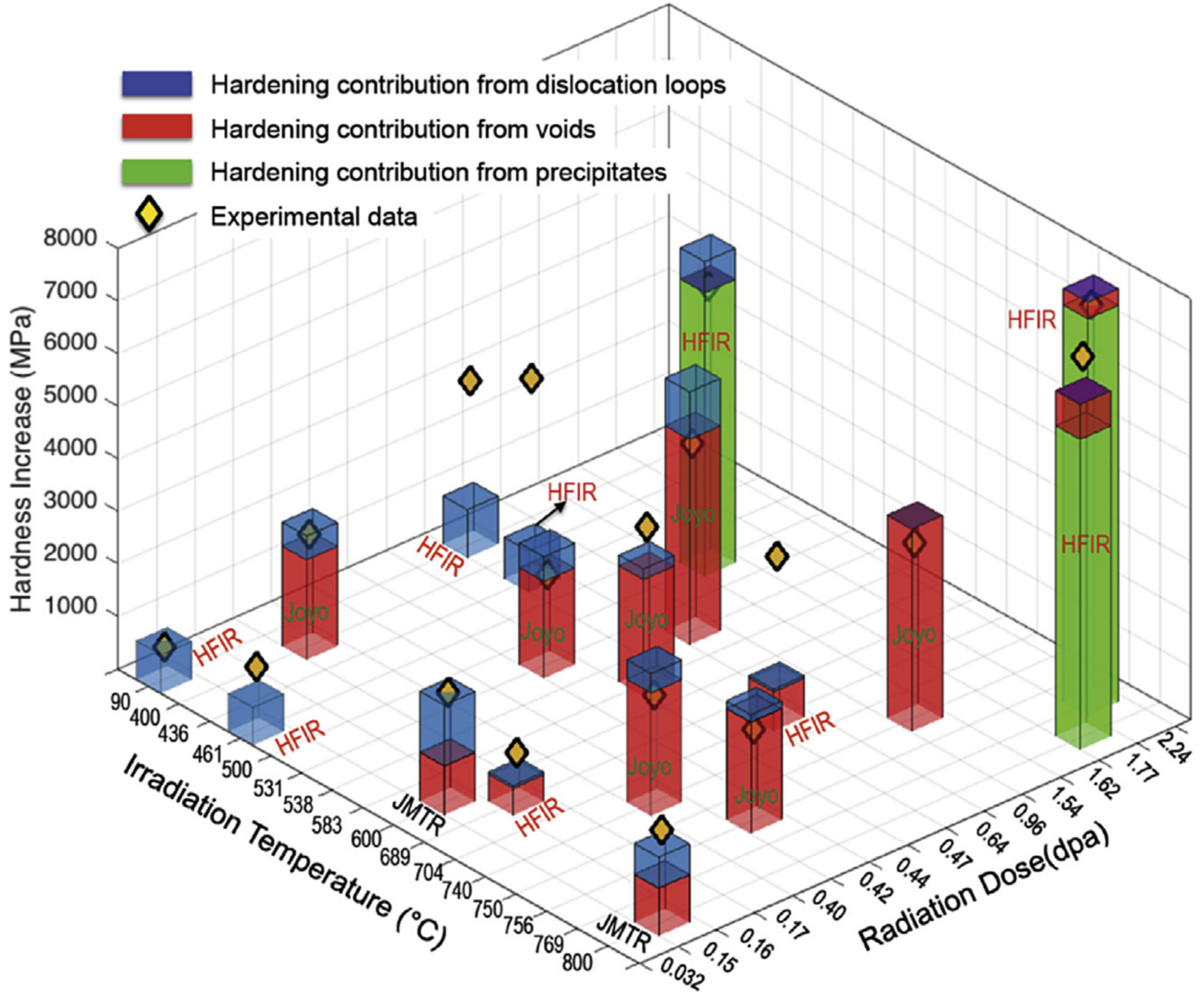
Sprayed W



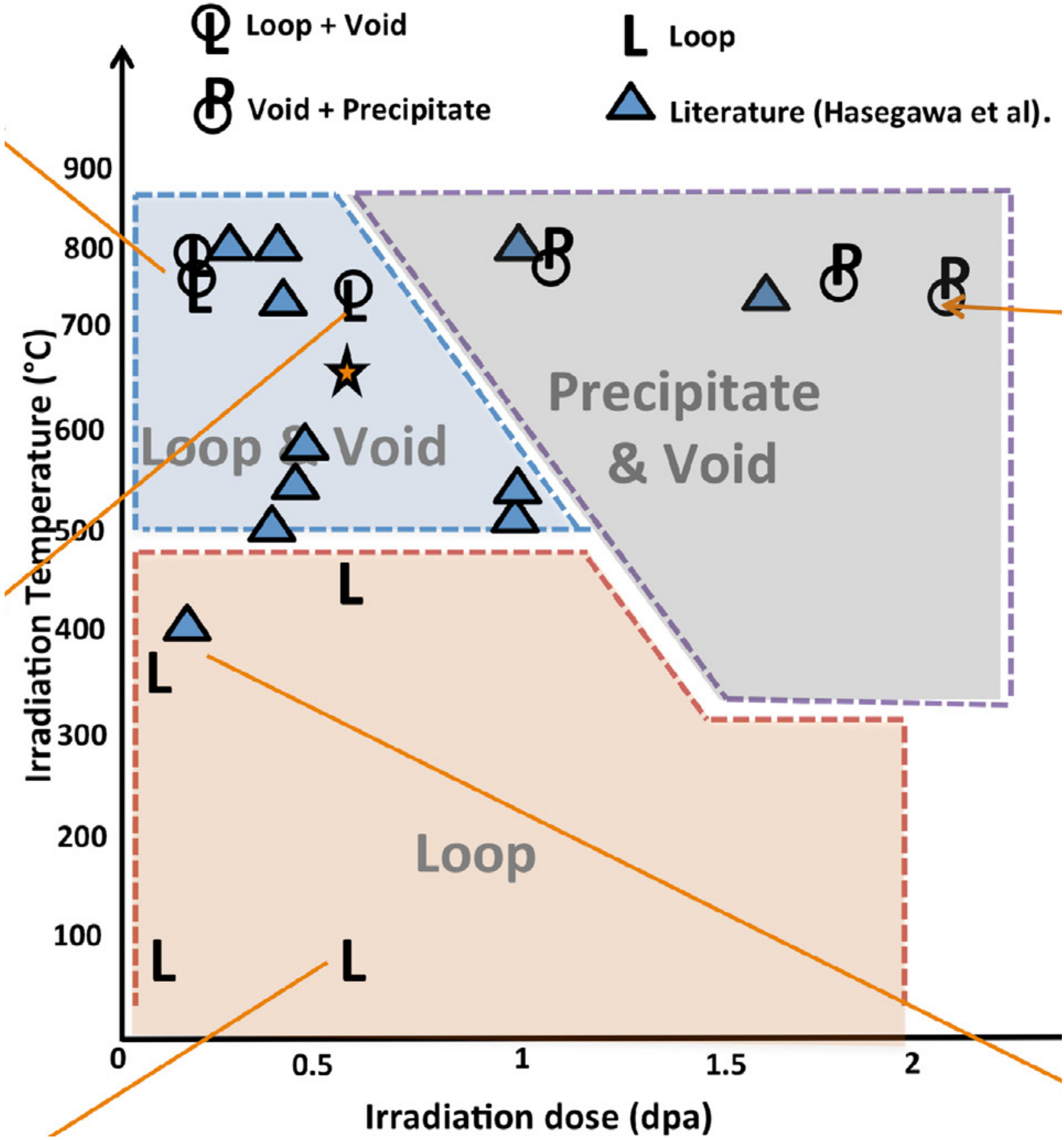
Y. J. Lee et al. | Int. J of Refractory Metals and Hard Materials 60, 99 (2016)

Mechanical properties

of n-irradiated materials



X. Hu et al. | JNM 480 235 (2016)

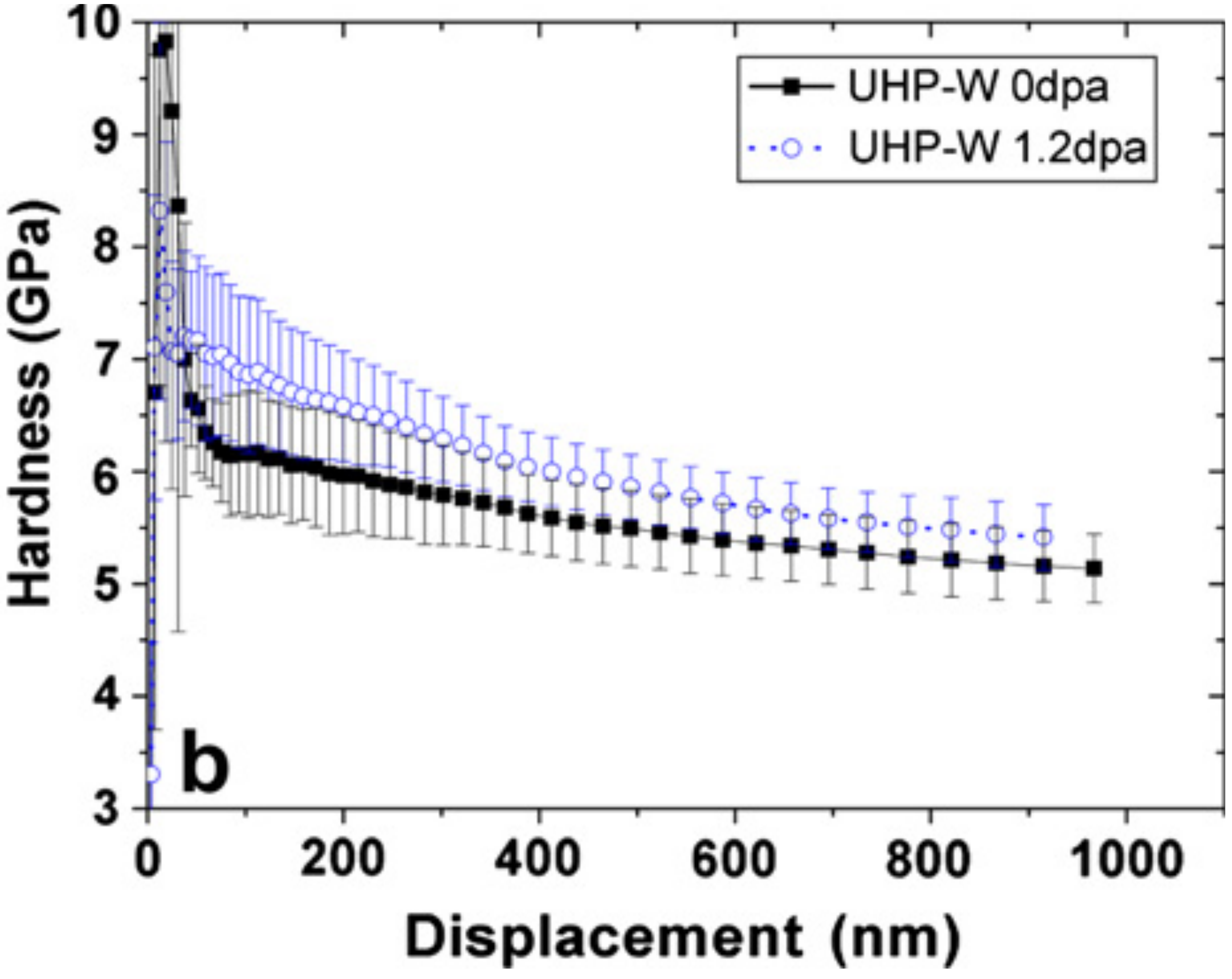


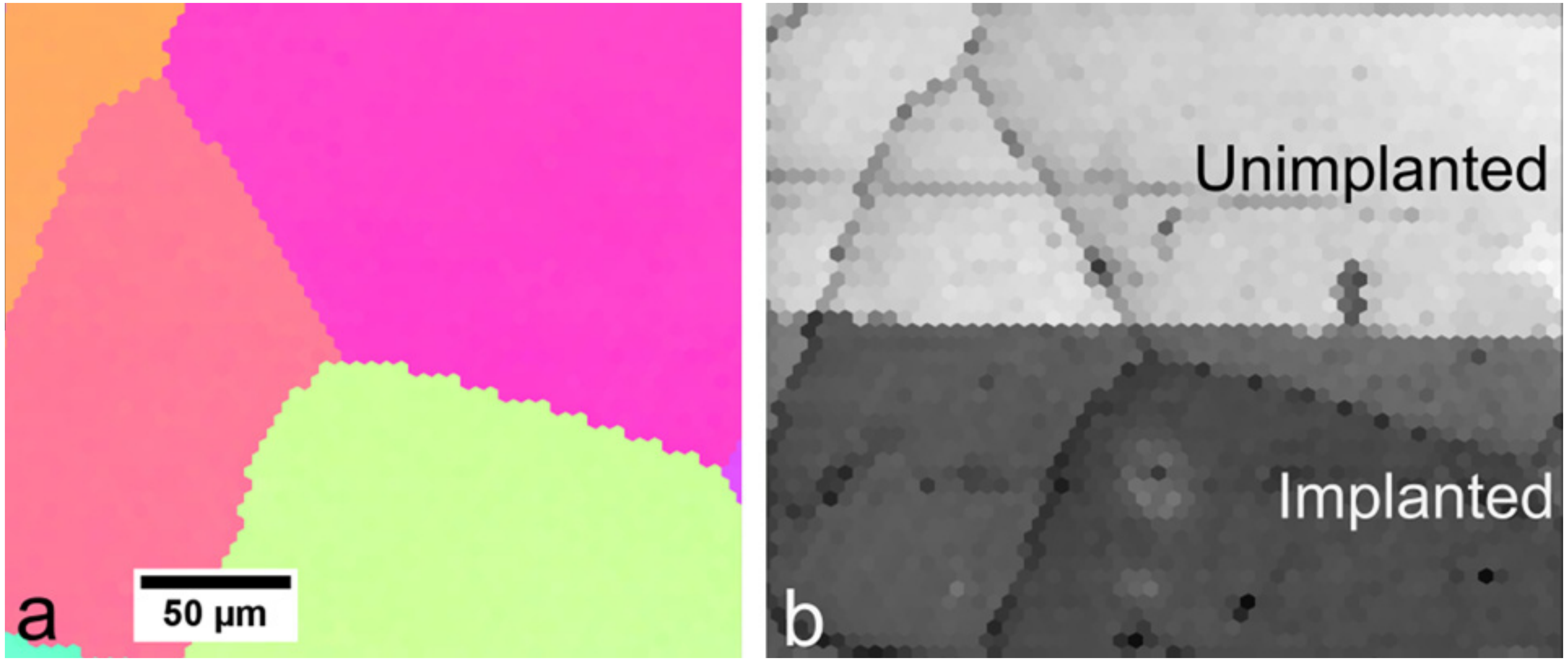
J. Marian et al. | Nucl. Fusion 57, 092008 (2017)

Grain boundaries remain nearly unchanged

Microstructure has changed though

self-ion irradiated W





(a) Inverse pole figure and (b) image quality map produced using EBSD

D.E.J. Armstrong et al. | JNM 432, 428 (2013)

Is GB transparent to neutron irradiation?

Is GB transparent to neutron irradiation?

PKA simulations

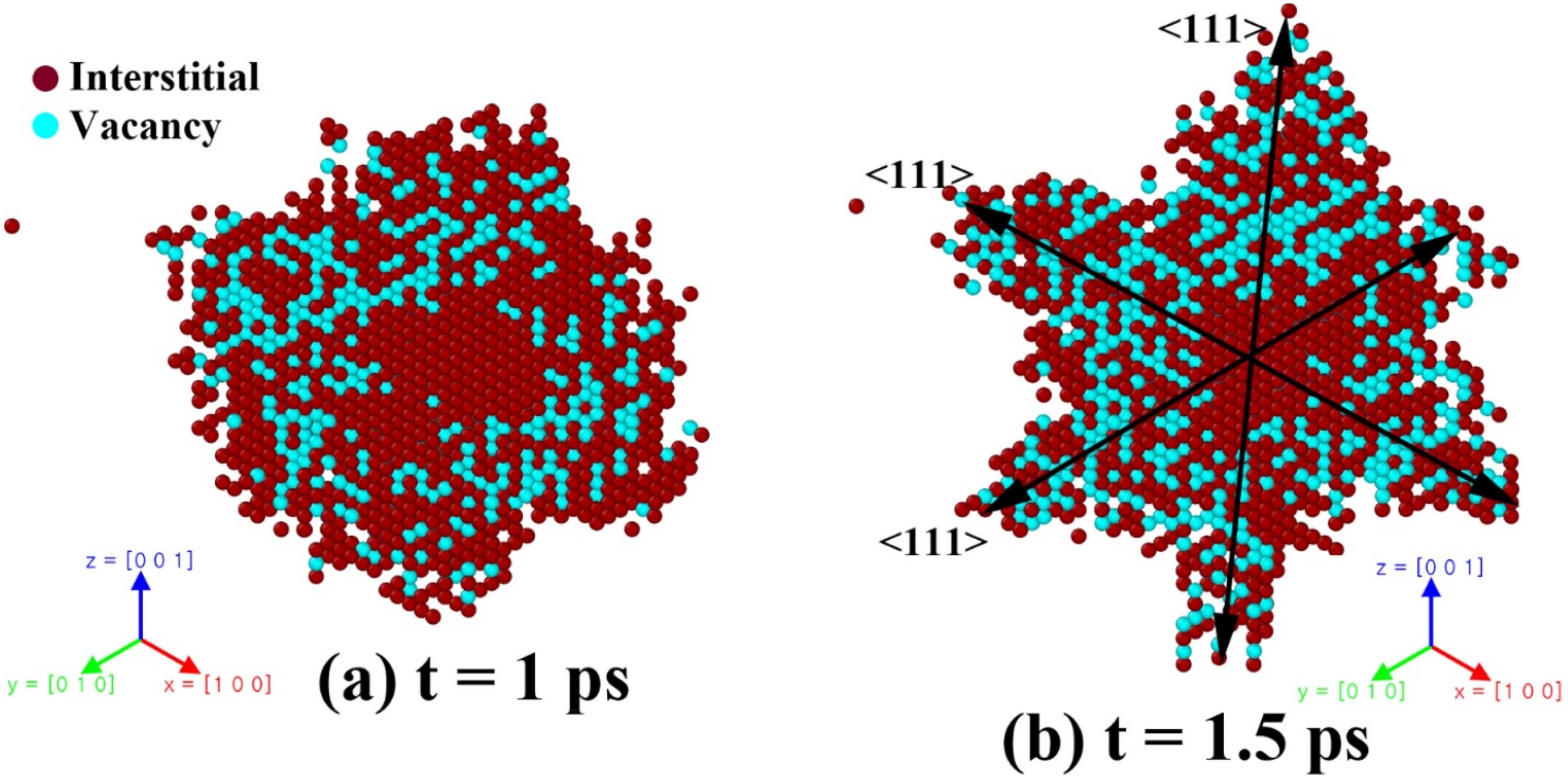
Primary Knock-on Atoms to simulate n-irradiated cascades

- Cascades
  - In periodic bulk
  - Near surface
  - Near grain boundary
    - Damage detection methods
    - Preliminary results

Irradiation damages

in single crystalline bulk

Wigner-Seitz (W-S) analysis

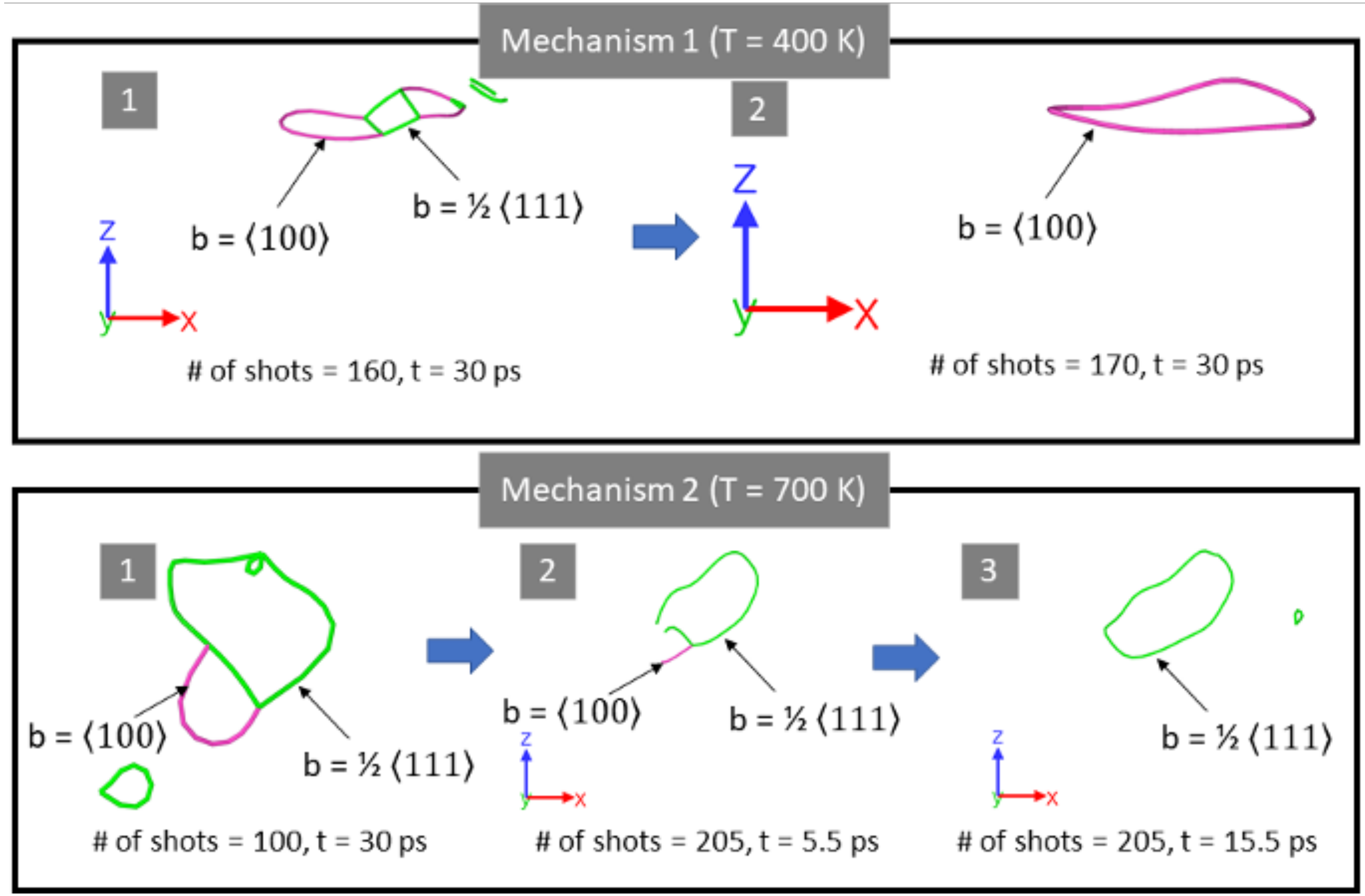


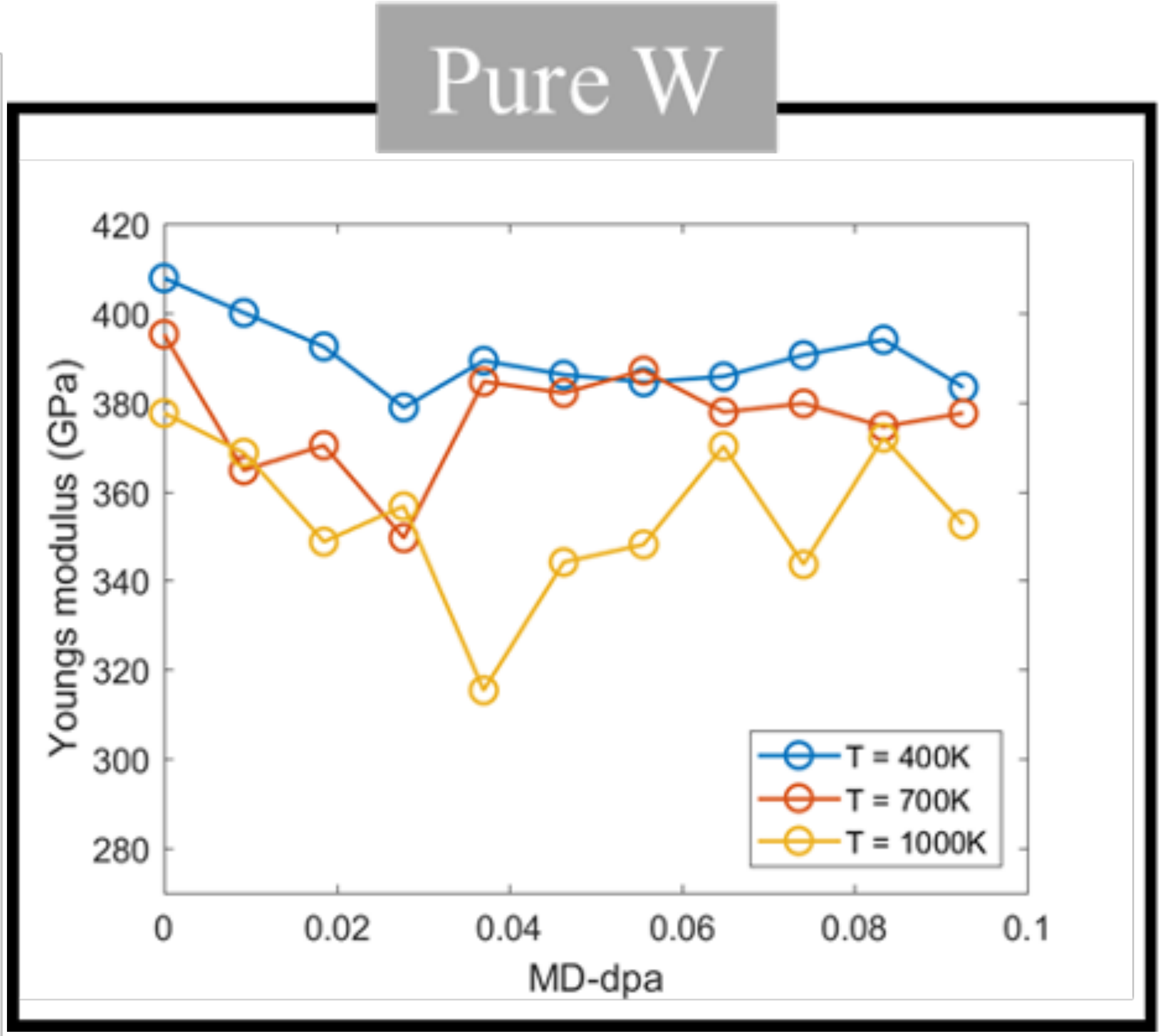
H.G. Lee, S. Yoo, B. Lee, and K. Kang | Nuclear Fusion 60 (2020)

FS-AT / ZBL as implanted by Fikar and Schaeublin

Total defect neutrality in periodic bulk

vacancies = # SIAs





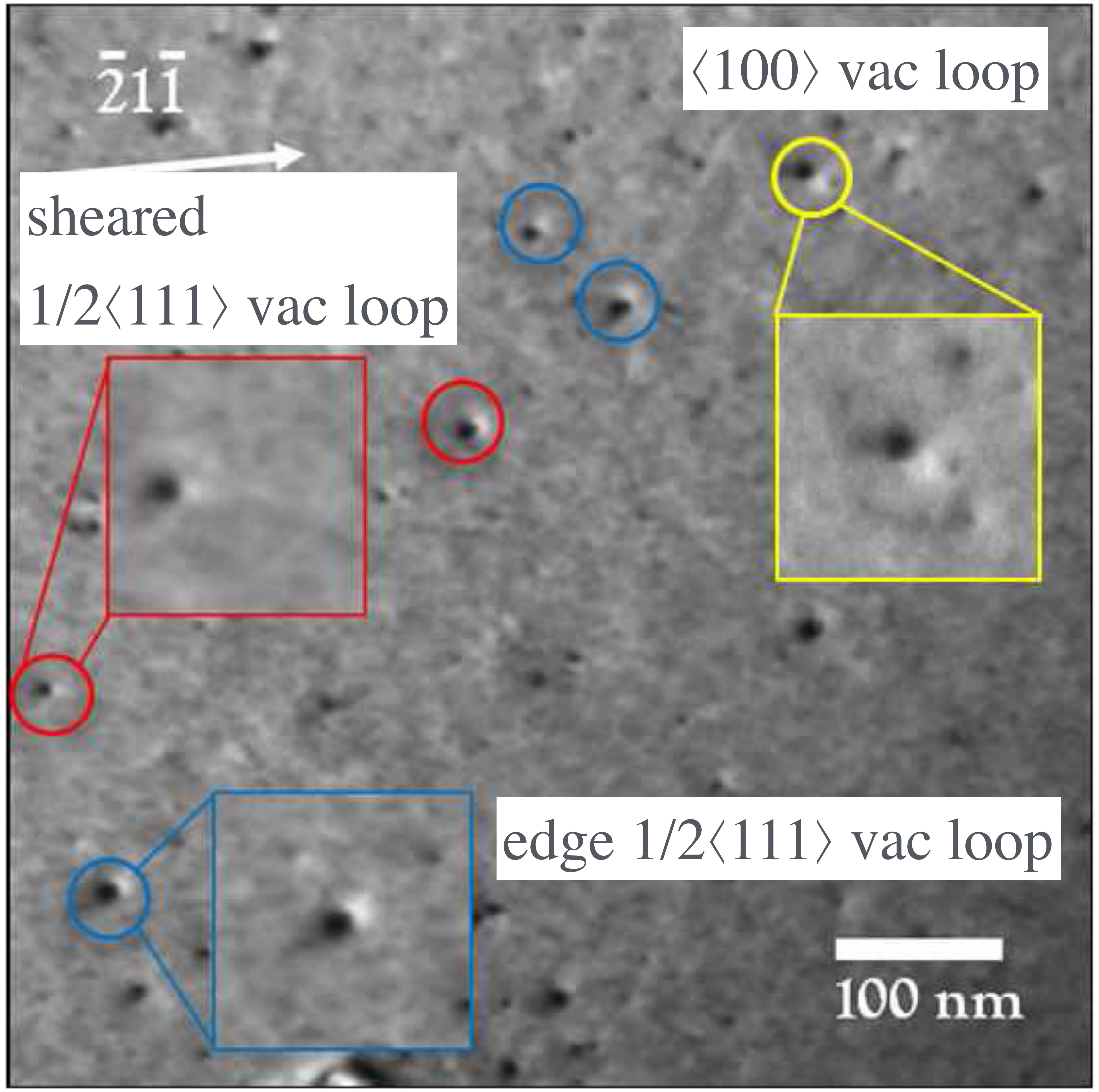
Young's modulus

H.G. Lee et al. | unpublished

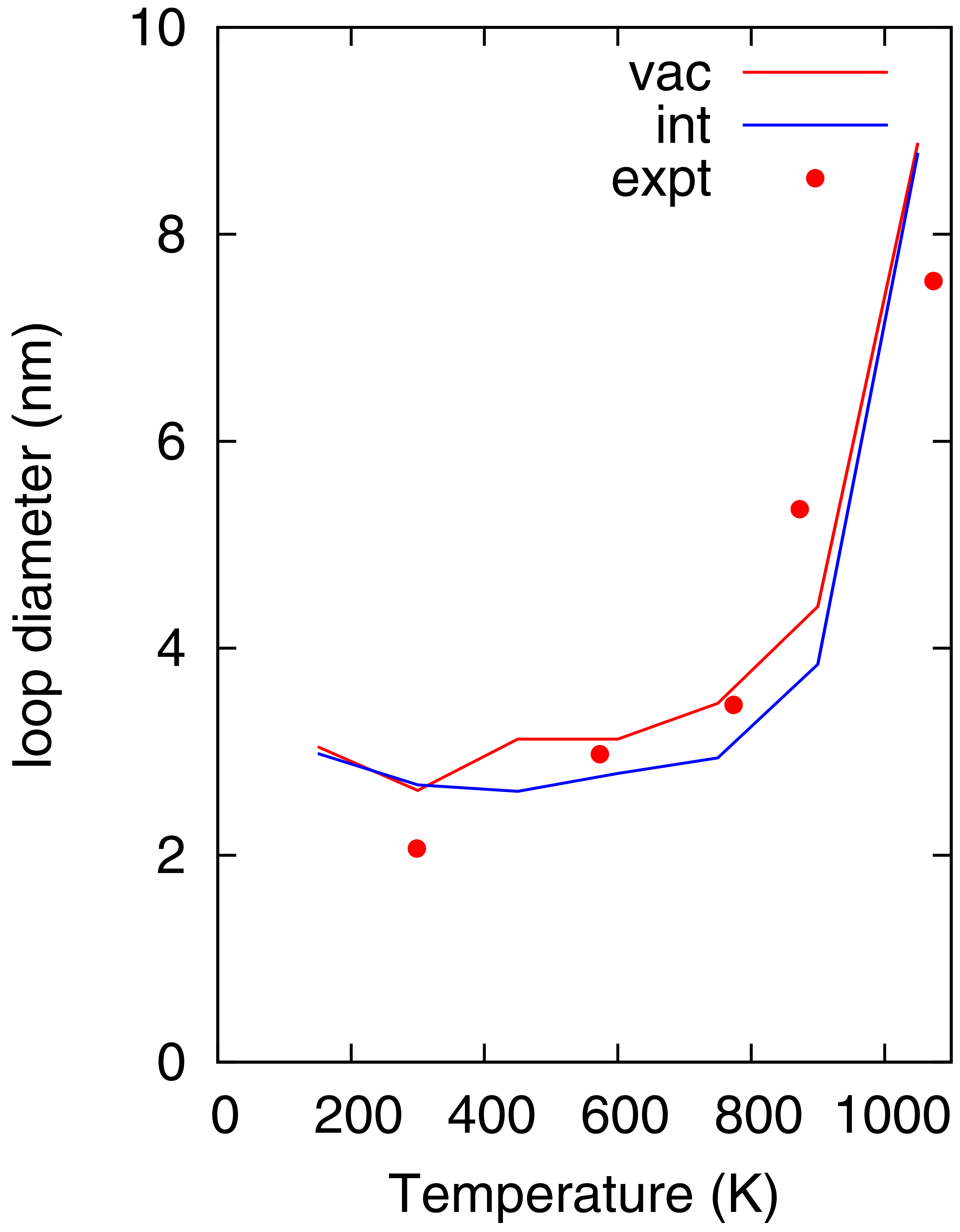
Irradiation damages

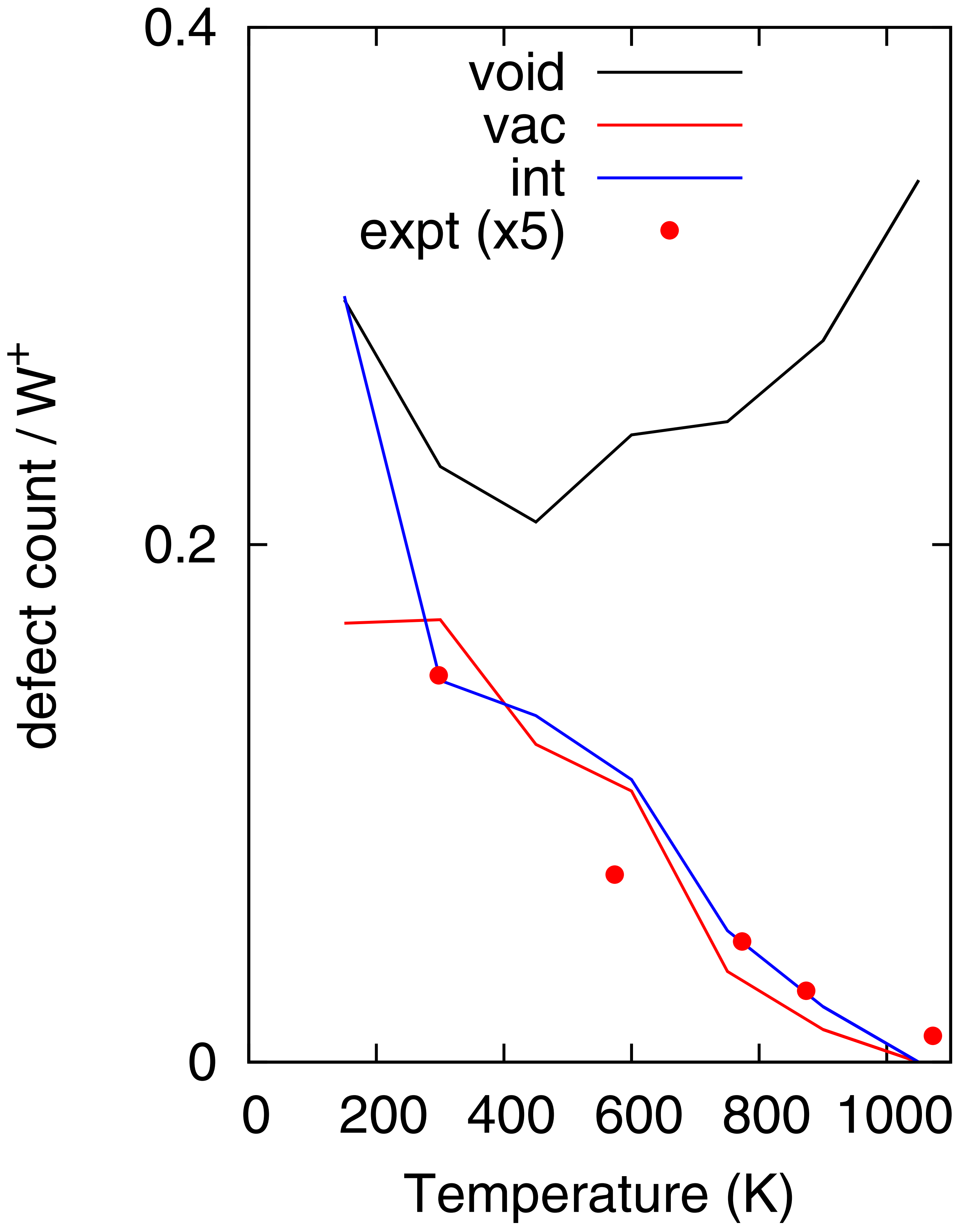
in W foils

~ 0.01 dpa w/ 150 keV W+ @ 300K



"the largest loops to be predominantly of prismatic 1/2⟨111⟩ type and of vacancy character"

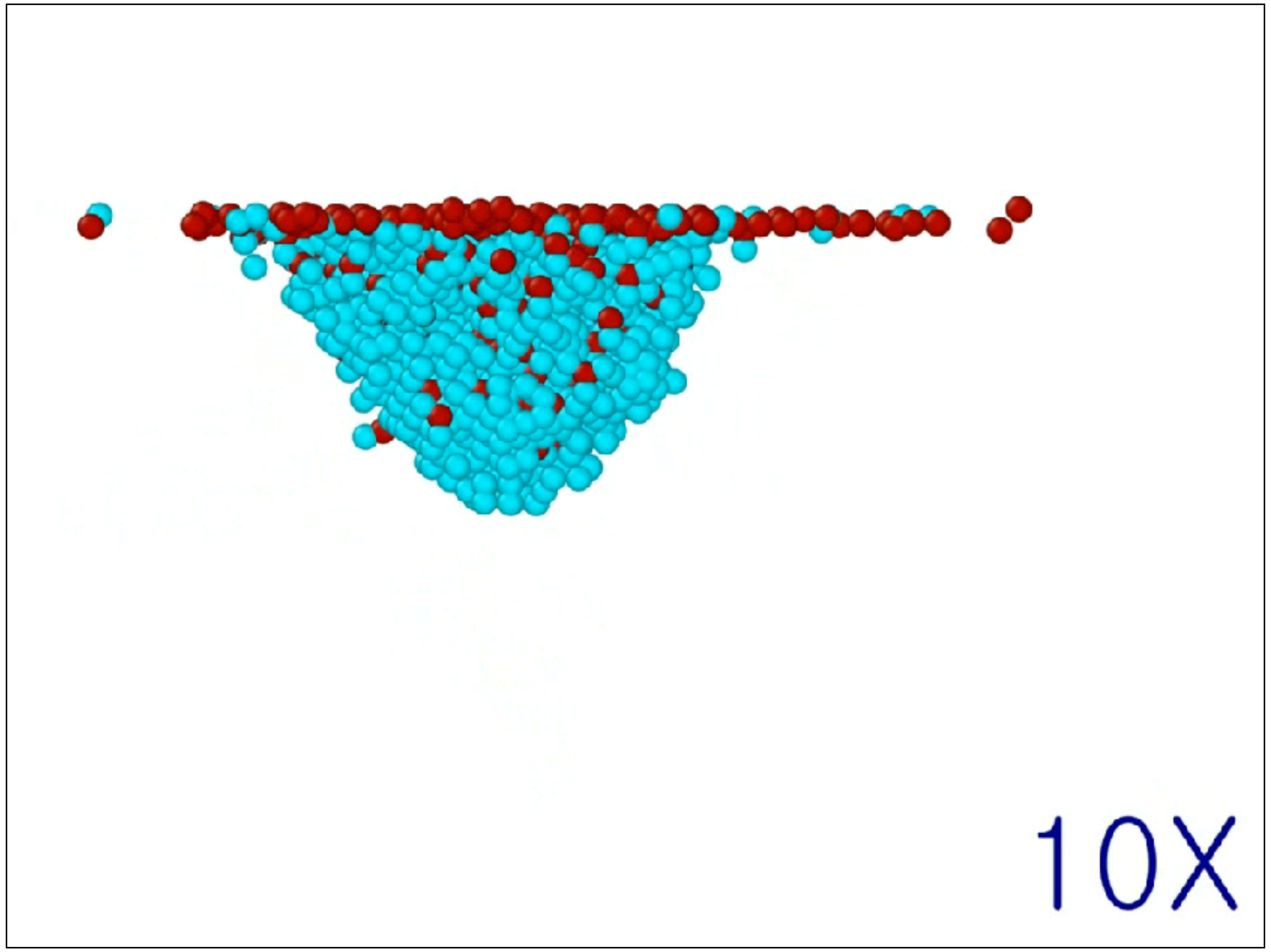




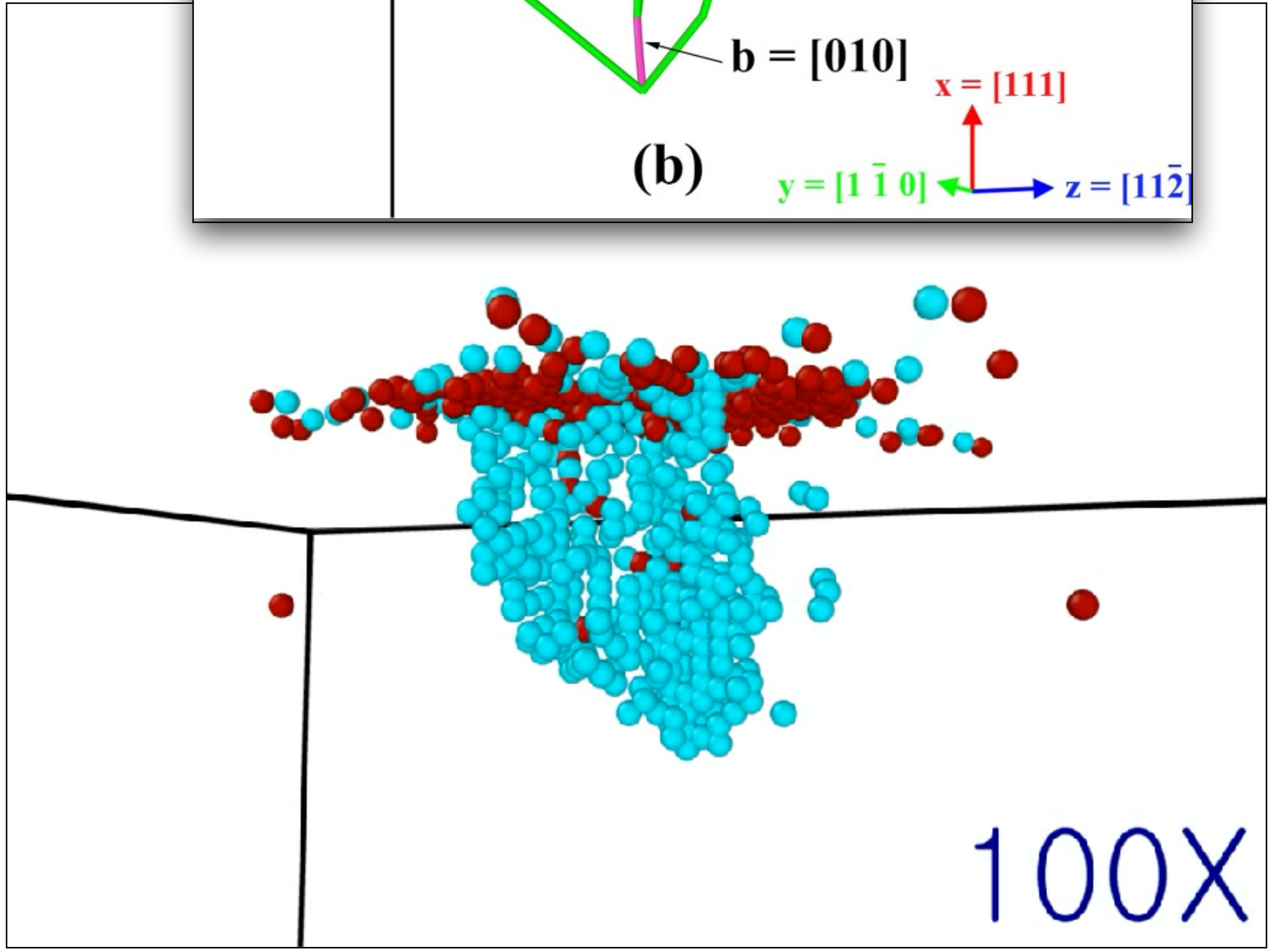
D. R. Mason et al. | J. Phys.: Condens. Matter 26 (2014) 375701

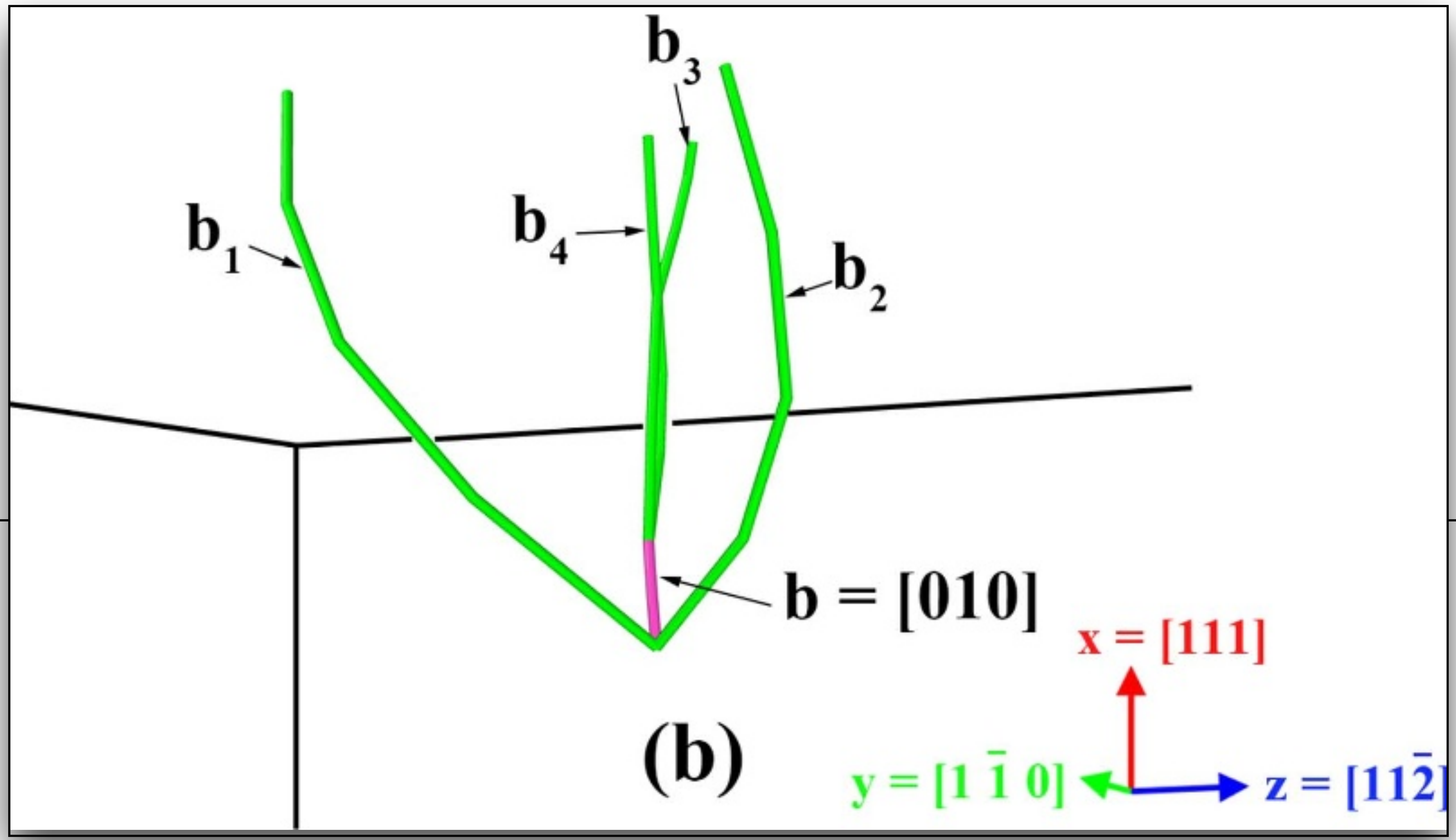
Irradiation damages

near surface



Mobile (vacancy) dislocation loop





Immobile (vacancy) dislocation network

Surface ~ a defect sink w/ infinite capacity

H.G. Lee et al. | Nuclear Fusion 60 (2020)

Irradiation damages

near grain boundary (GB)

Grain boundary ~ a defect sink w/ **finite** capacity

Common Neighbor Analysis (**CNA**) showing non-BCC atoms

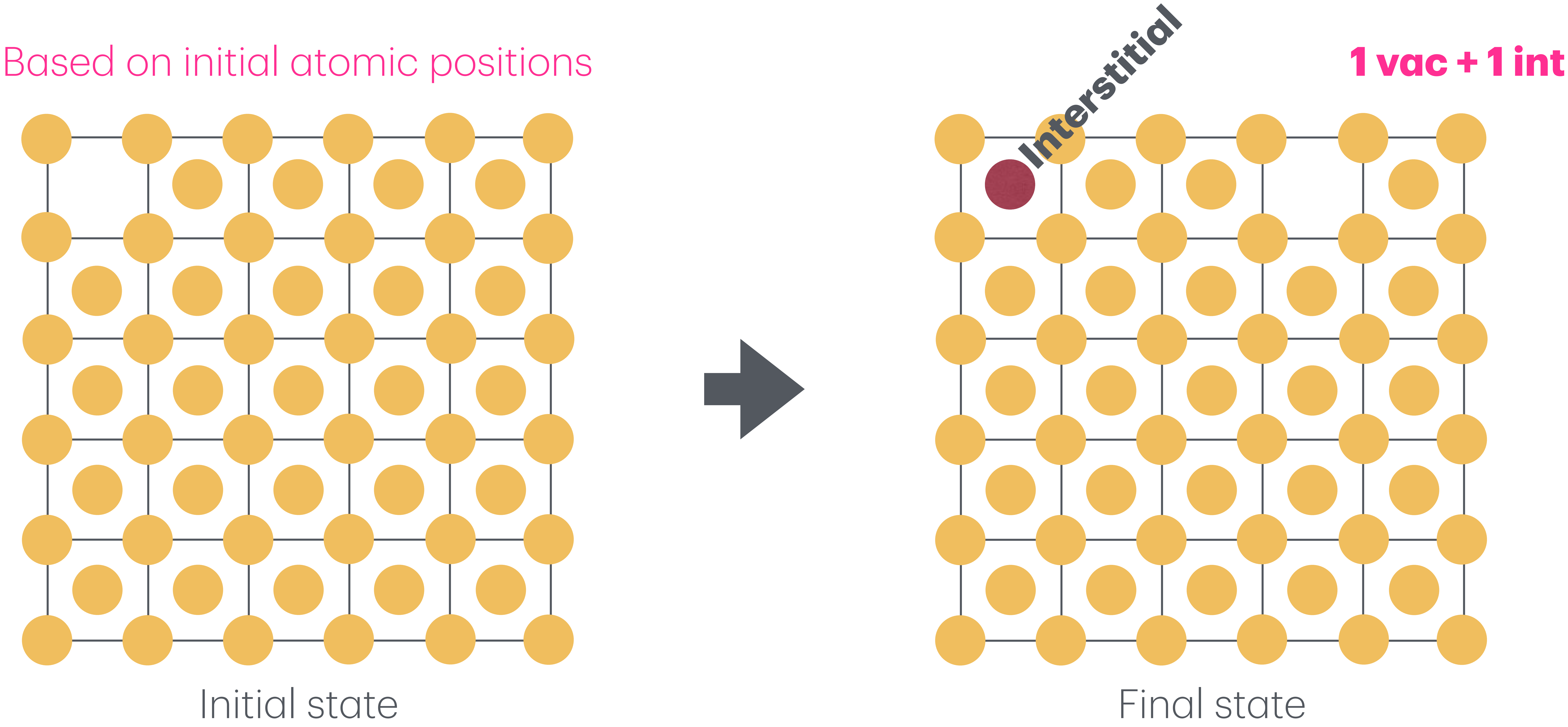
GBs absorb defects

Then what?

- Possible scenarios
  - Diffusion inside GBs
  - Dislocations
  - **Crystal growth**
    - May be in the form of GB motion for small-area boundaries

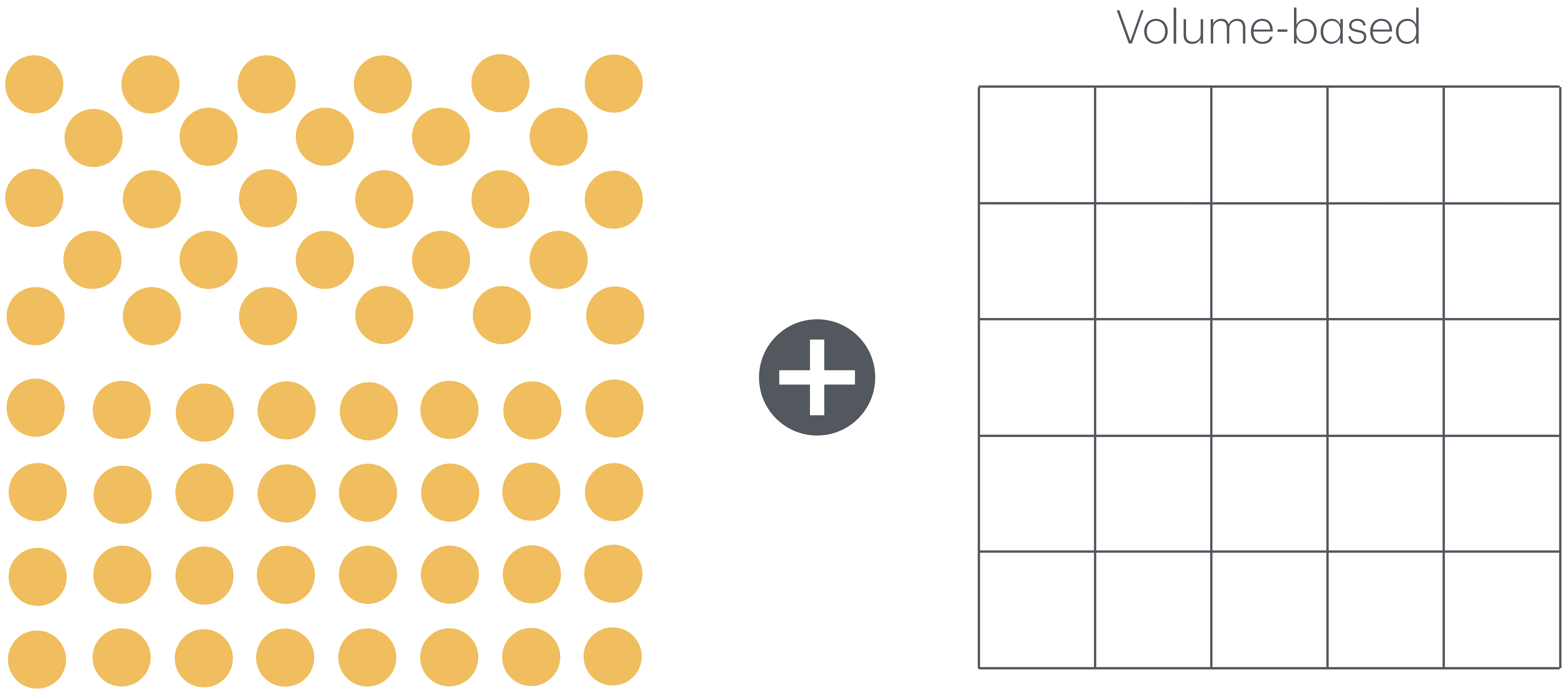
We need defect counts

Wigner-Seitz as implemented in popular tools



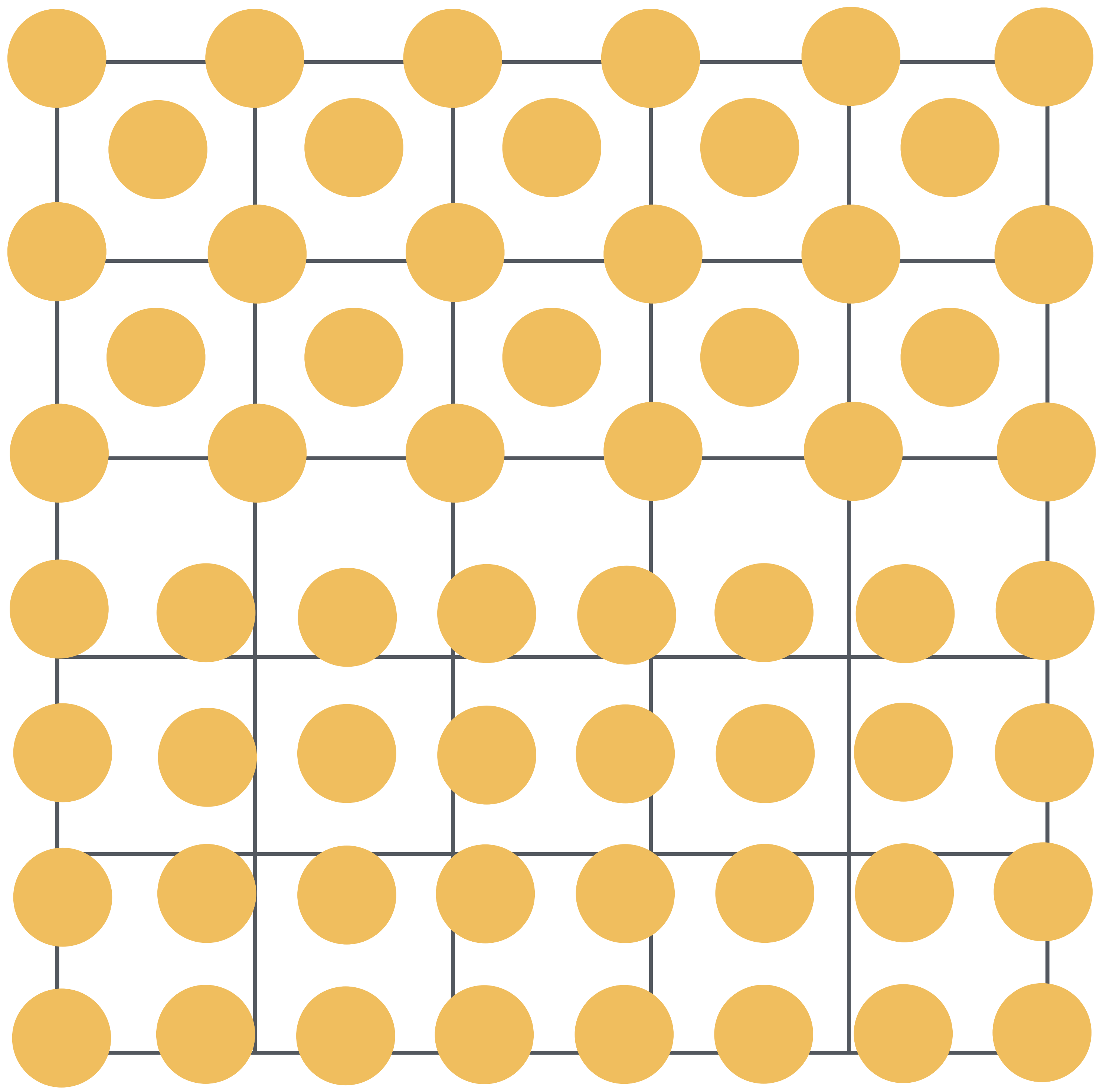
W-SO

with a fictitious perfect lattice



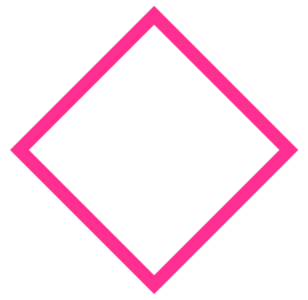
W-SO

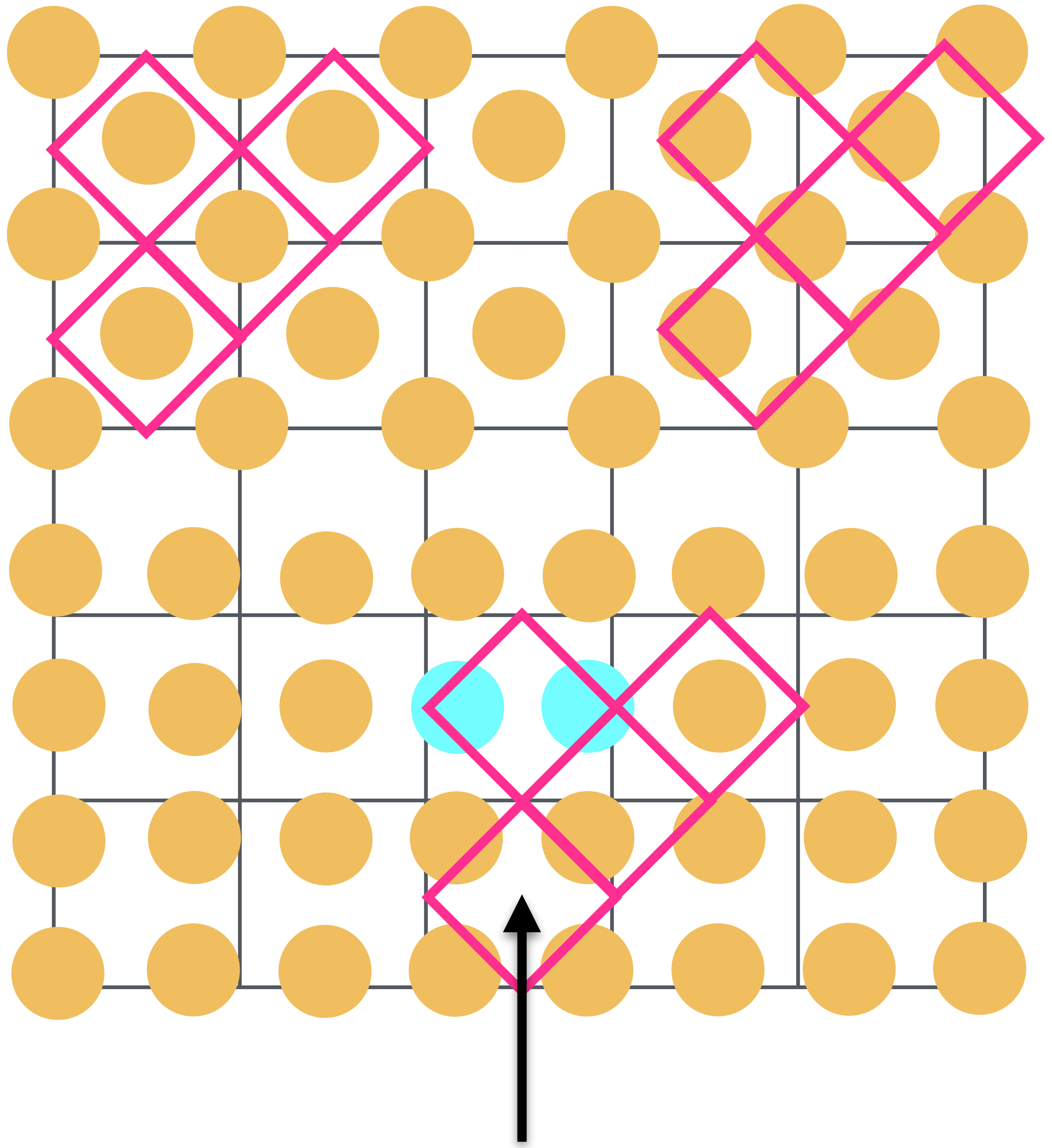
with a fictitious perfect lattice



W-SO

fails in polycrystalline structures





W-S cell

(Primitive cell)

Translation of reference lattice **hardly** matters

Rotation matters!!

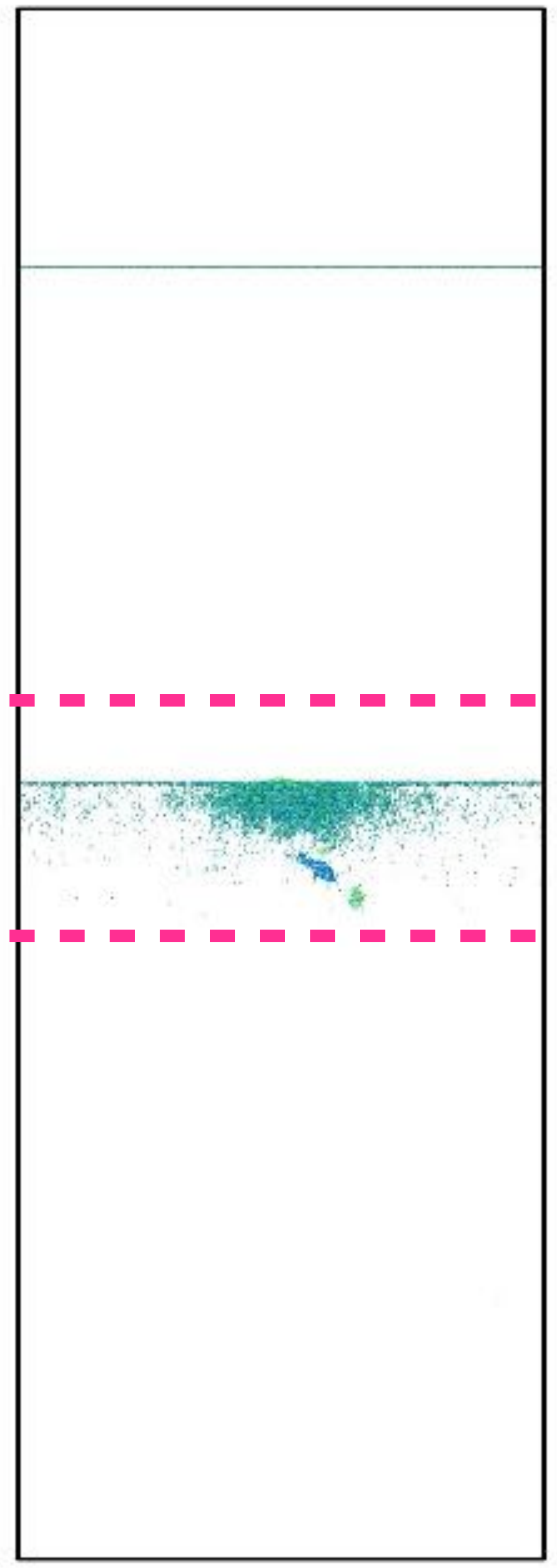
Interstitials

Interstitial-vacancy pair FALSE detection

W-S

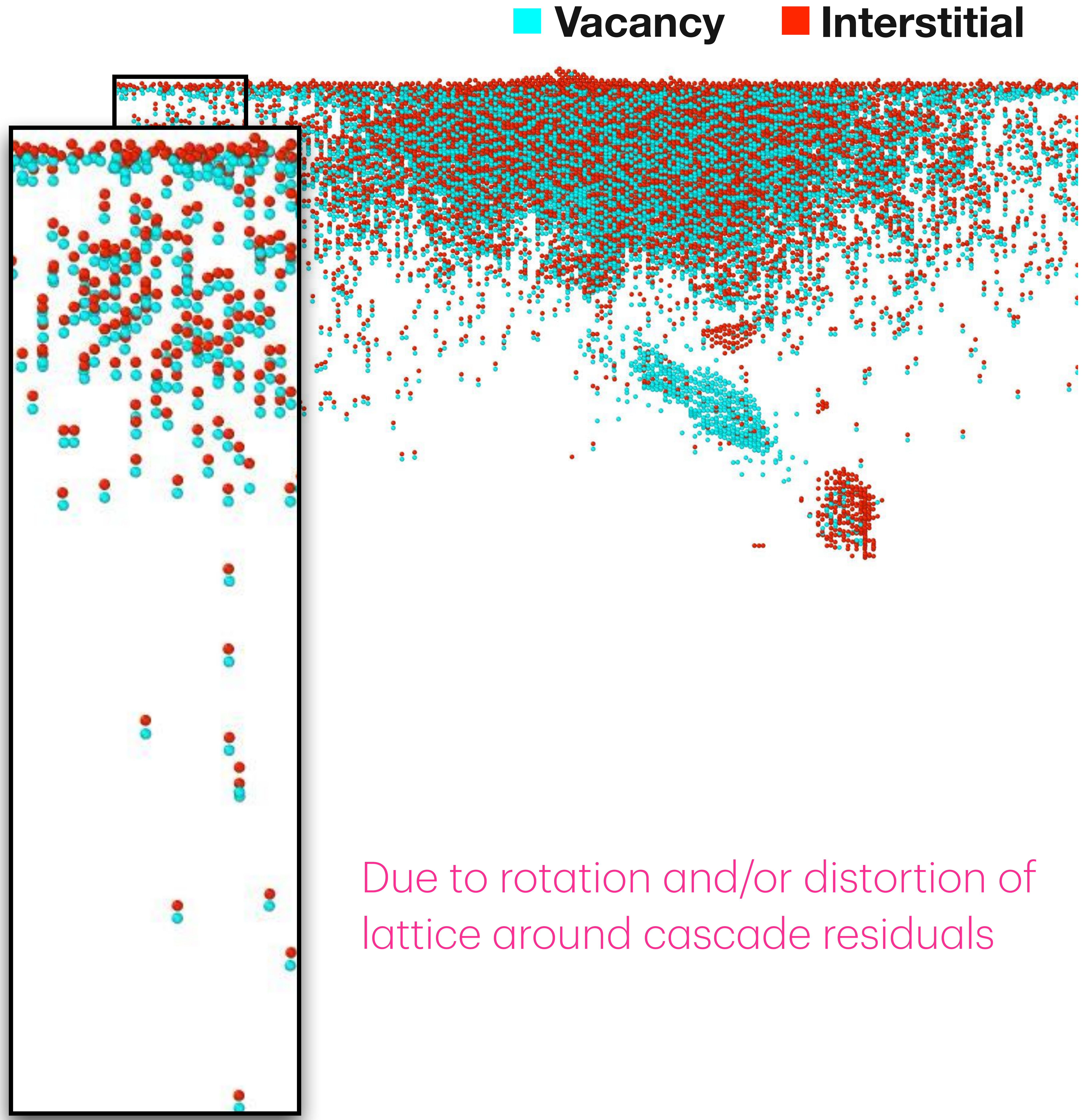
fails even for a clean GB

<100>



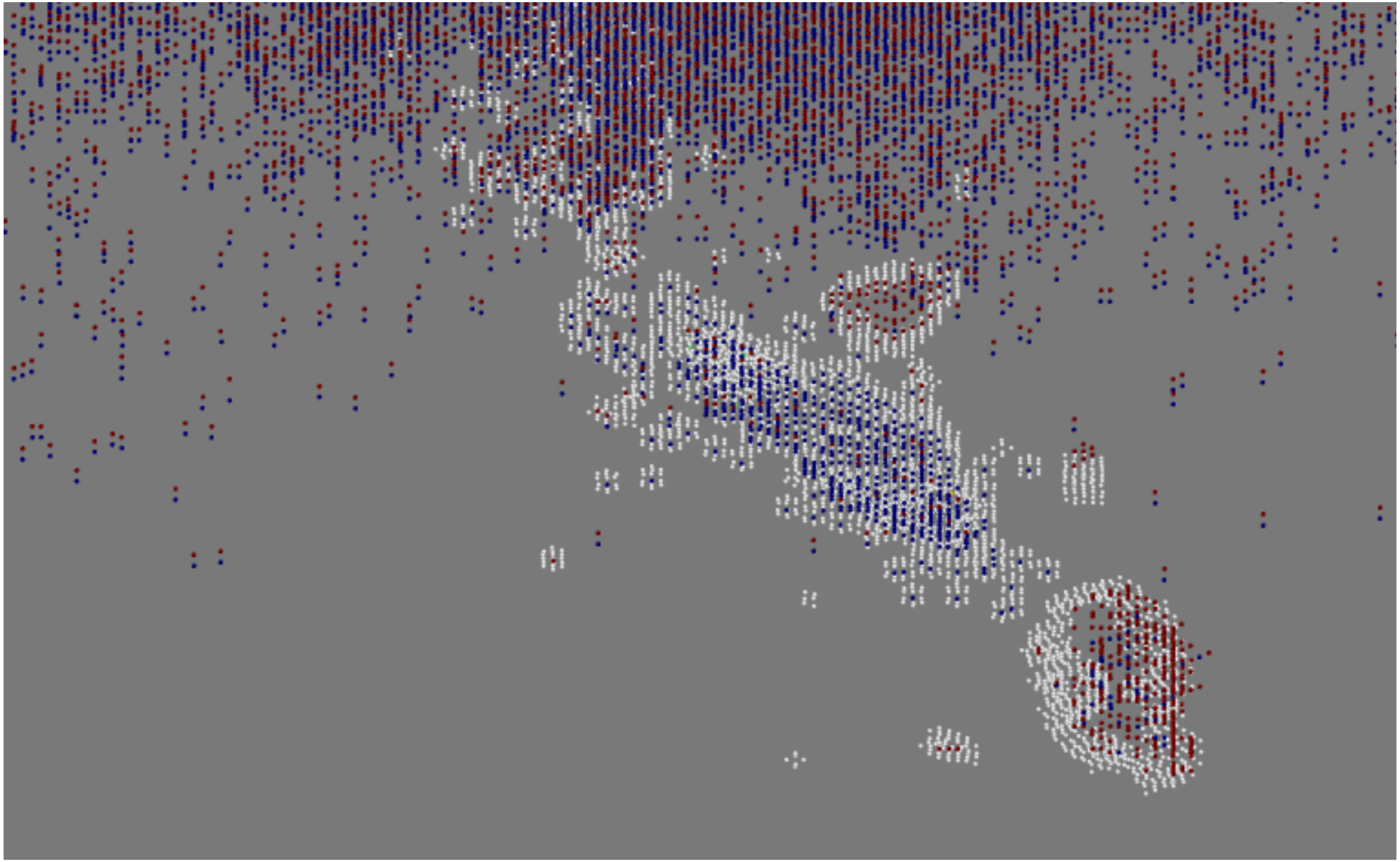
<111>

100 nm x 100 nm x 300 nm
PKA Energy = 300 keV @ 823K
PKA location = 1nm from GB

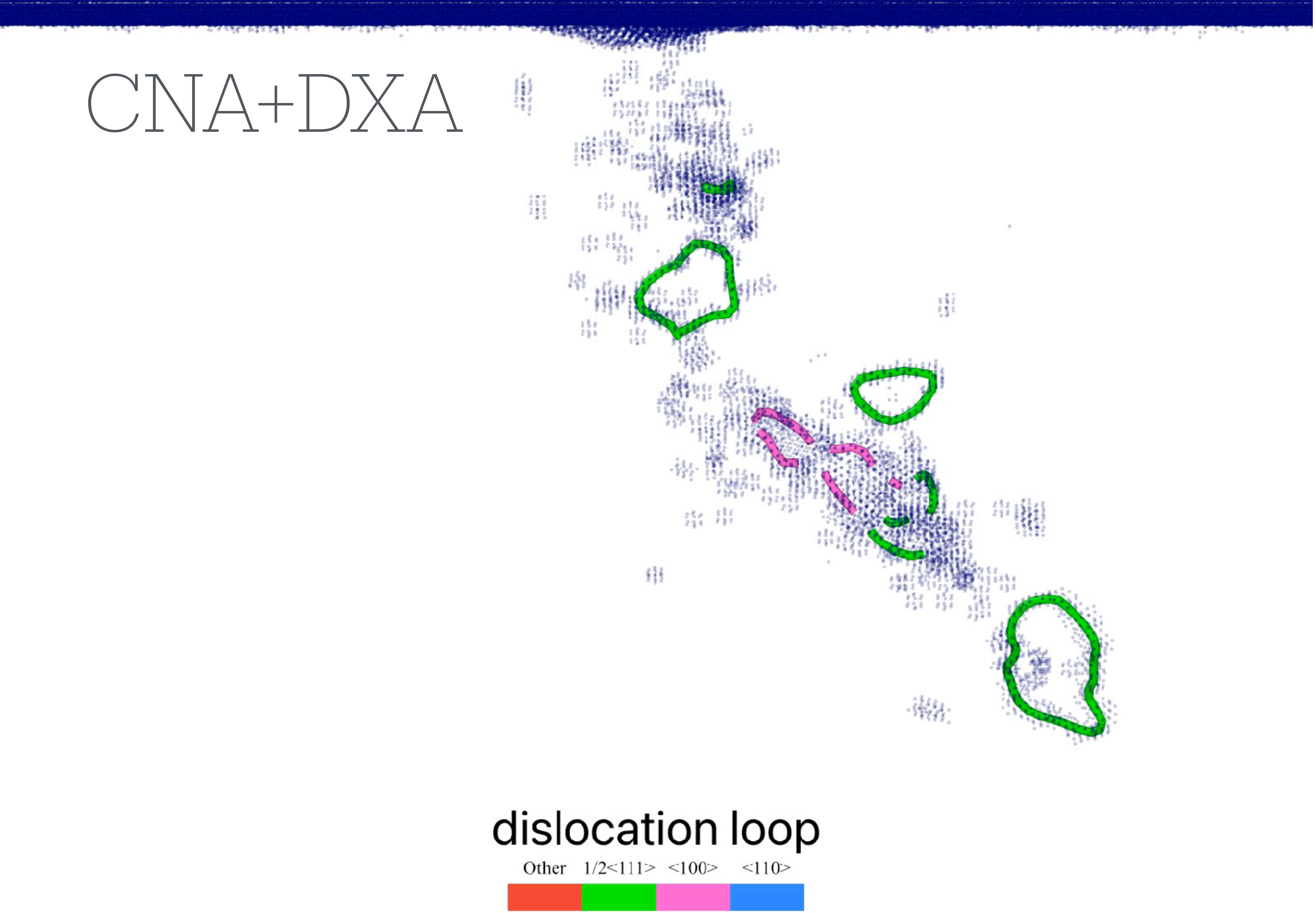


Due to rotation and/or distortion of lattice around cascade residuals

CNA+WS

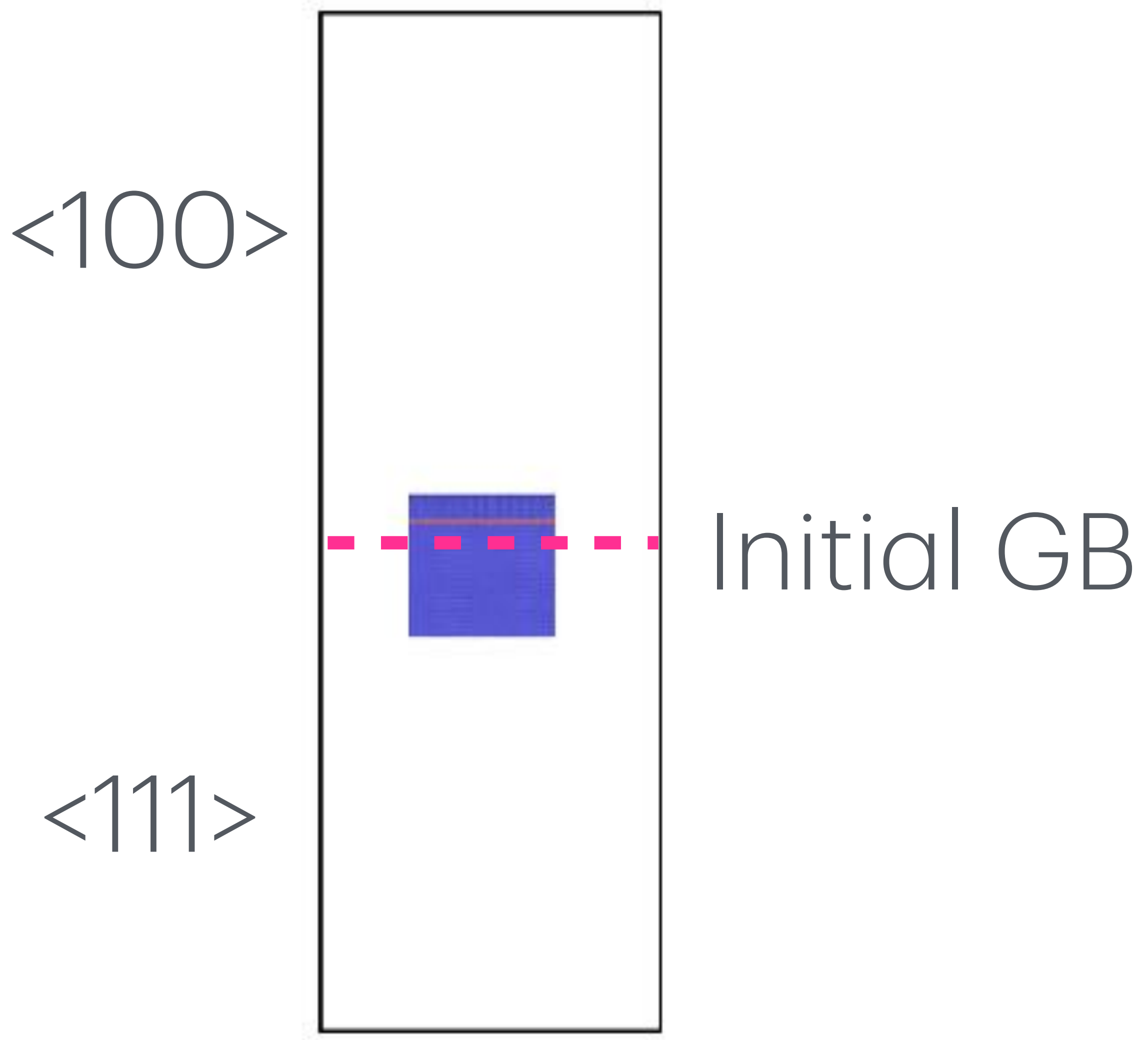


CNA+DXA



How to separate defects

in GB from those in bulk w/ defect type info?



bcc <100>/<111>

100 nm x 100 nm x 300 nm

PKA Energy = 300 keV @ 823K

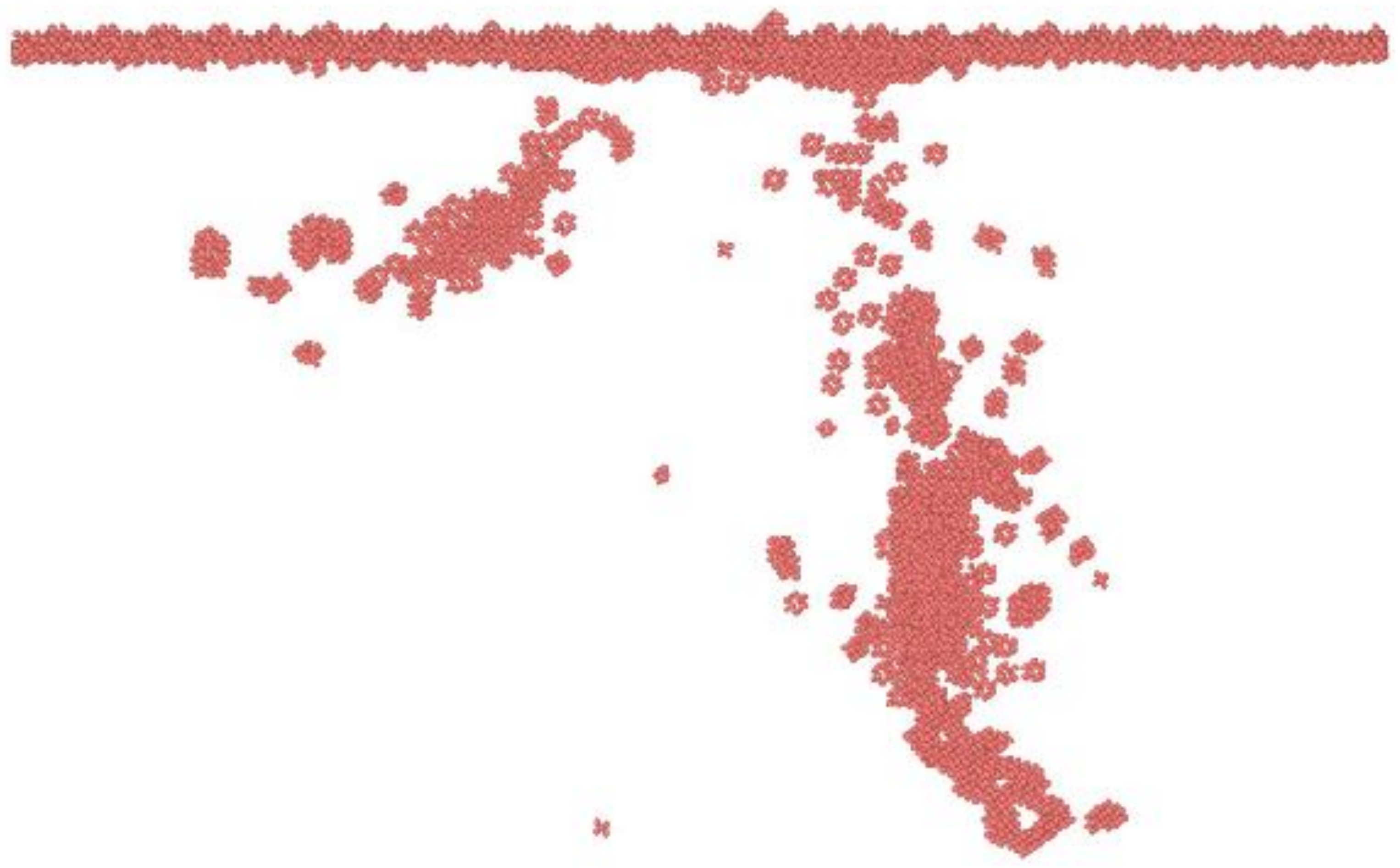
0 ps

defect count = 65,798

CNA only tells you either crystalline or other

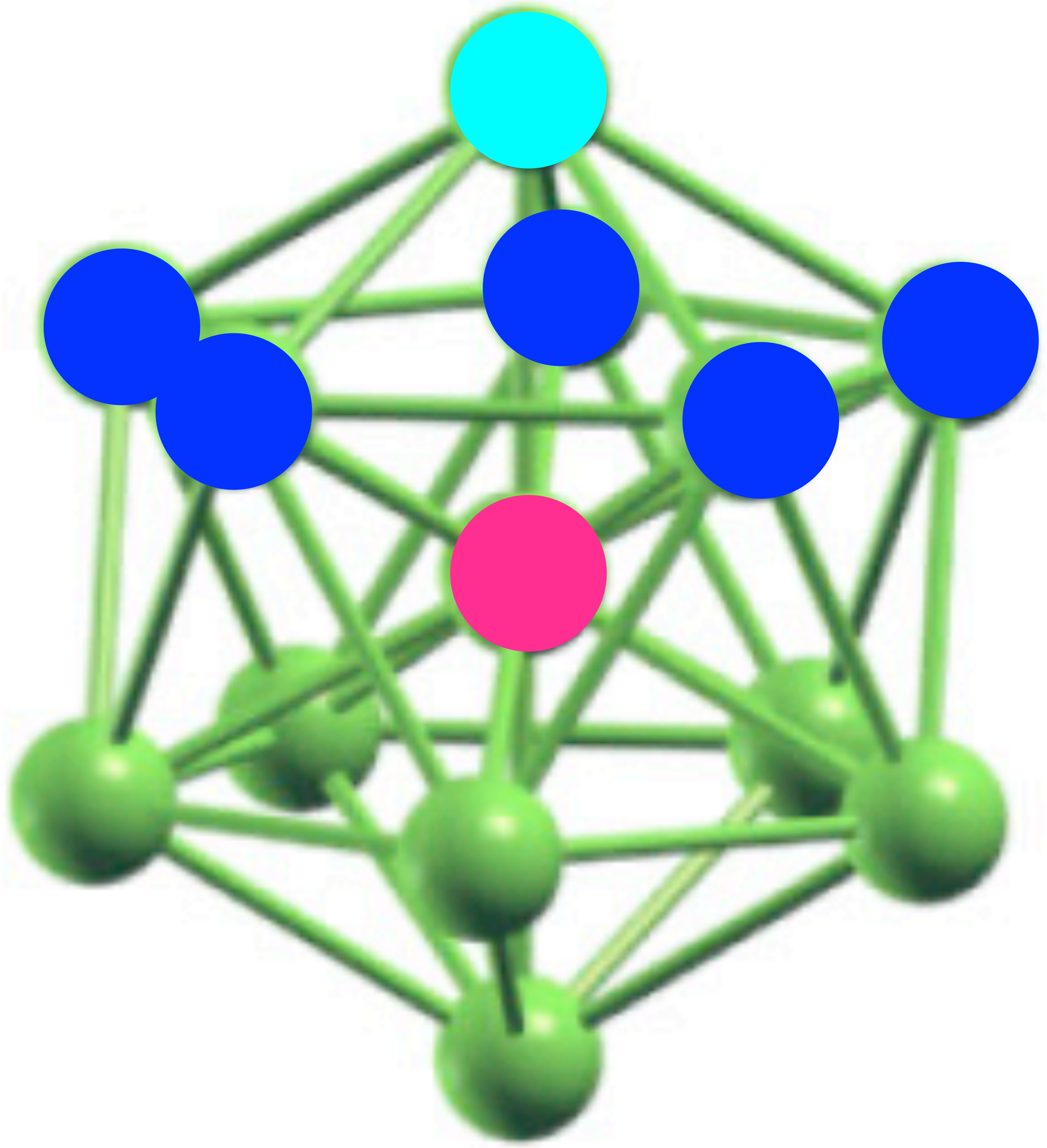
36.13 ps

defect count = 70,170



Deep inside

CNA

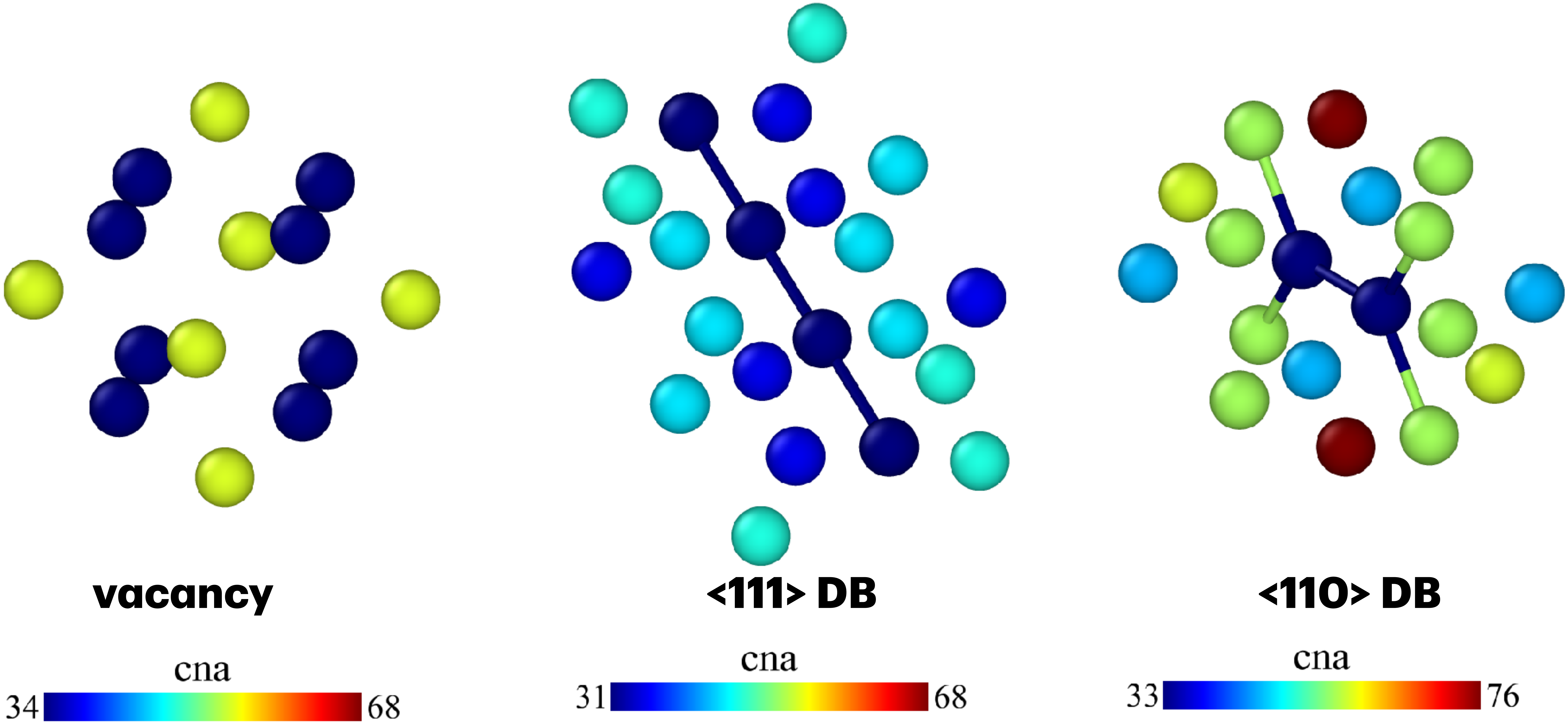


Bonded pairs	Stable liquid (2000 K)	Supercooled liquid (1700 K)	Ordered structure			
			bcc	fcc	hcp	ISRO
1101	0.04	0.02				
1201	0.12	0.08				
1211	0.06	0.04				
1301	0.07	0.06				
1311	0.22	0.19				
1321	0.09	0.09				0.71
1411	0.04	0.04				
1421	0.07	0.08		1.00	0.50	
1422	0.09	0.13			0.50	
1431	0.11	0.14				
1441	0.00	0.01	0.43			
1531	0.01	0.01				
1532	0.01	0.01				
1541	0.05	0.07				
1551	0.02	0.03				0.29
1661	0.00	0.01	0.57			

atom of interest
probe neighbor
common neighbors

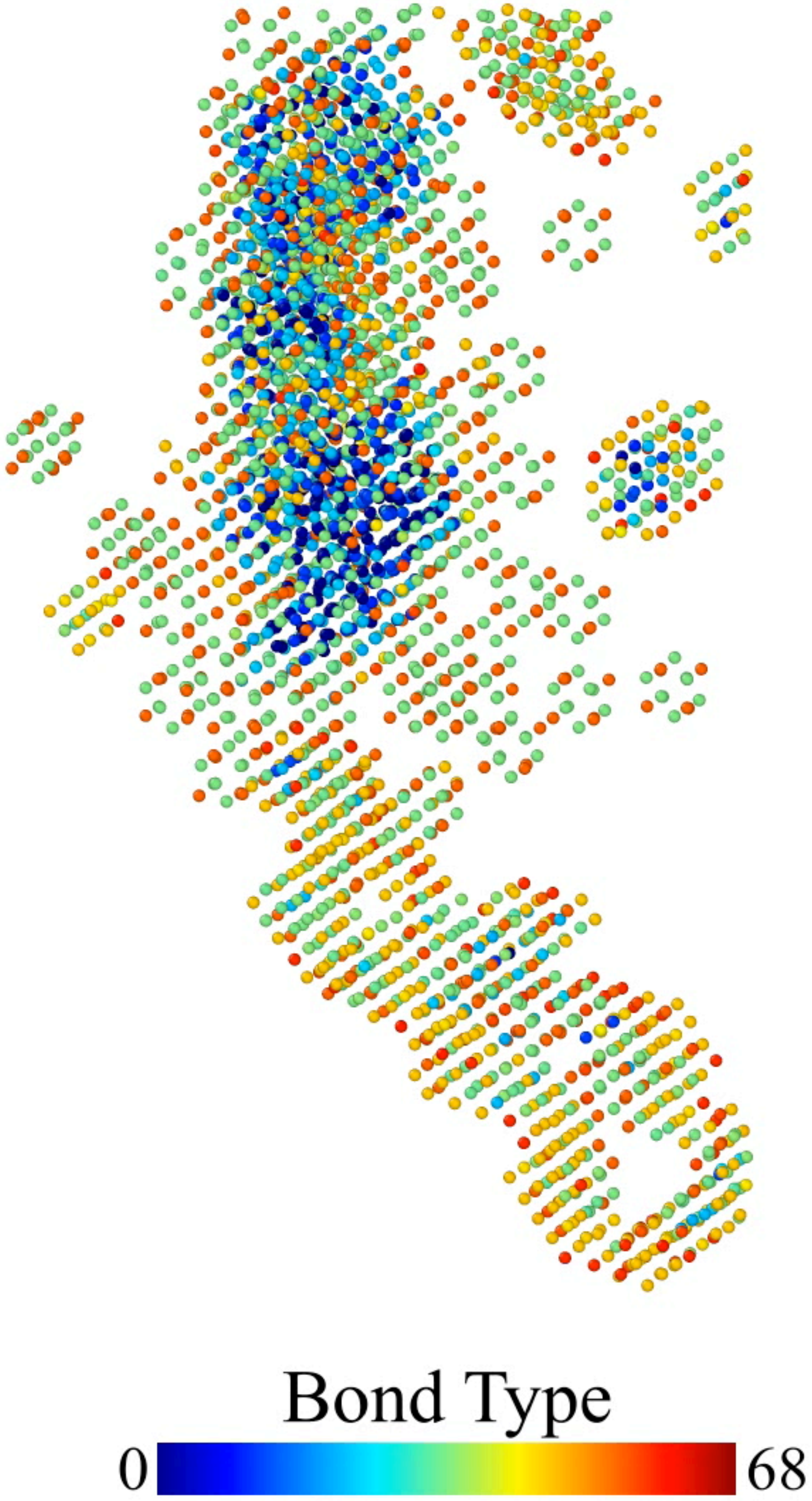
B. Lee et al. | JCP 129, 024711 (2008)

CNA goes beyond non-bcc

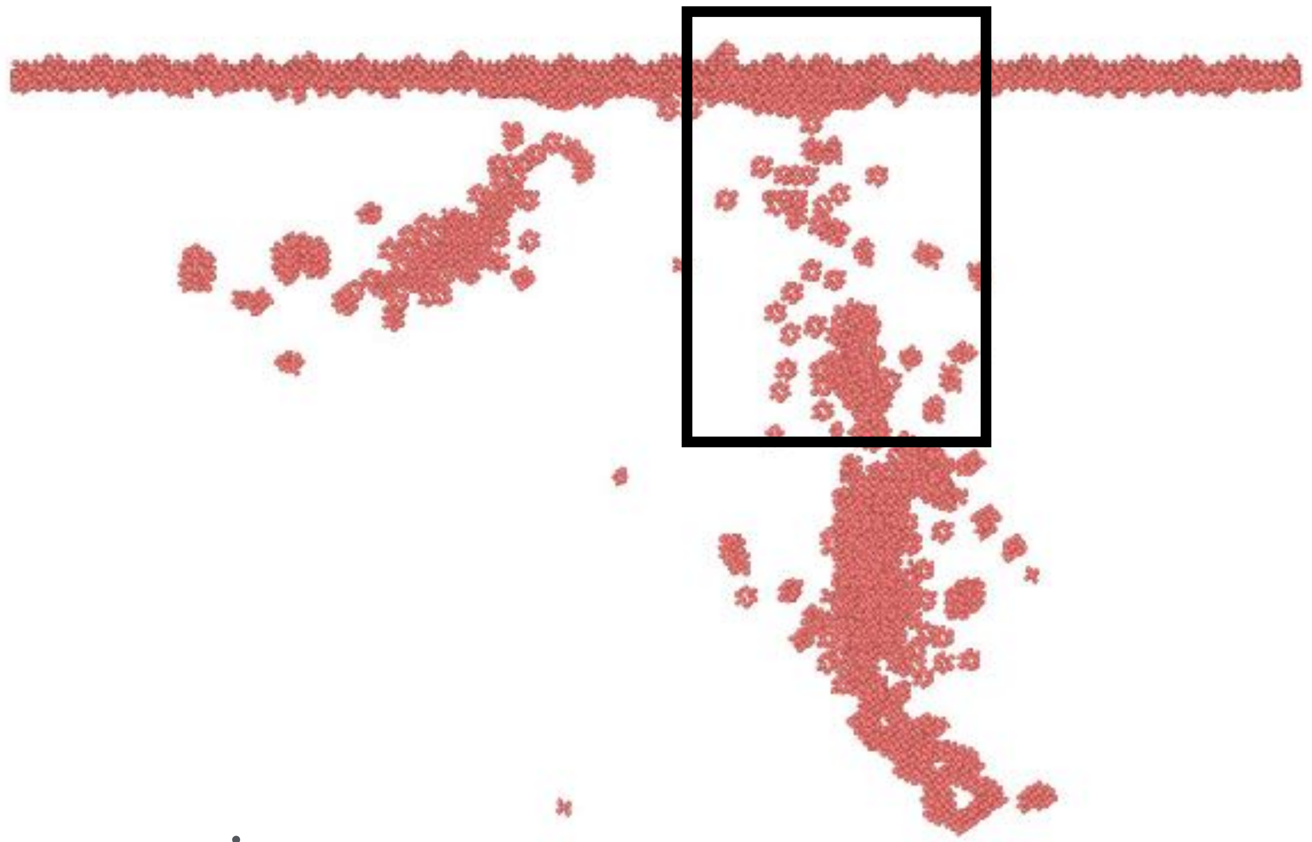


CNA

with bond types

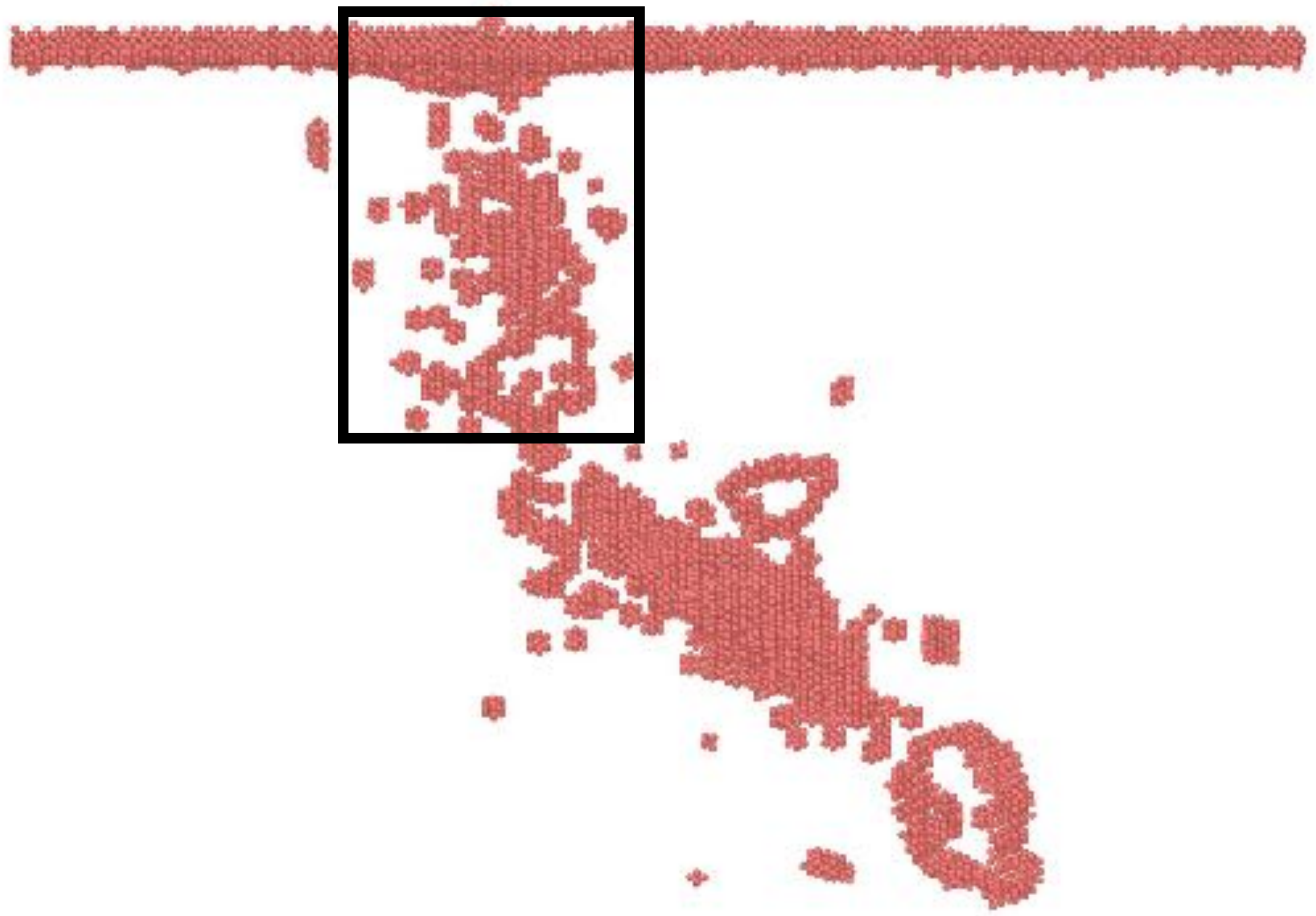


Crystal growth
from GB



Front view

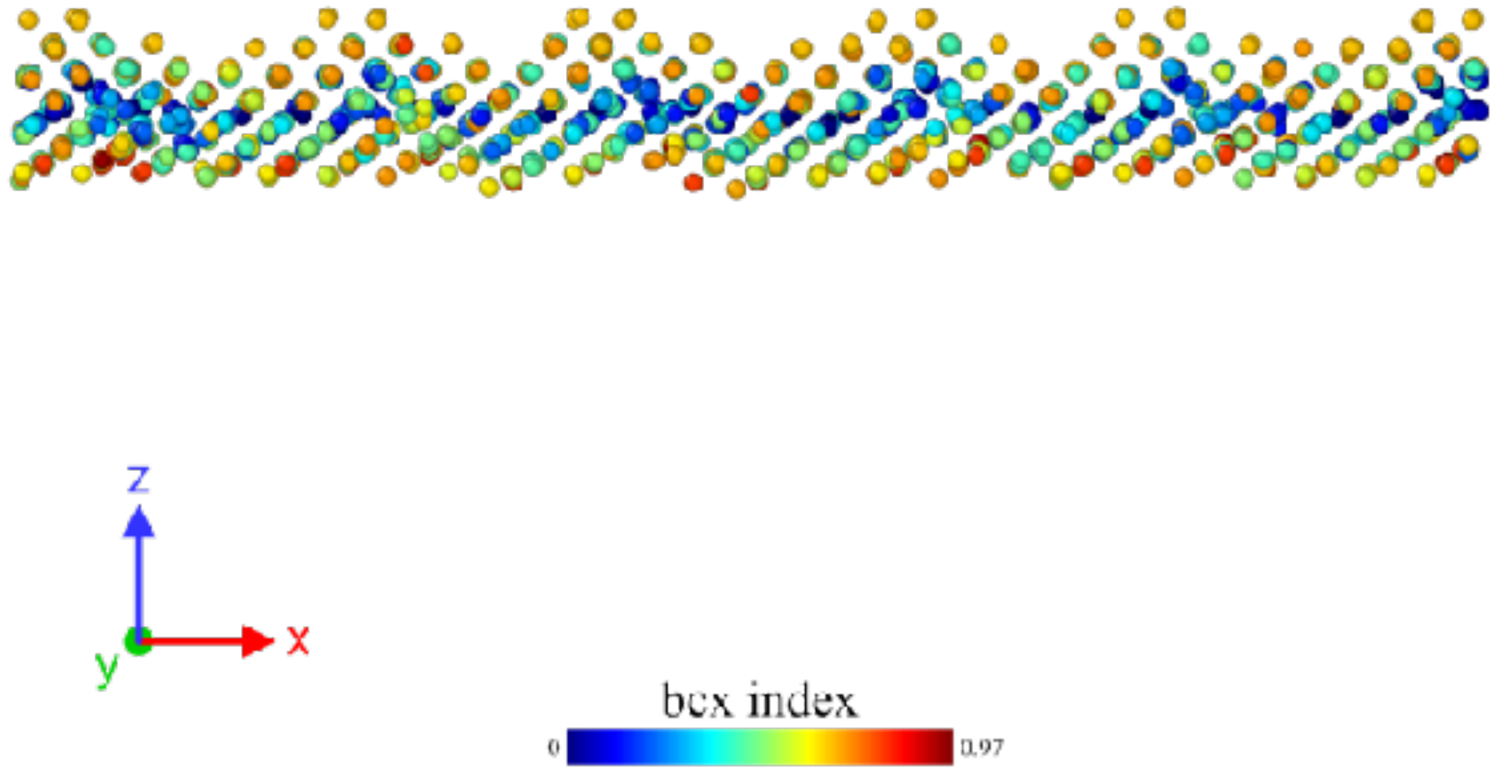
Side view



0 ps

GB atoms : 3,771

Bulk defects : 0



36.13 ps

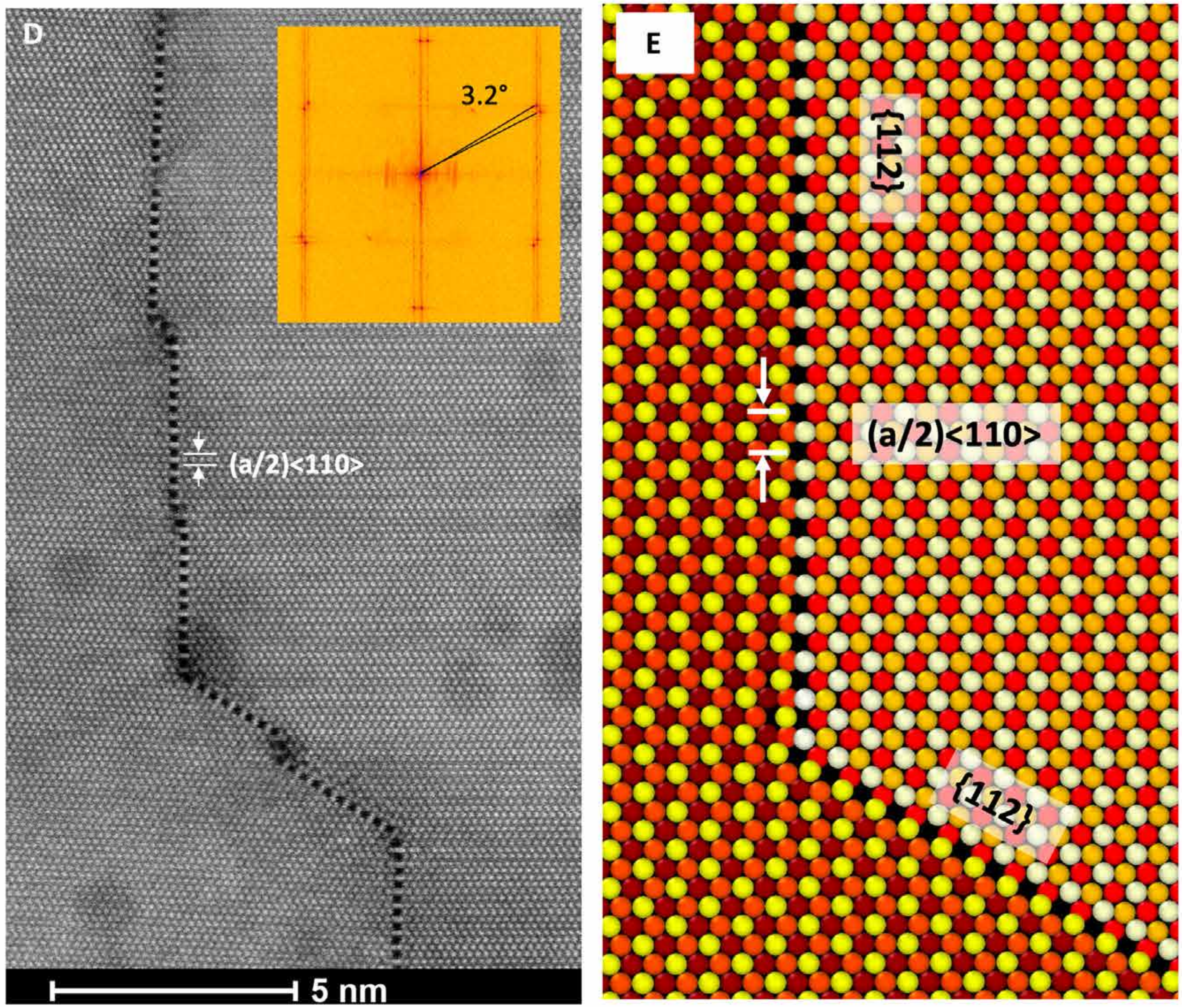
GB atoms : 3,686

Bulk defects : 1,118

CNA w/ bond type results

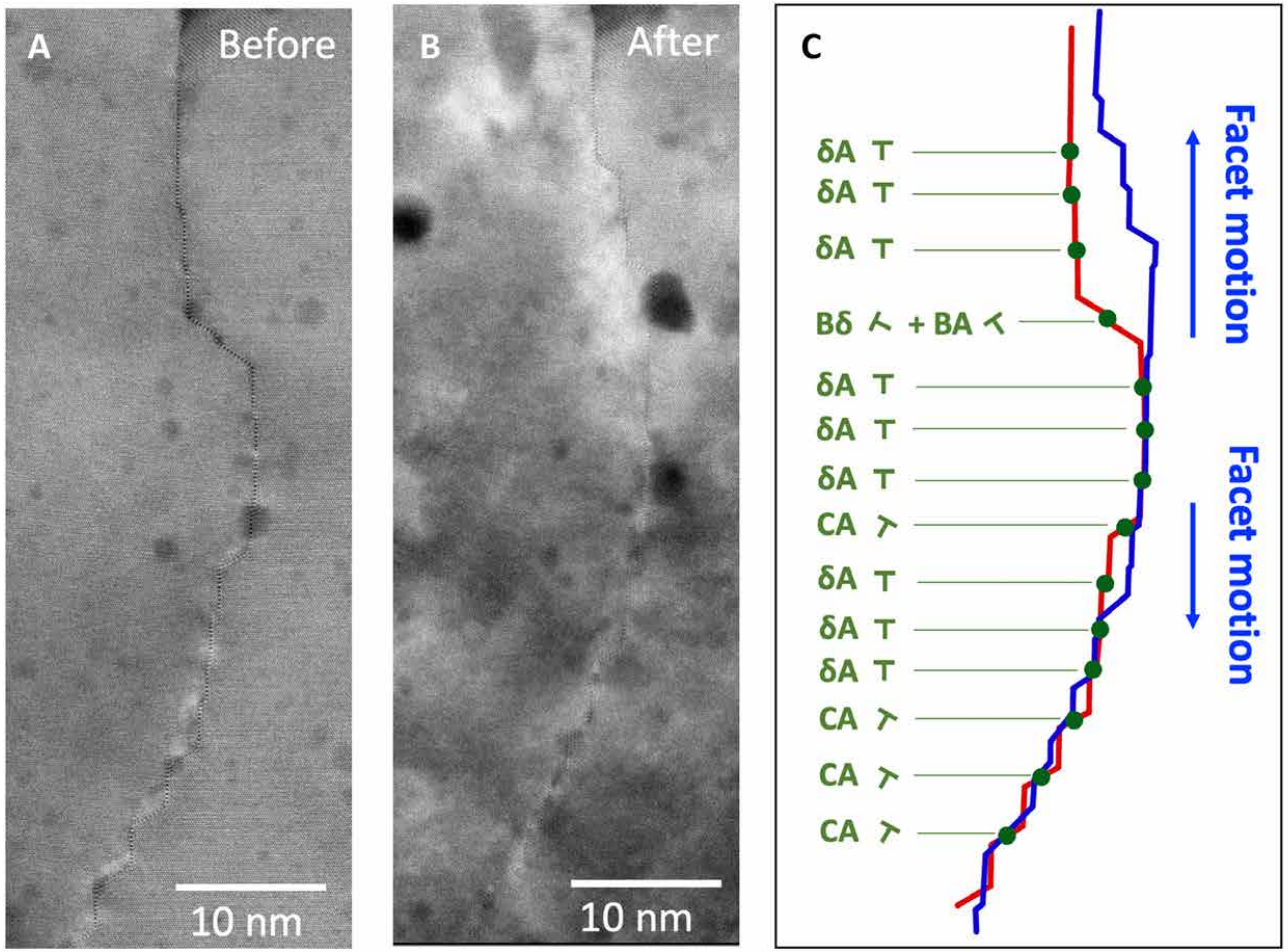
Irradiation damages

near GB



Pt Σ3 {112} GBs

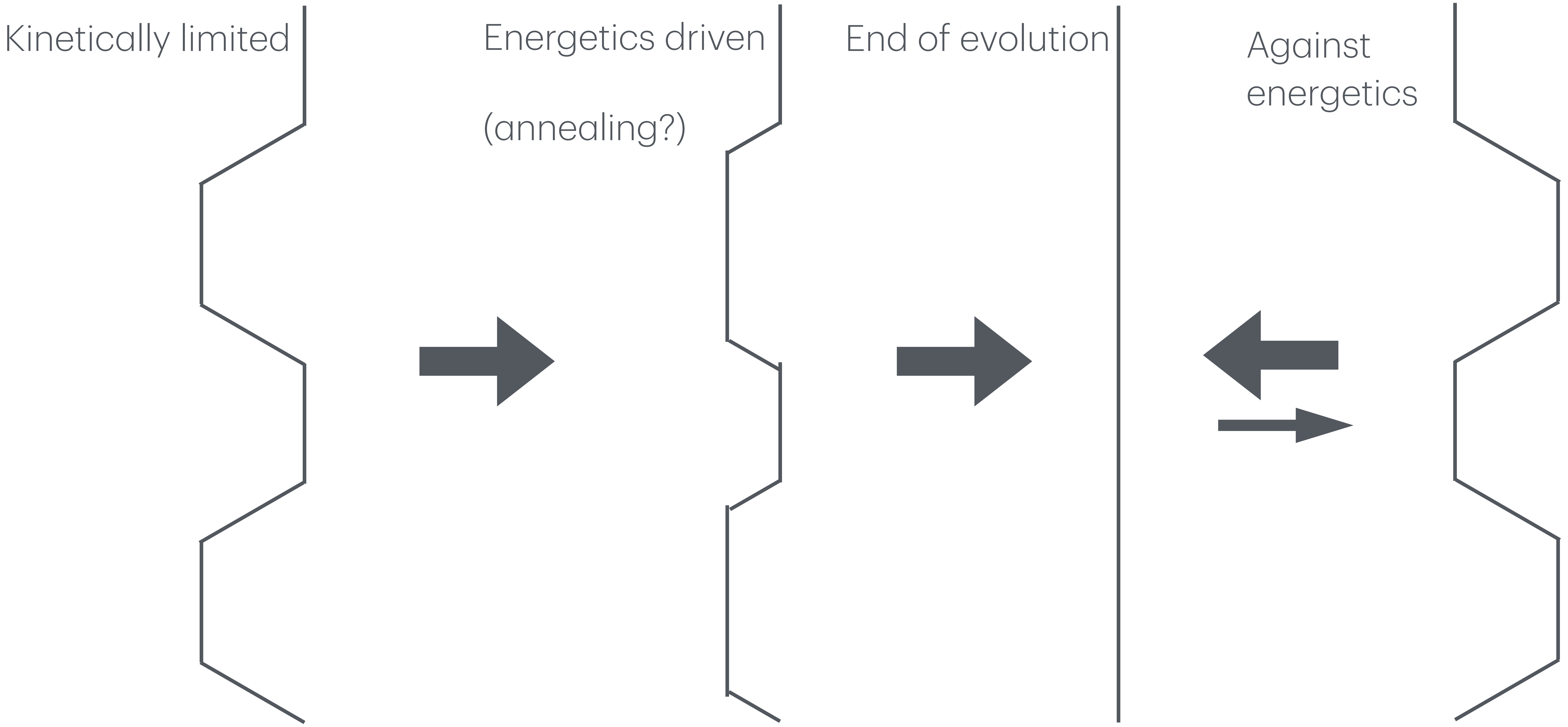
~ 1 dpa w/ 2.8 MeV Au4+



C. M. Barr et al. | Sci. Adv. **8**, eabn0900 (2022)

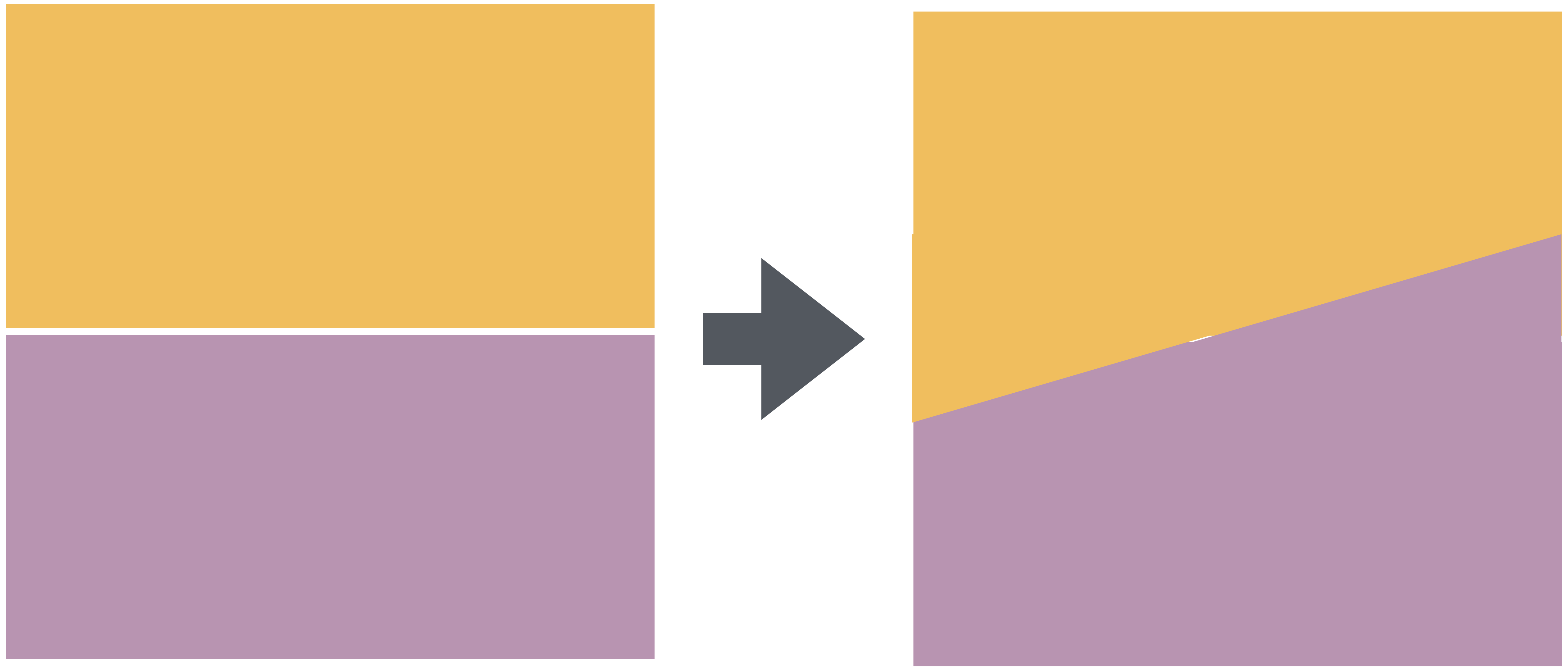
End of evolution scenario?

Moving Vs Flattening?



GB energetics

to find optimum



- Nucleation
  - Crystal growth
  - Dislocations
- Energetics
  - GB facet/surface energies
  - GB area

Is GB transparent to neutron irradiation?

Likely… as far as GB degradation goes

GB is a defect sink, and the source of other defects

It will be interesting to see how GBs do

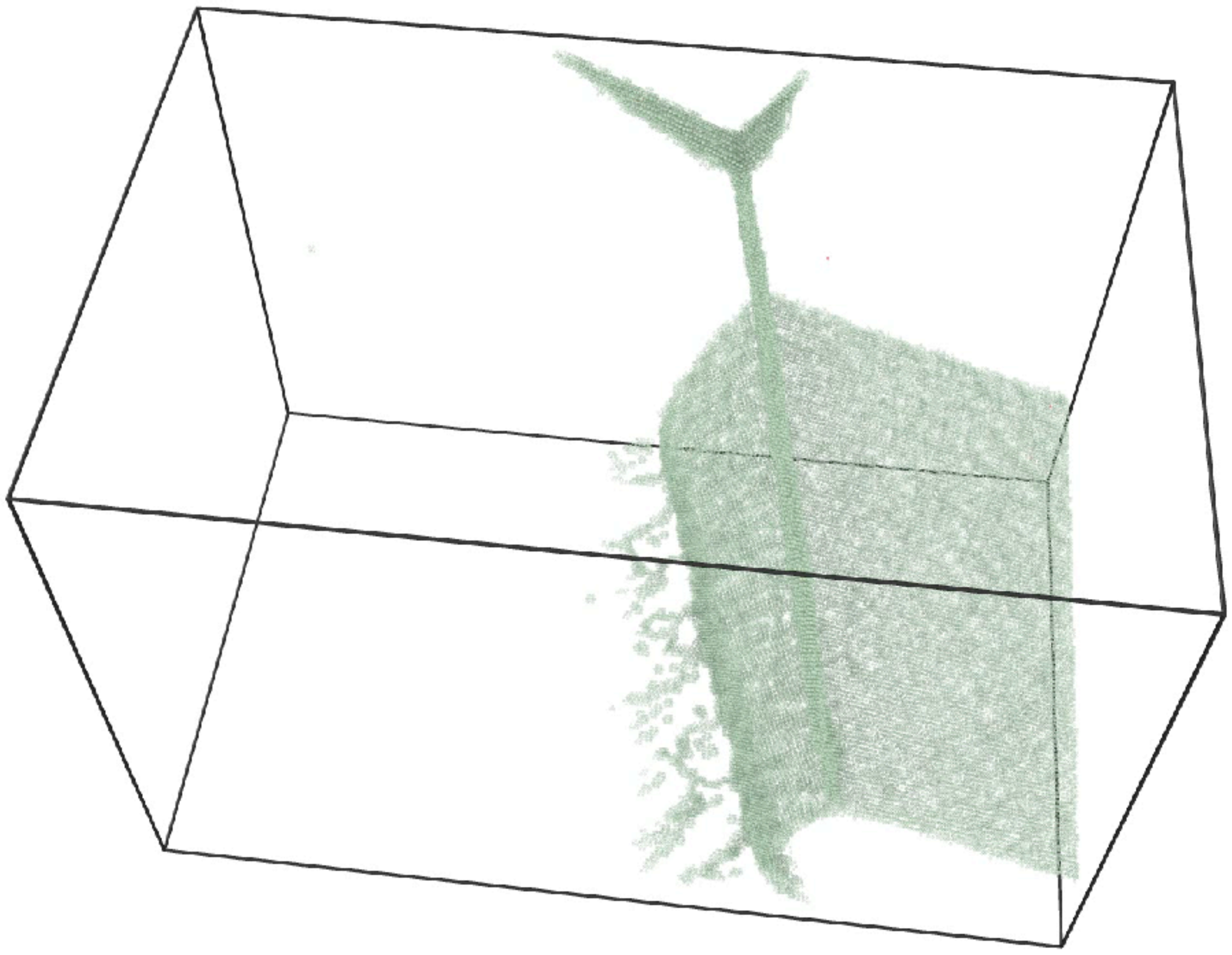
in the presence of transmutation and hydrogen

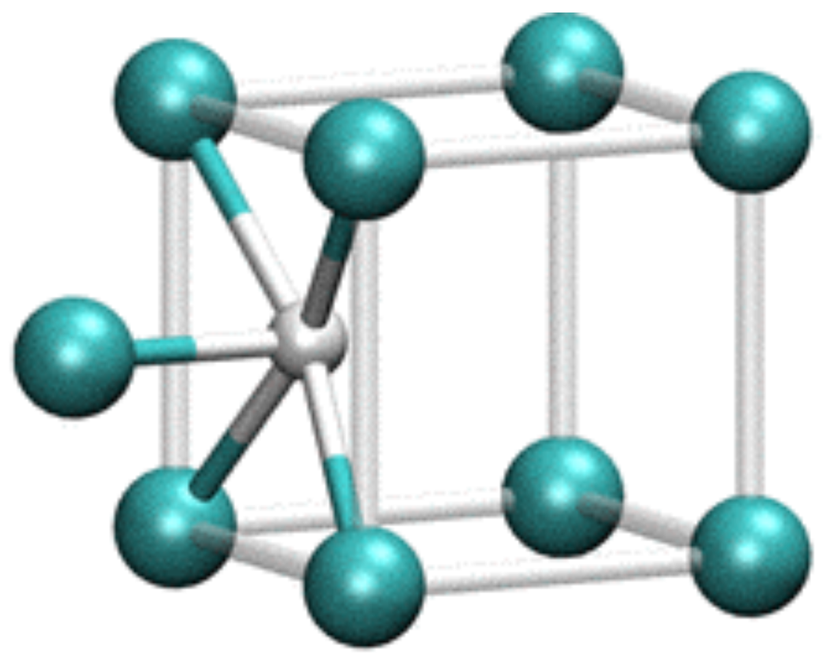
Remarks

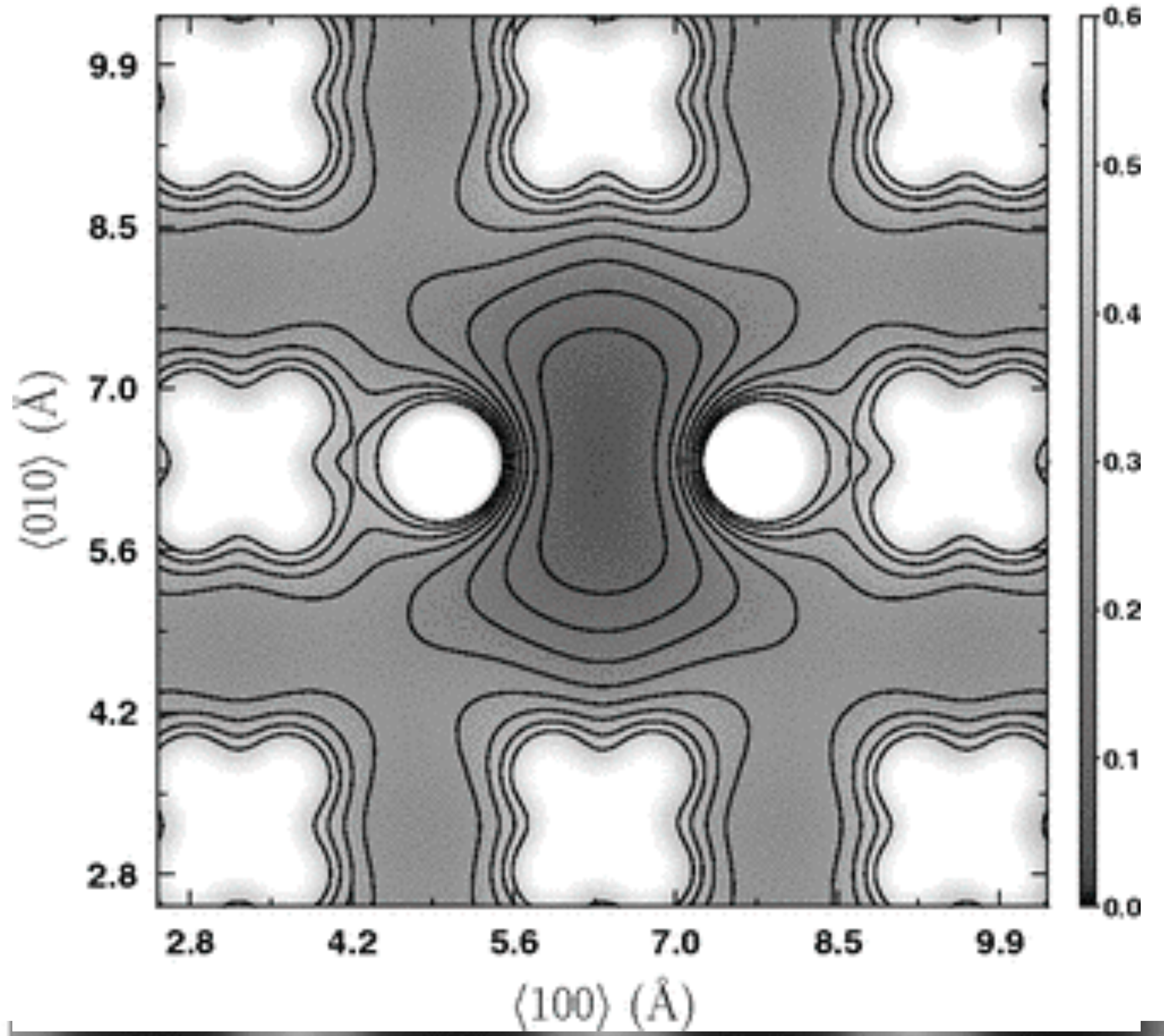
During irradiation

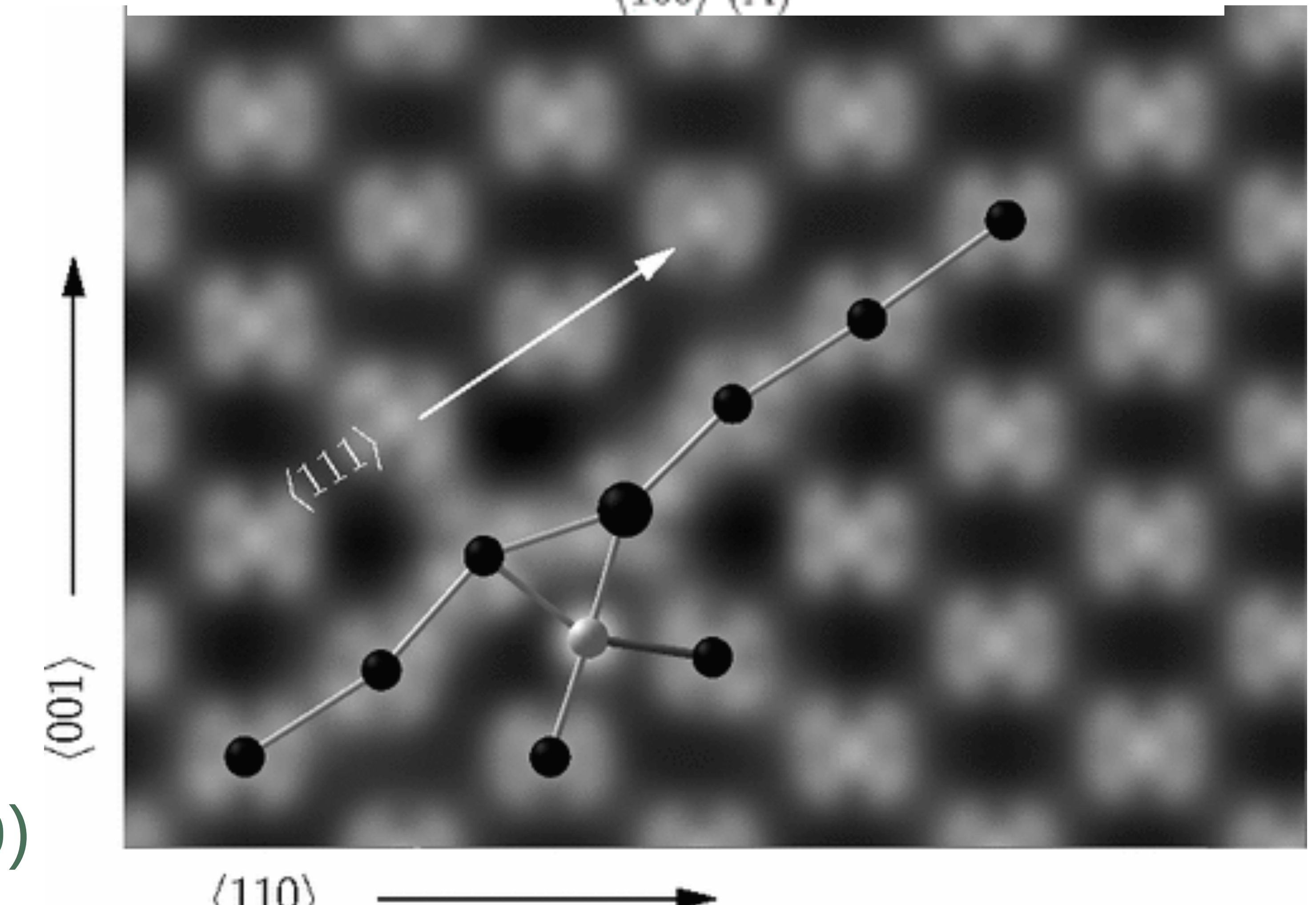
- CNA seems promising for detections of various defects including GBs
  - **Fine-tuning in progress**
- Irradiation may stabilize the microstructure?
  - GBs may realign to reduce energy penalty
  - GB energy reduction **= grain growth?**

Future outlook









Y. Shin et al. | unpublished

K. Heinola et al. | Phys. Rev. B 82, 094102 (2010)

Thank you!