Computational investigation of radiation damage in $YBa_2Cu_3O_7$ superconducting tapes for nuclear fusion applications

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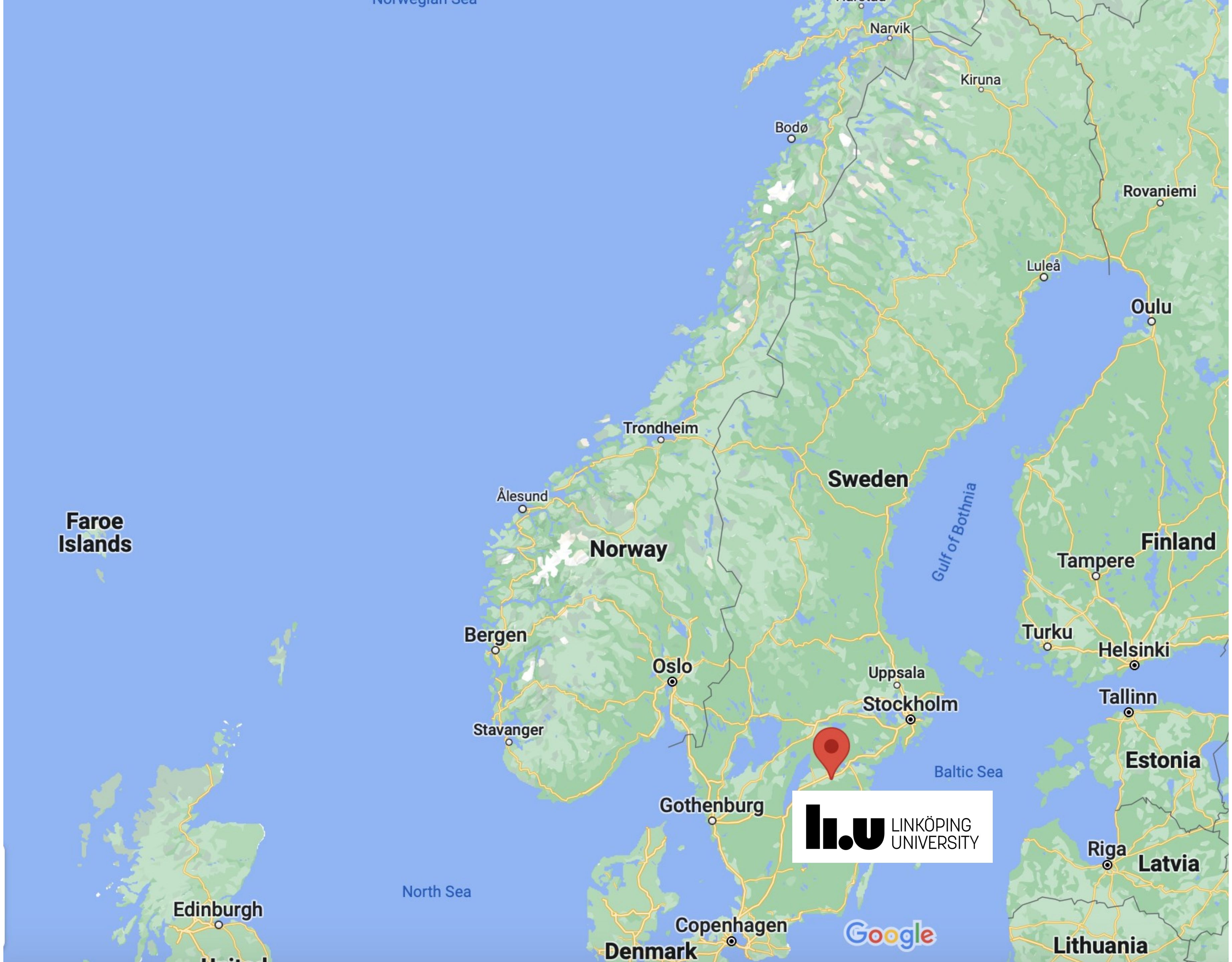
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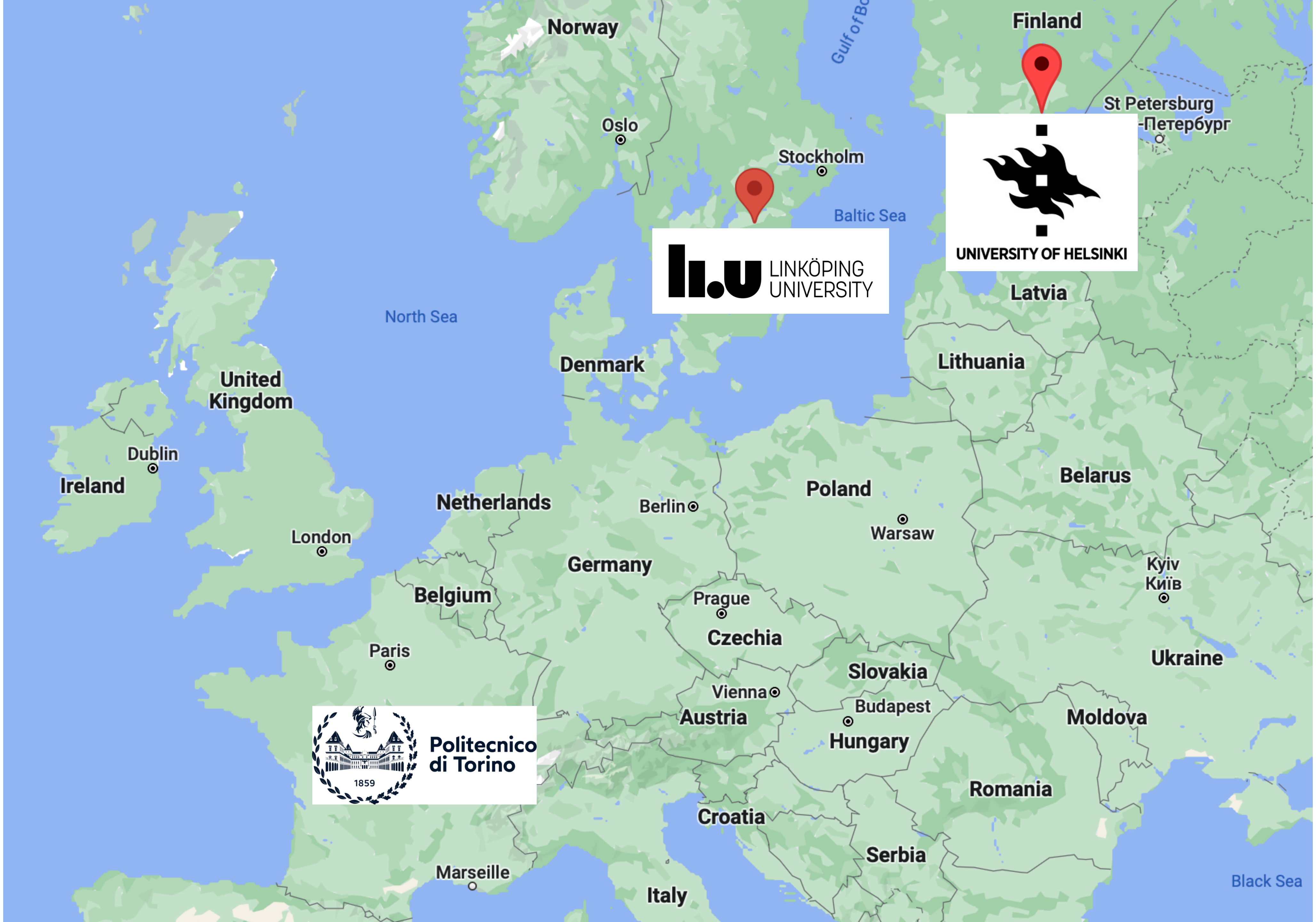

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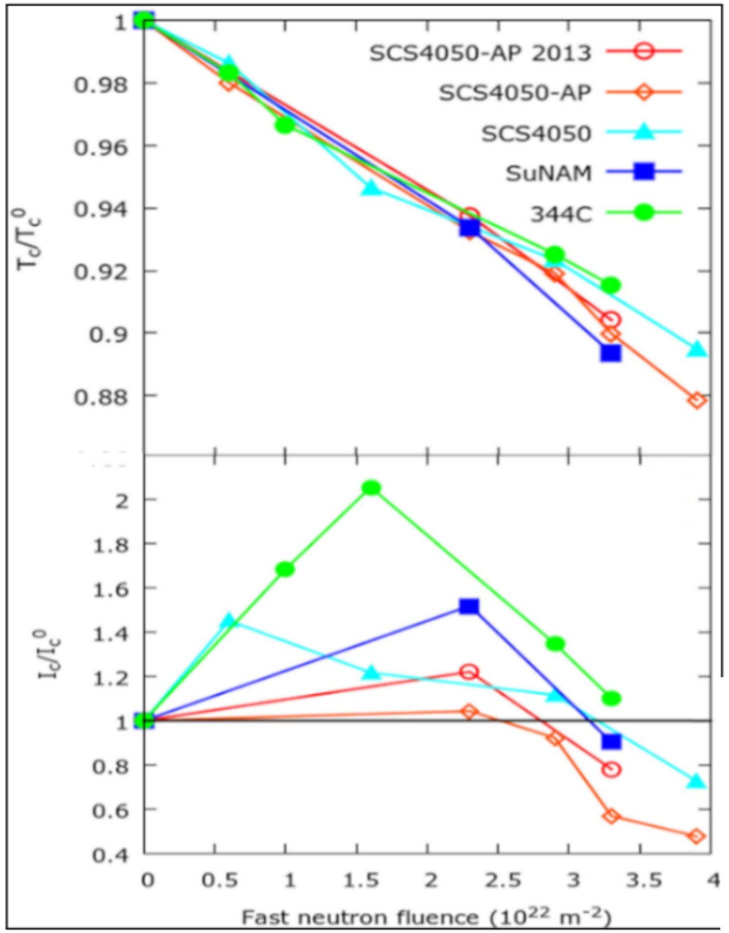
Magnetic confinement approach – ARC reactor

Compact fusion reactors such as ARC

Magnetic confinement approach – ARC reactor

Compact fusion reactors such as ARC



Fischer *et.al.* SuST (2018)

Neutron damage affects SC properties

- Enhances **carriers scattering** that **decreases** $\boldsymbol{T_c}$
- Defects act as **pinning centers** that **increase** $\boldsymbol{j_c}$
- The effect on J_c is difficult to be predicted and depends on the pristine pinning landscape

Magnetic confinement approach – ARC reactor

Compact fusion reactors such as ARC

Fischer *et.al.* SuST (2018)

Neutron damage

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Need to evaluate expected damage and its effects on HTS in ARC

Expected radiation environment and damage for YBCO tapes in compact fusion reactors

Superconductor Science and Technology

PAPER

Expected radiation environment and damage for YBCO tapes in compact fusion reactors

D Torsello[5,6,1,2], D Gambino[5,3], L Gozzelino[1,2], A Trotta[4] and F Laviano[1,2]

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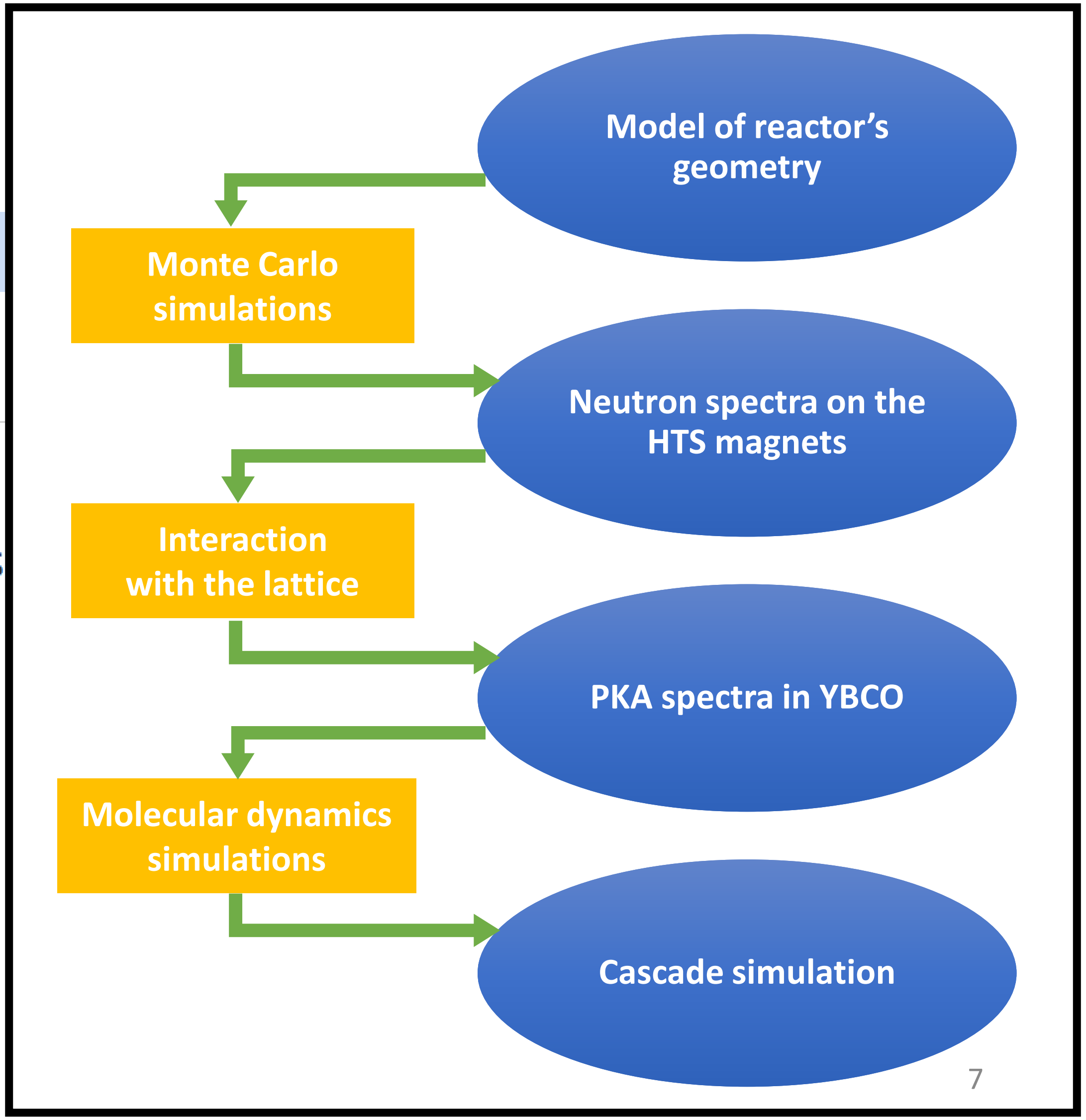
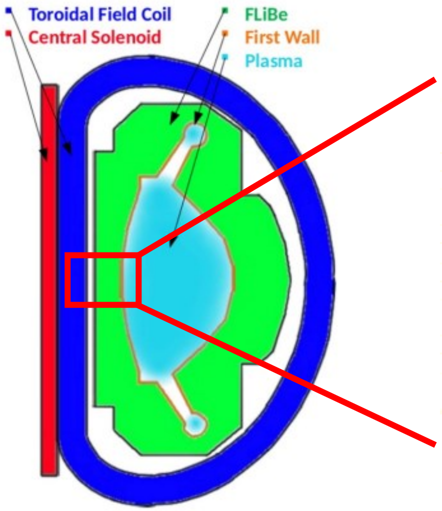


Neutron transport

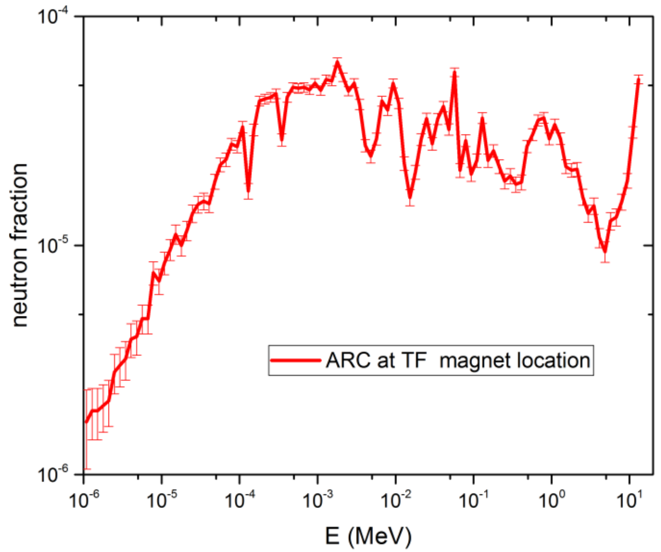
Parameter	ARC (expected in 10 years)	TRIGA (Fischer*et al* [12])
Fast neutron fluence (neutrons cm^{-2})	1.6×10^{19}	4.0×10^{18}
dpa	0.52	0.02
H yield (appm dpa^{-1})	0.5	0
He yield (appm dpa^{-1})	10.6	0

PHITS
Particle and Heavy Ion Transport code System

Model of reactor's geometry → **Monte Carlo simulations** → **Neutron spectra on the HTS magnets**



Component	Material	Density (g cm^{-3})	Thickness (cm)
FW	W	19.25	0.1
VV	Inconel steel	8.44	1
Molten salt	F_4Li_2Be	1.94	2
Multiplier	Be	1.85	1
VV	Inconel steel	8.44	3
Molten salt	F_4Li_2Be	1.94	100
VV	Inconel steel	8.44	3
TF	$YBa_2Cu_3O_7$	6.40	20



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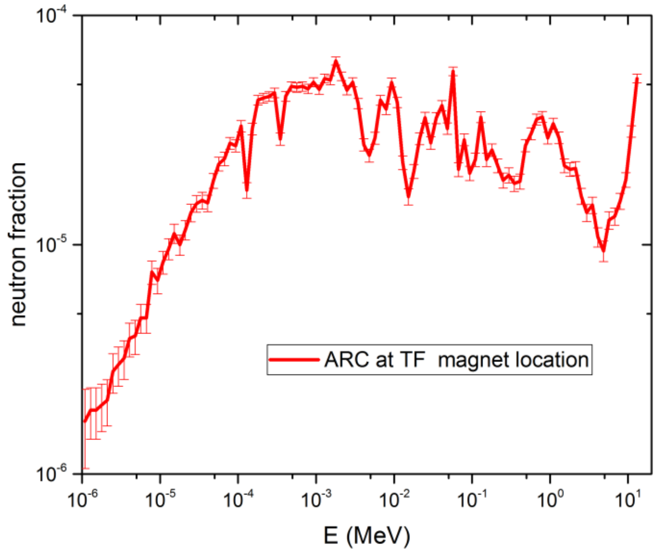
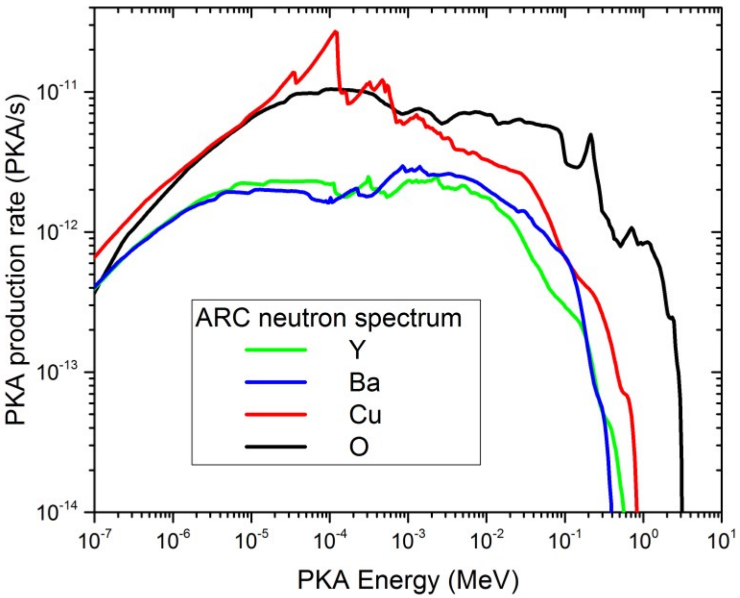
Neutron-lattice interaction

PKA-SPECTRA

Neutron spectra on the HTS magnets → **Interaction with the lattice** → **PKA spectra in YBCO**



- Primary Knock-on Atom (PKA) spectra needed for MD simulations
- Complex spectra result from elastic and inelastic interactions



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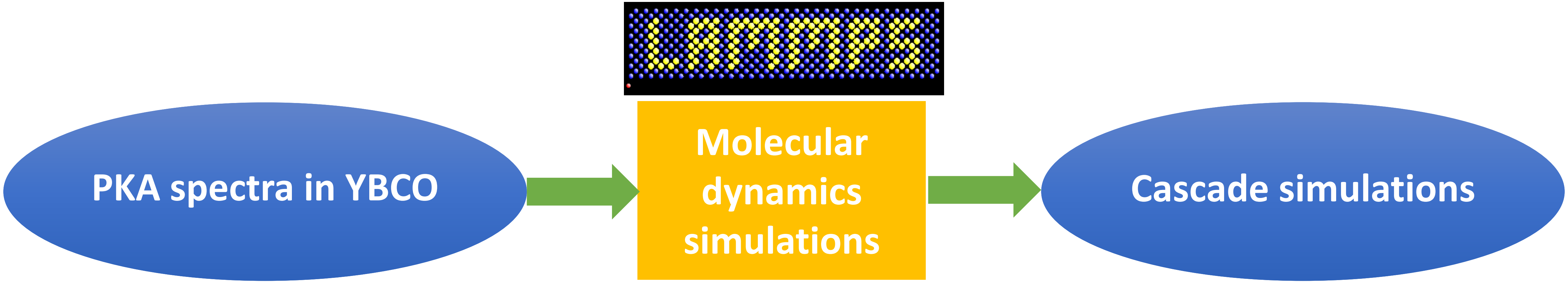
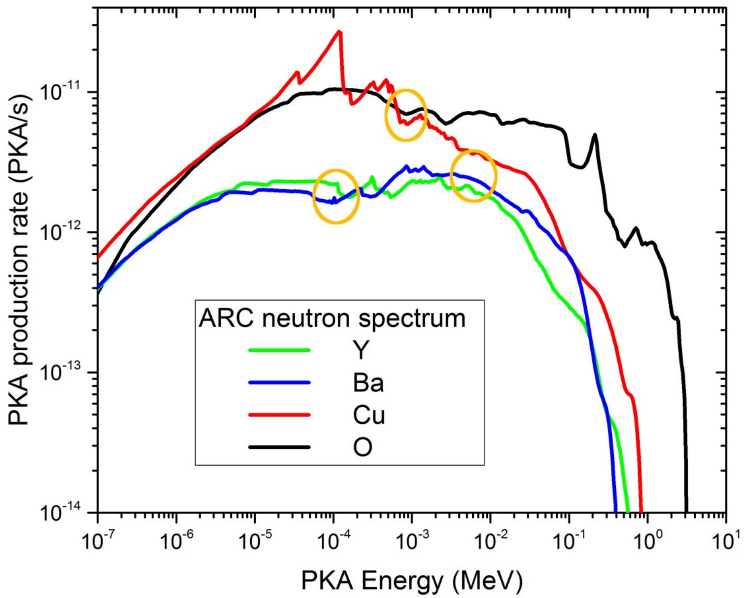
Cascade simulation





- Collision cascade simulations
- Results:
  - Defect size vs energy
  - Defect morphology
  - Defect recombination
  - Temperature transients

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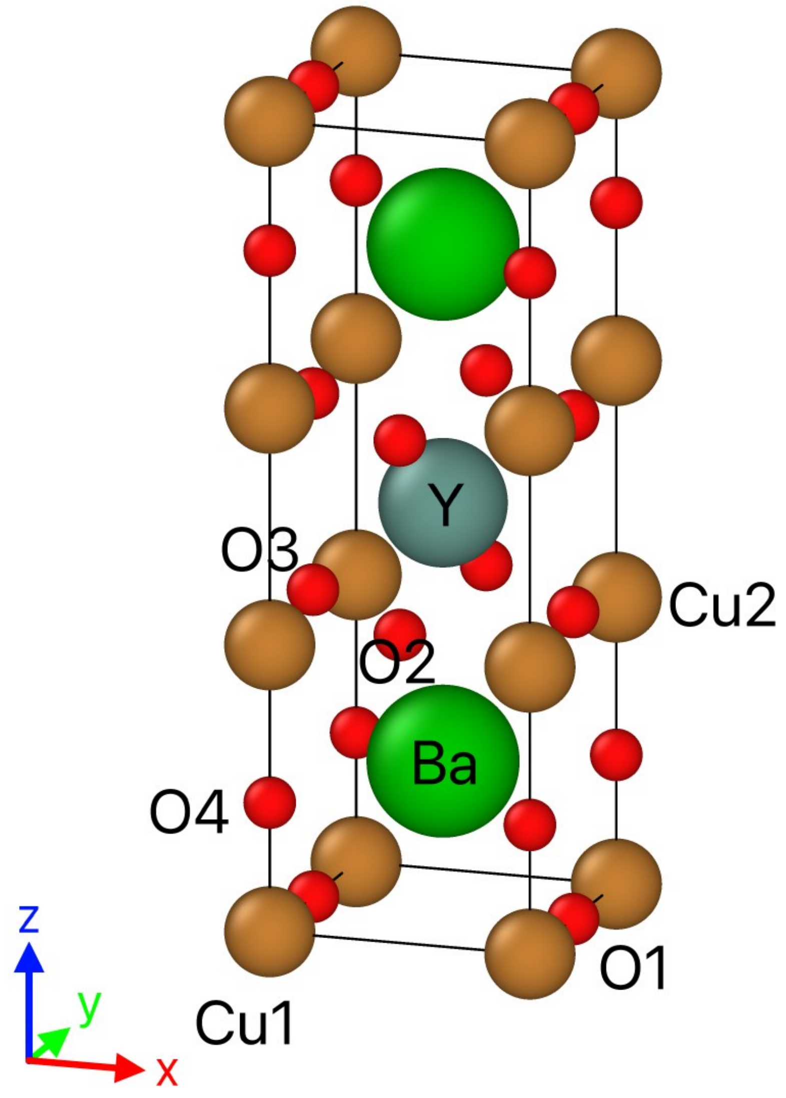
$YBa_2Cu_3O_7$ (YBCO)

- Ceramic material
- Available interatomic potential: Buckingham+Coulomb fitted to DFT results (Gray et al., Supercond. Sci. Technol. 35, 035010 (2022))
  - Ziegler-Biersack-Littmark screened nuclear repulsion included

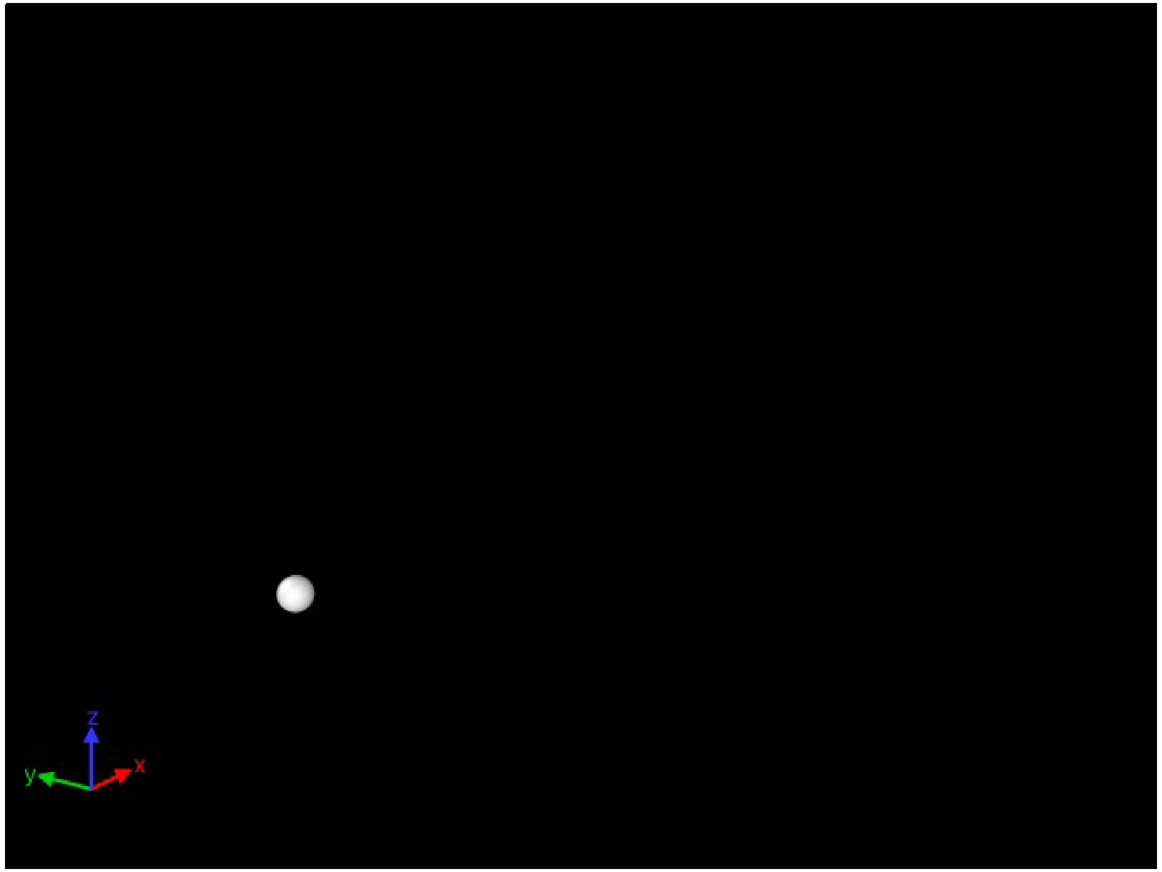


MD –collision cascade simulations

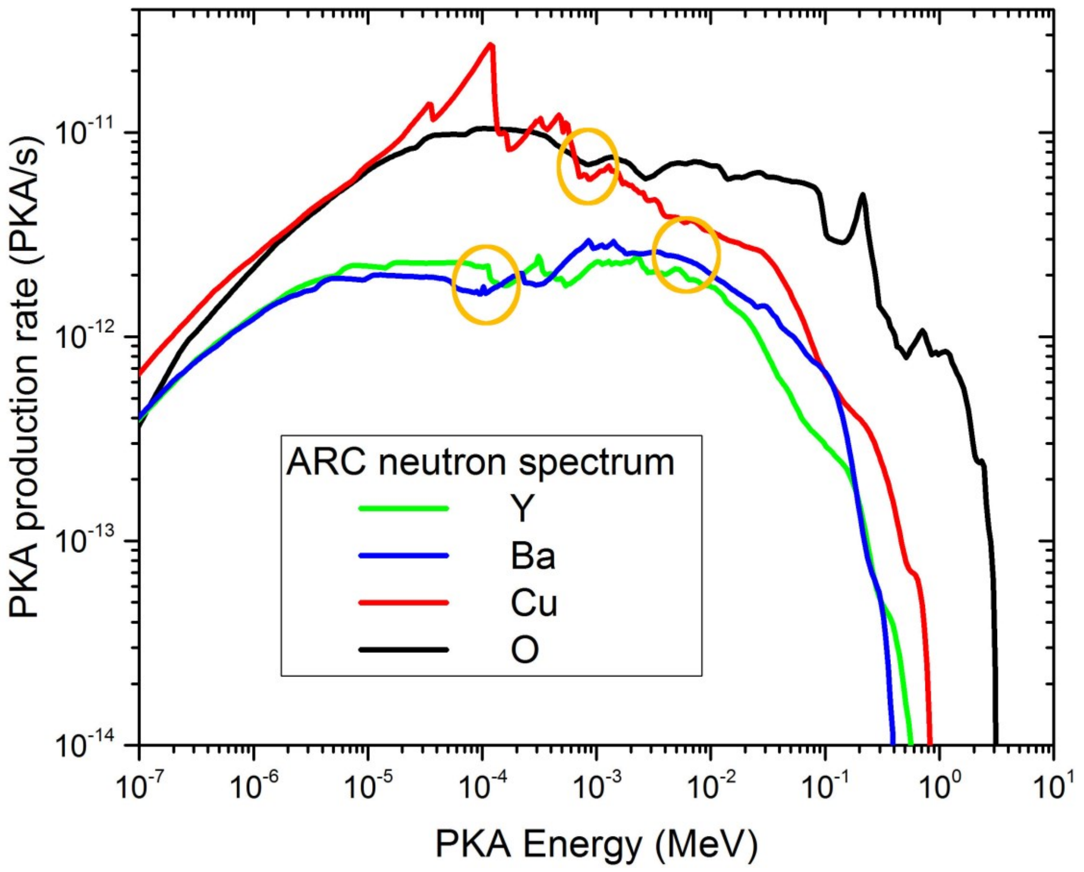
Workflow:

- same as Gray et al., SUST 35, 035010 (2022))

- Large cells (1-100 million atoms)
- Initial equilibration (NpT-ensemble)
- Collision cascade performed in NVE-ensemble within a sphere
- Outer atoms thermostatted to dissipate excess energy
- PKA launched with initial velocity according to spectrum



MD – Initial conditions

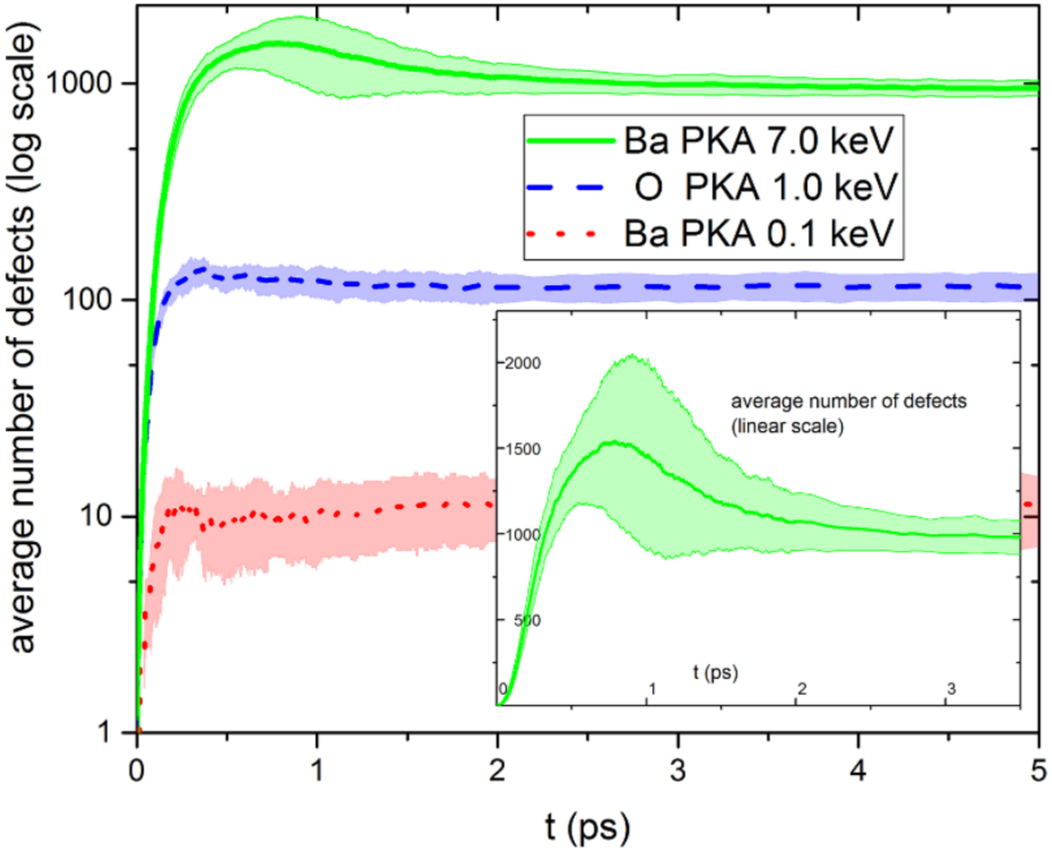


Ba PKA		
T (K)	20	300
E_k PKA (keV)	0.003	-
	0.1	0.1
	7	7
	110	110

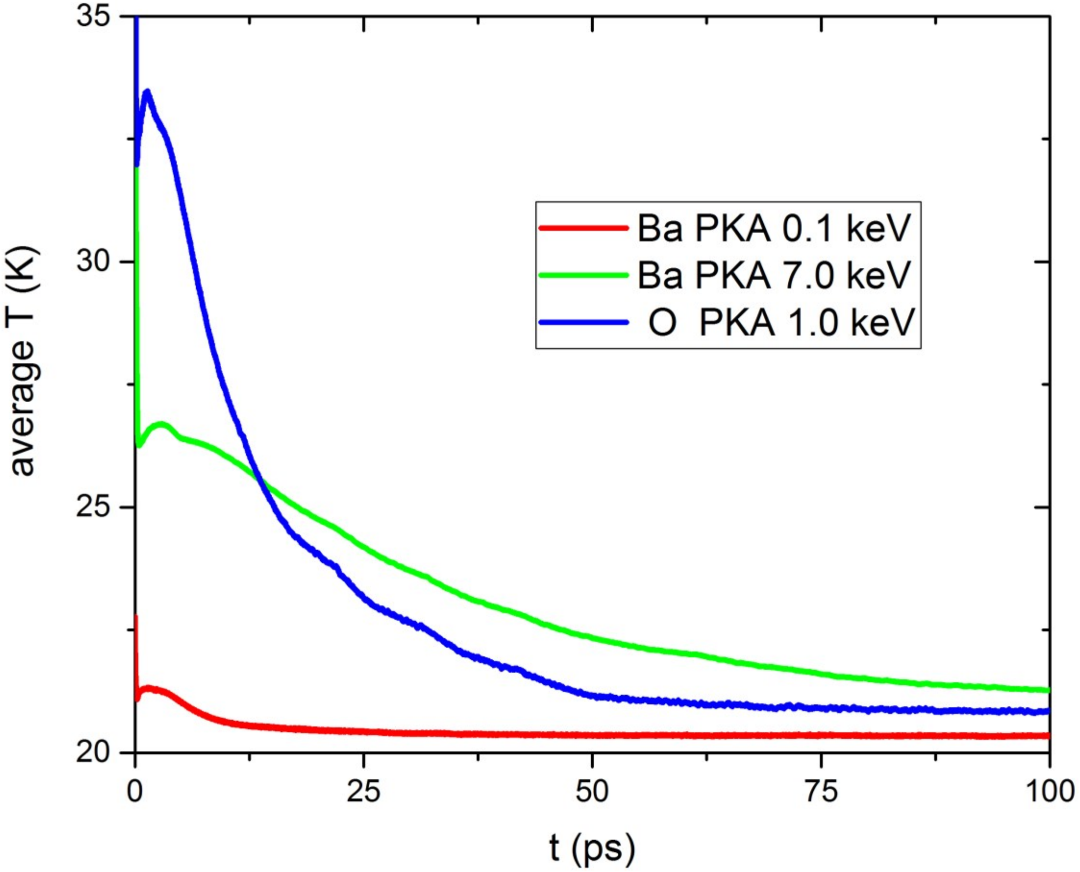
O PKA		
T (K)	20	300
E_k PKA (keV)	1	1

MD – Results

Average number of defect vs time



Temperature vs time



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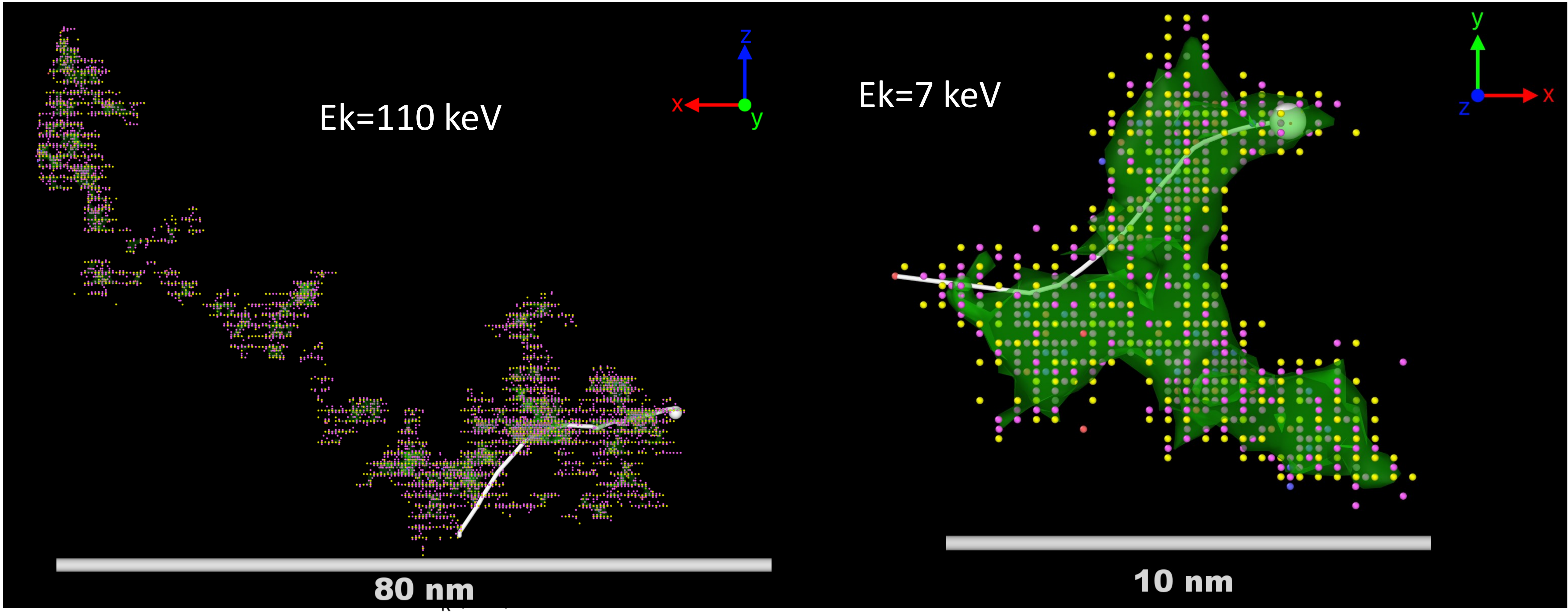
MD – Results



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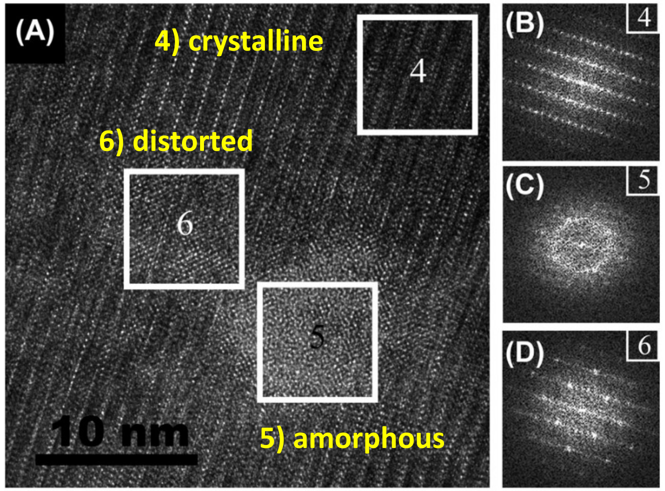
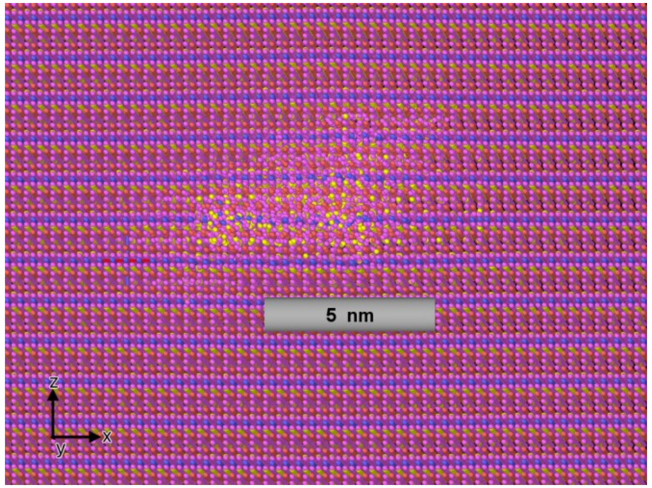
Additional analysis and model refinement – Ongoing work

Additional analysis

- Comparison with experiments (often T_{room})
  - TEM



From Linden et al., Journal of Microscopy 286, 3-12 (2022), neutrons from TRIGA MARK II



Snapshot from MD

Additional analysis and model refinement – Ongoing work

Additional analysis

- Comparison with experiments (often T_{room})
    - TEM

Model refinement

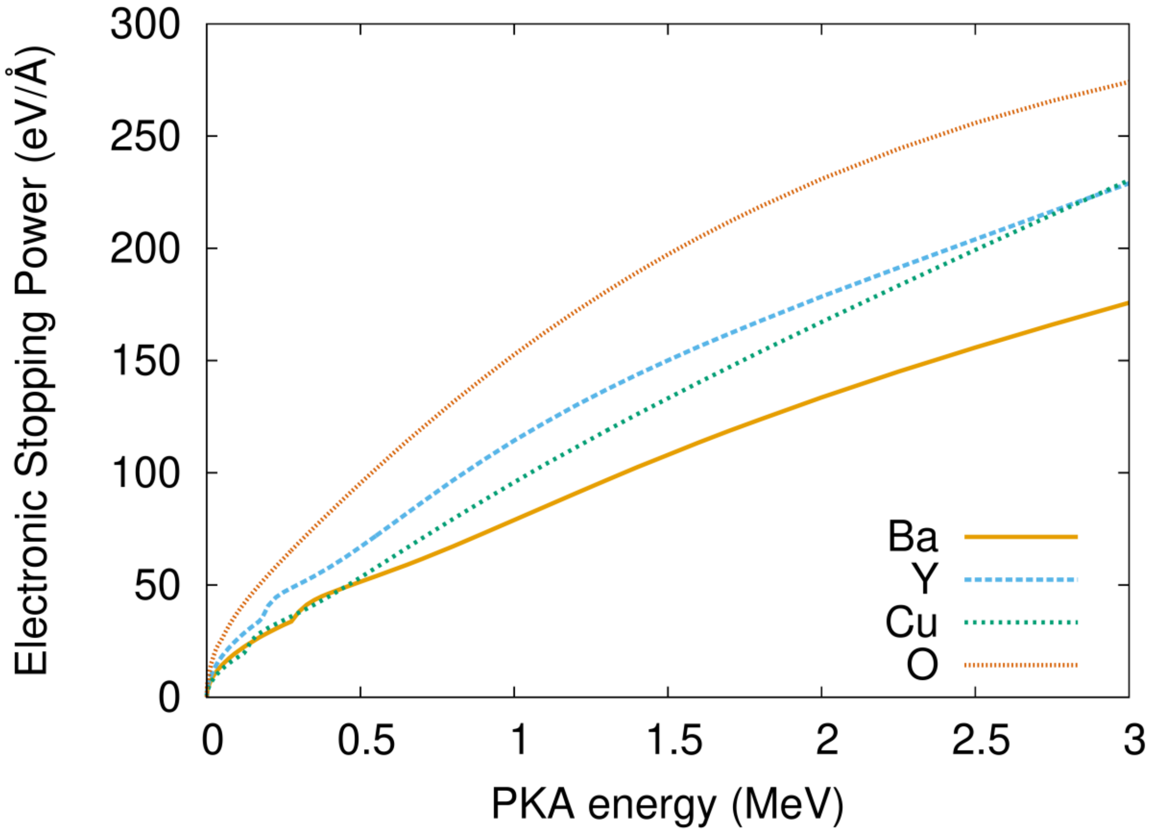
- Include electronic system:
    - Electronic stopping power
    - Two-temperature MD
- Complete PKA and energy investigation

Electronic stopping power

Model Refinement

Electronic stopping power

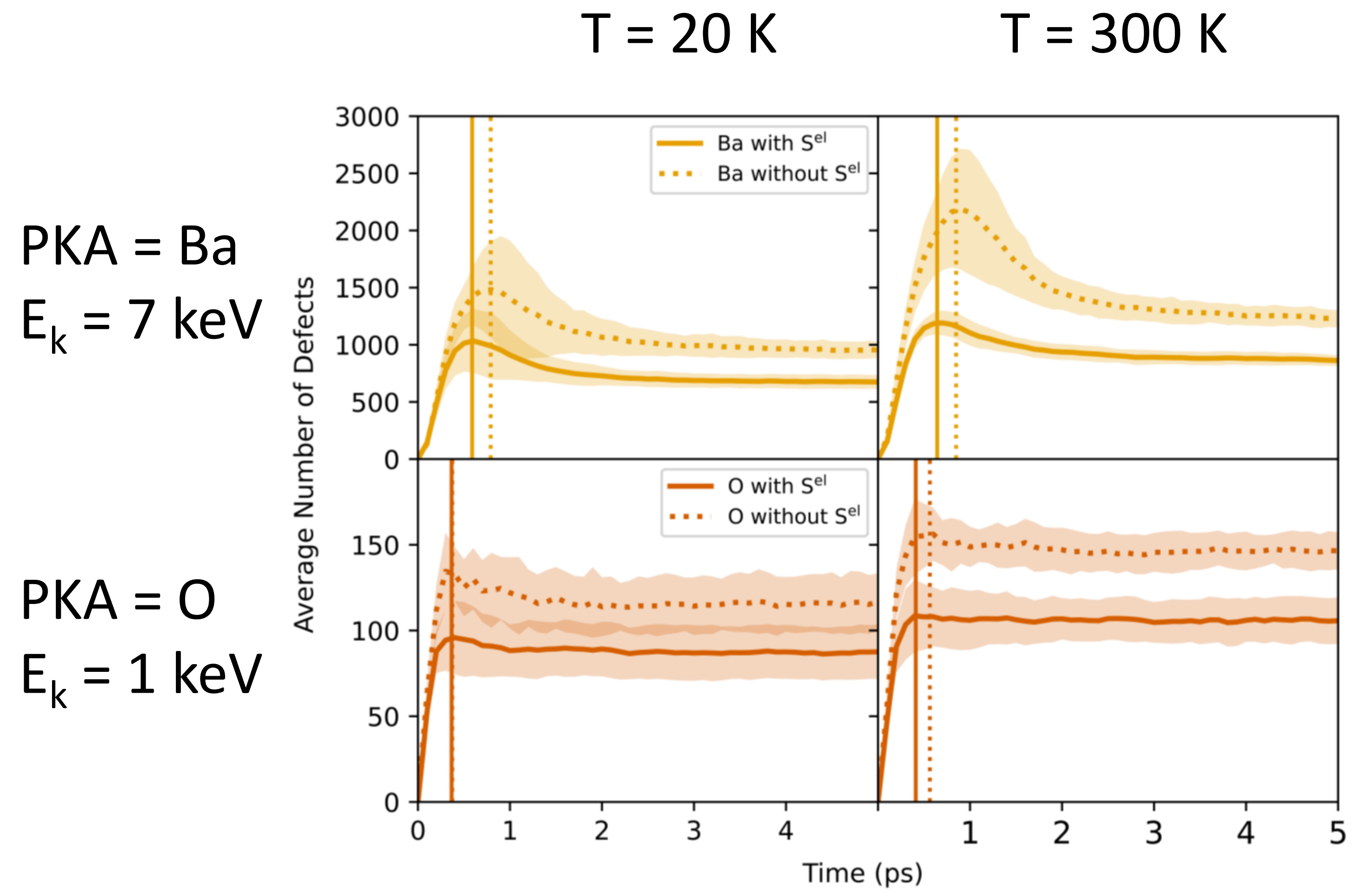
- Fast (keV) displaced ions interact with electrons
- Electronic stopping power calculated with SRIM
- Included in MD simulations as friction term



Electronic stopping power – Results

Effect of electronic stopping:

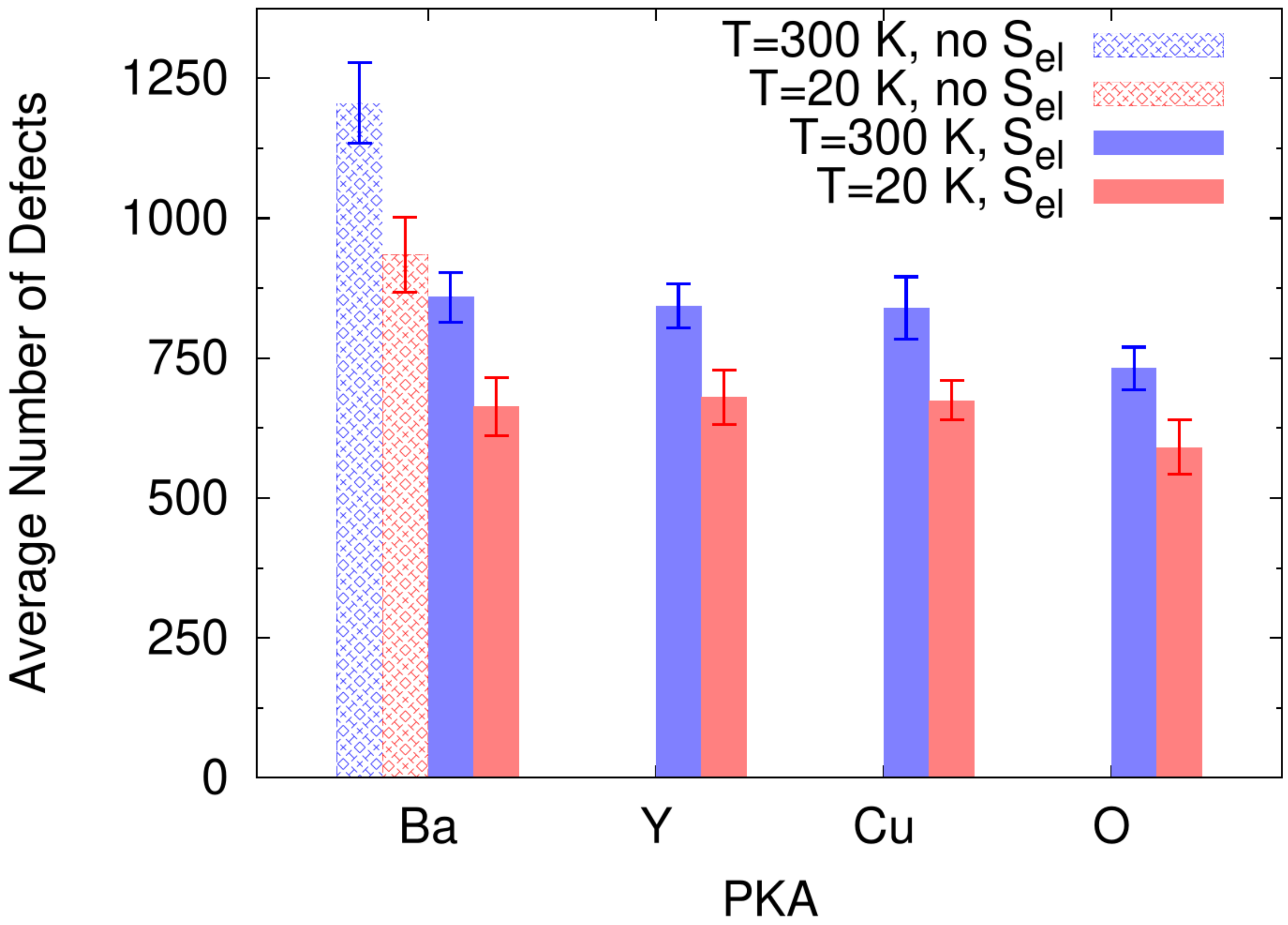
- Reduction of maximum and final number of defects
- Species and temperature dependent effect



Complete PKA and energy investigation

Model Refinement

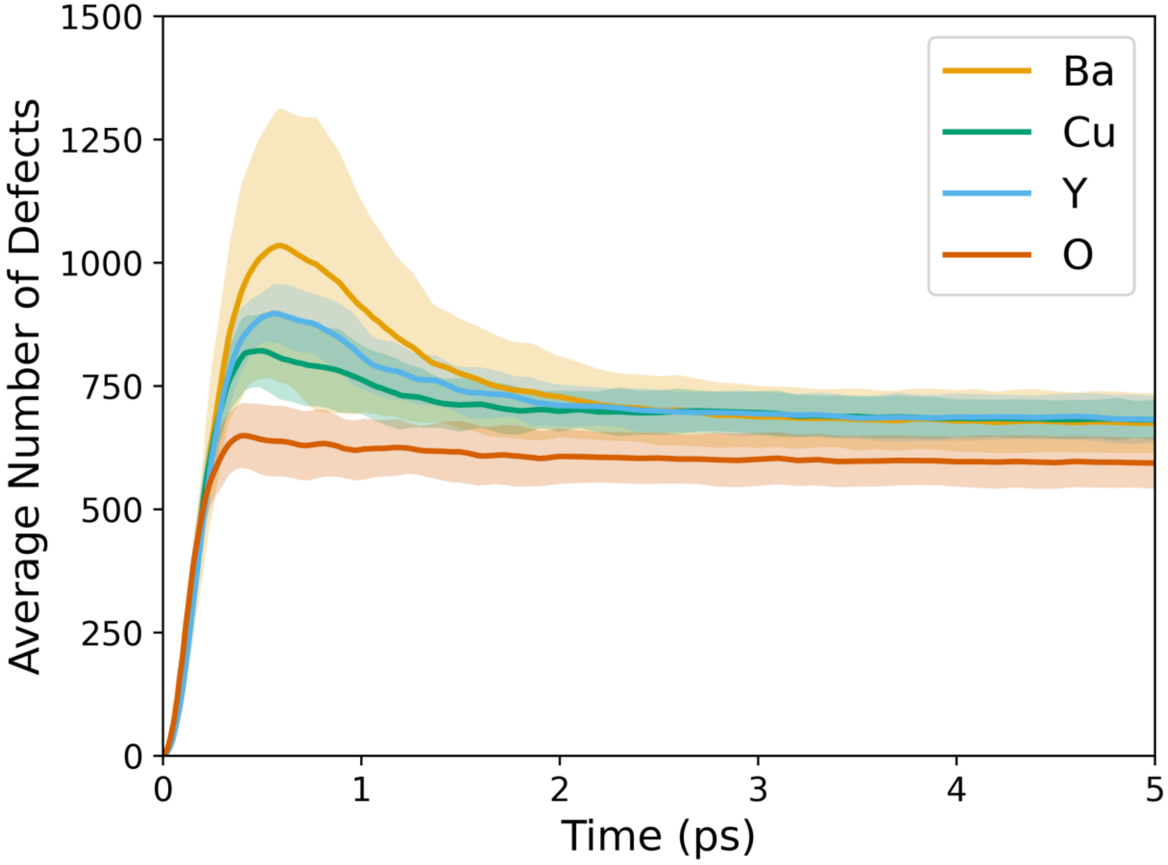
Defects vs PKA (E_k = 7 keV)



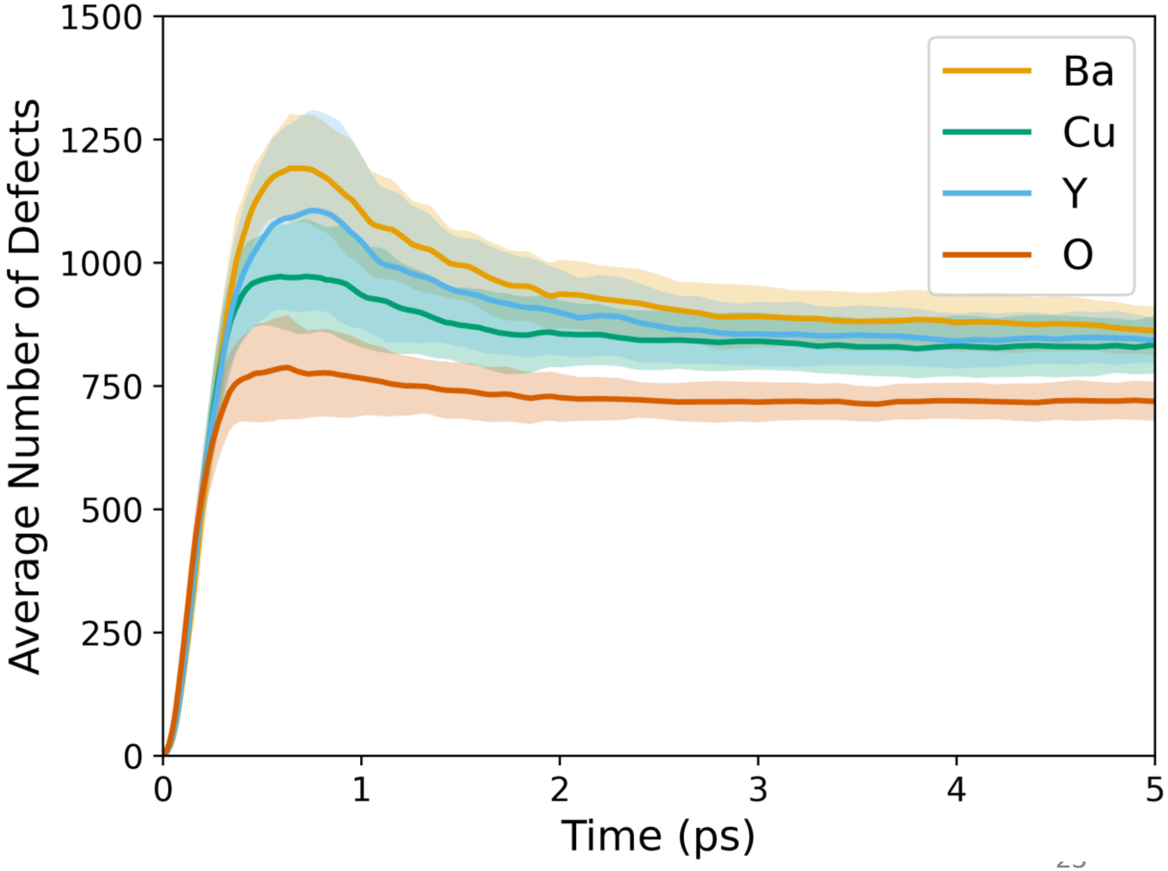
Defects vs PKA (E_k = 7 keV)

Mass (a.u.)	
Ba	137.33
Y	88.90
Cu	63.55
O	15.999

T = 20 K

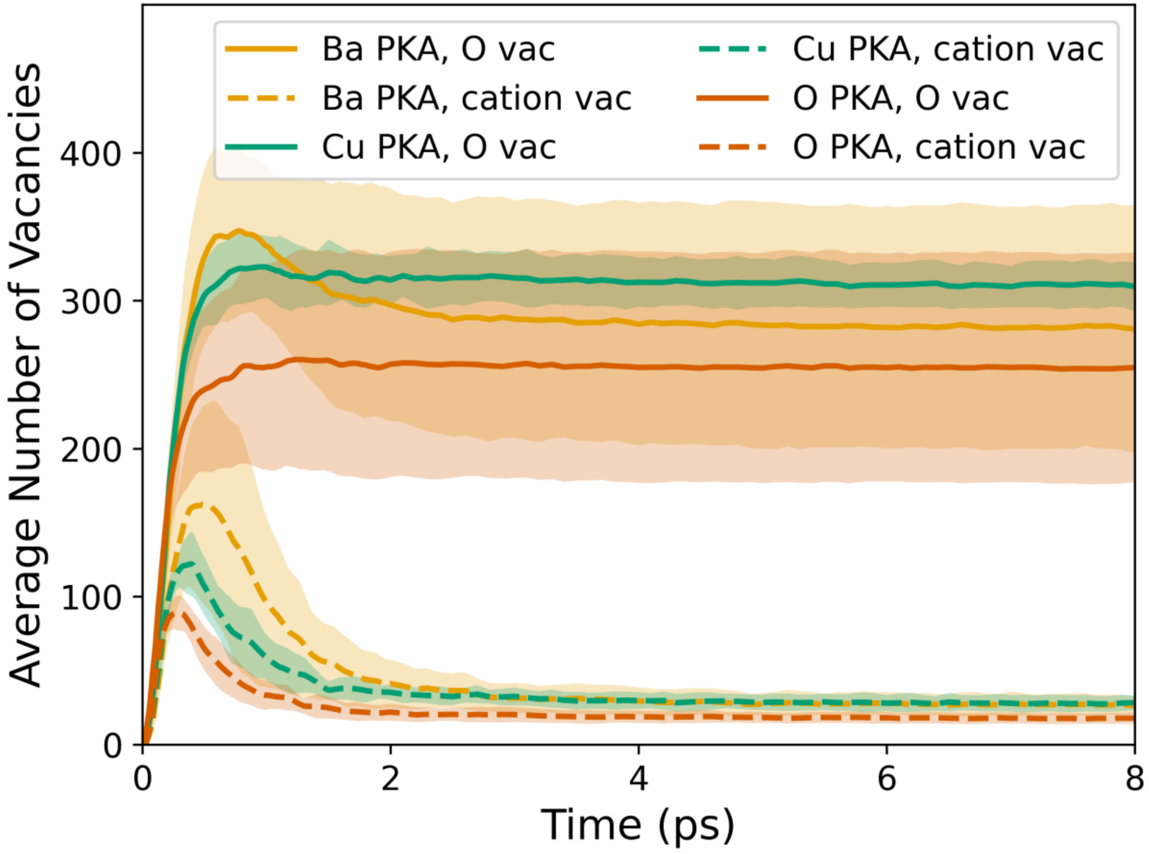


T = 300 K



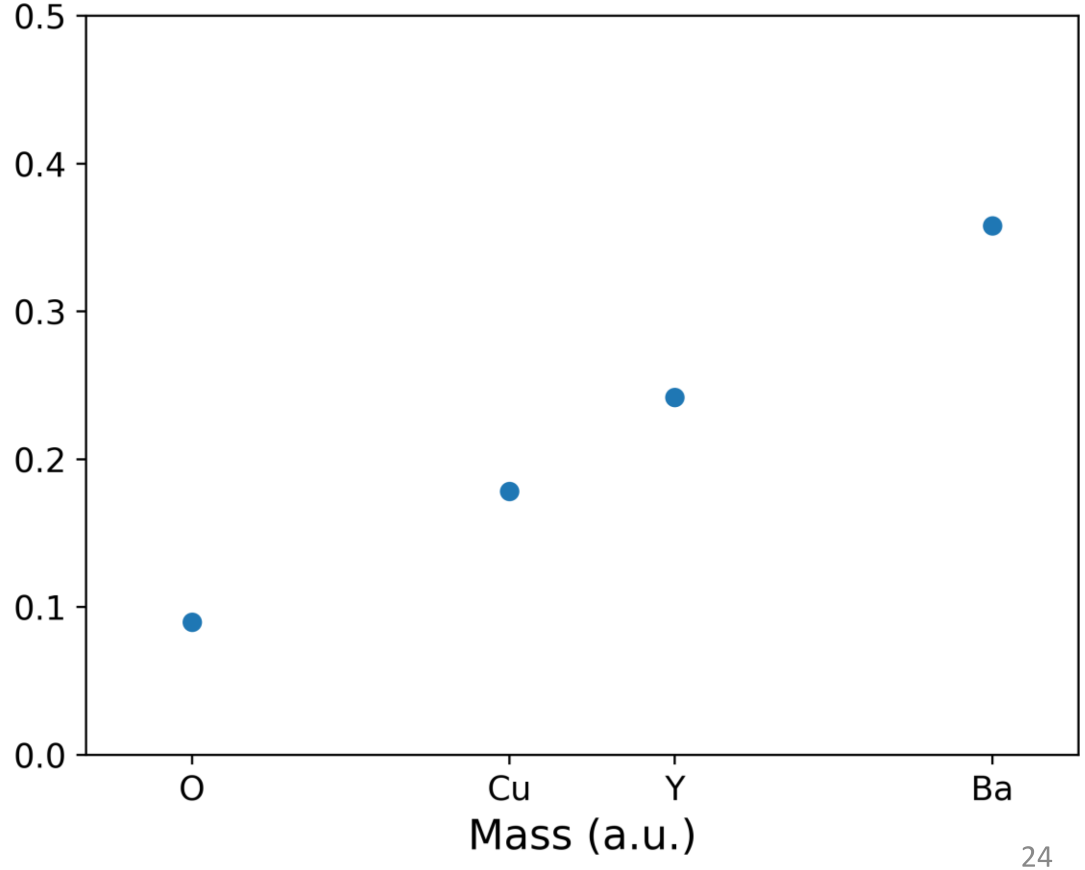
Number of vacancies vs PKA (E_k = 7 keV)

O vs cation vacancies



Recombination rate

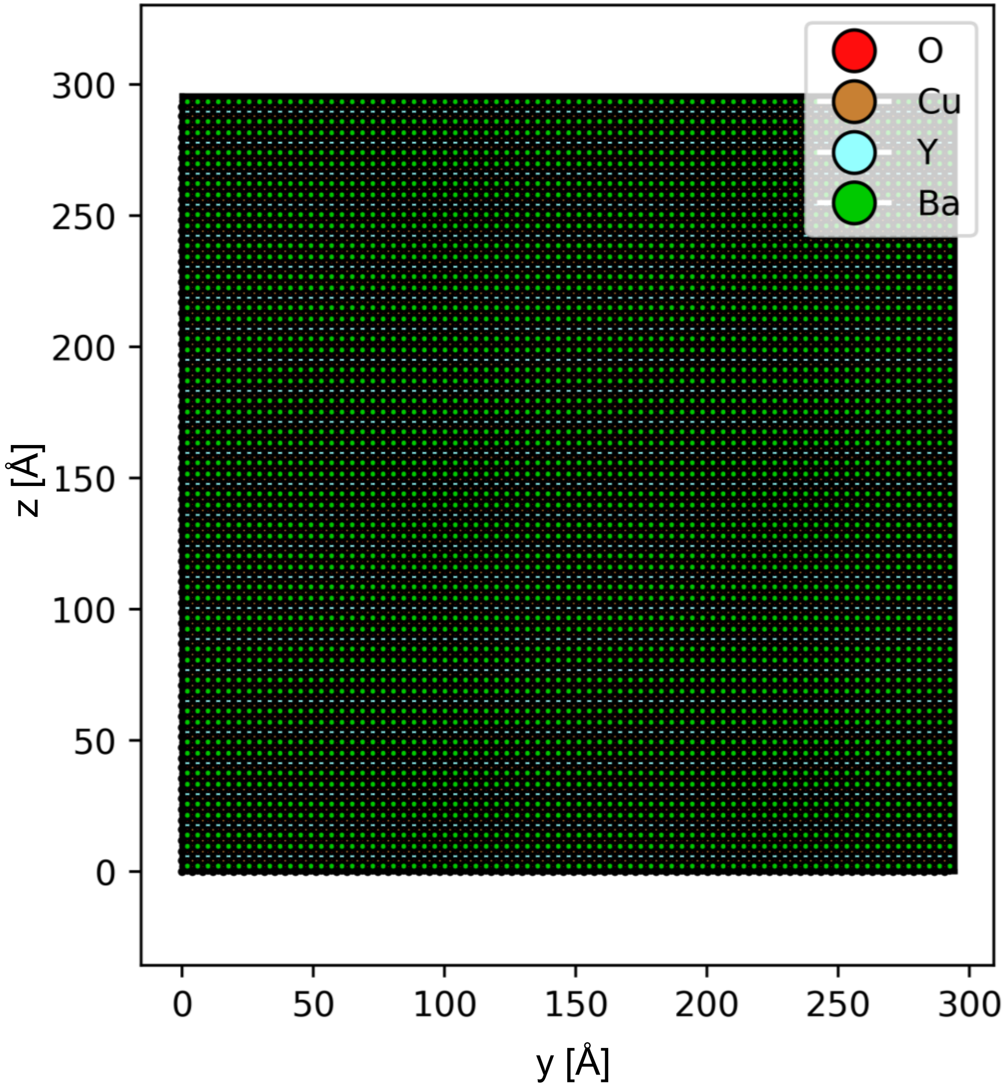
$$= 1 - N^{\text{final}}/N^{\text{peak}}$$

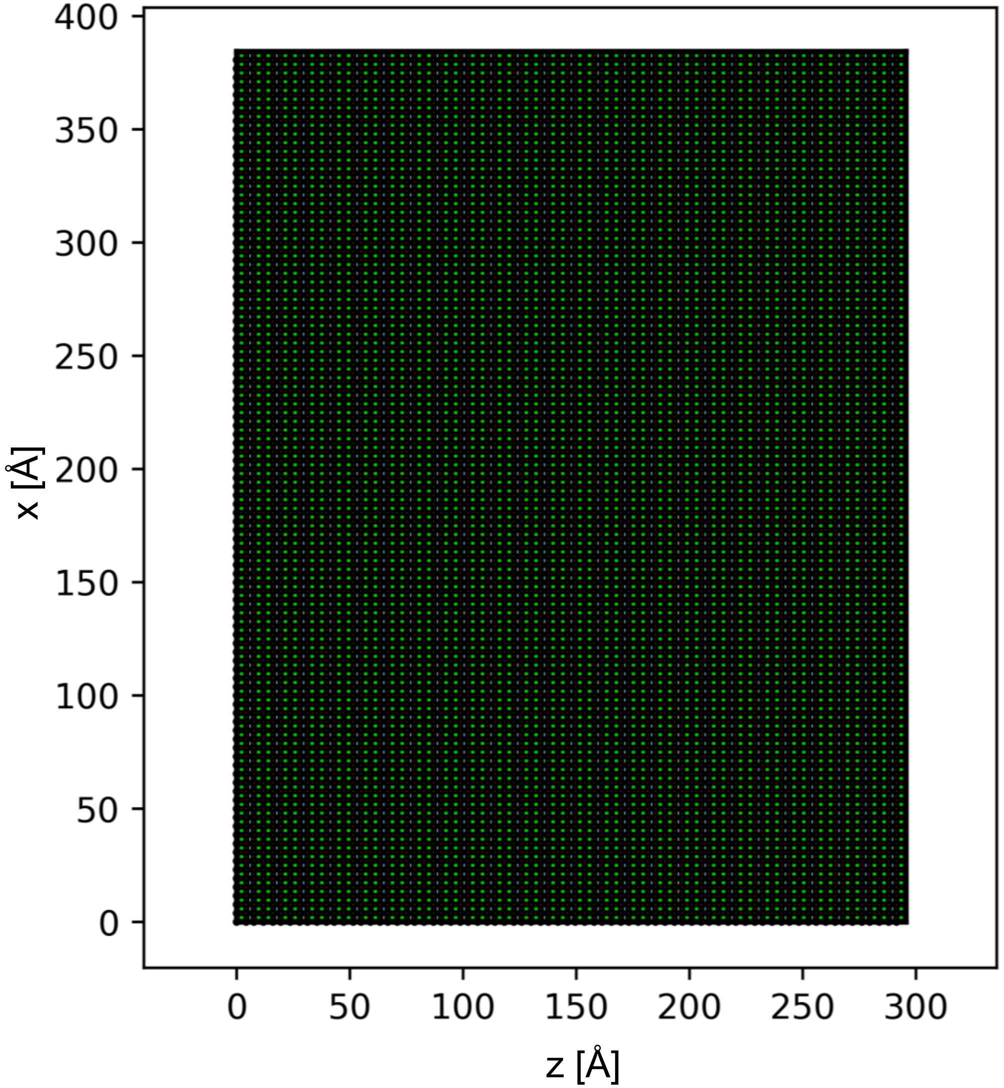


TEM image simulation

Additional analysis

TEM reconstructions – Ideal lattice





abTEM: Jacob Madsen and Toma Susi, *Open Research Europe* 1:24, 2021

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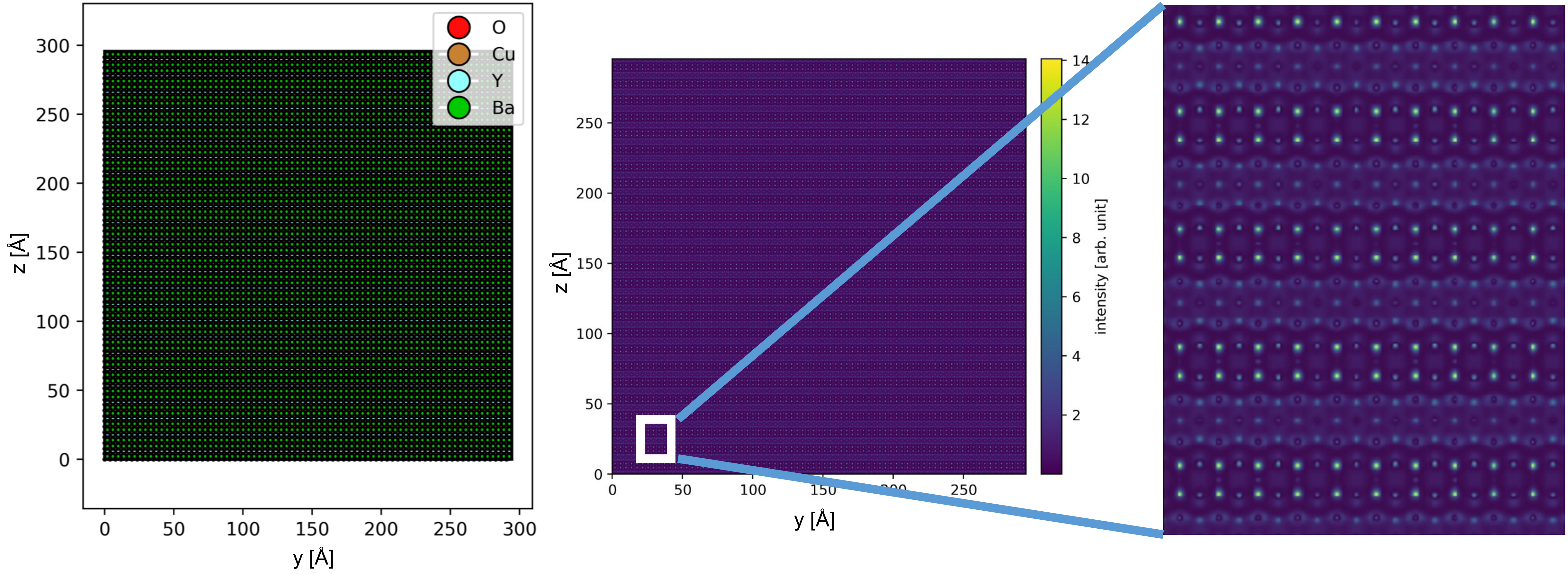
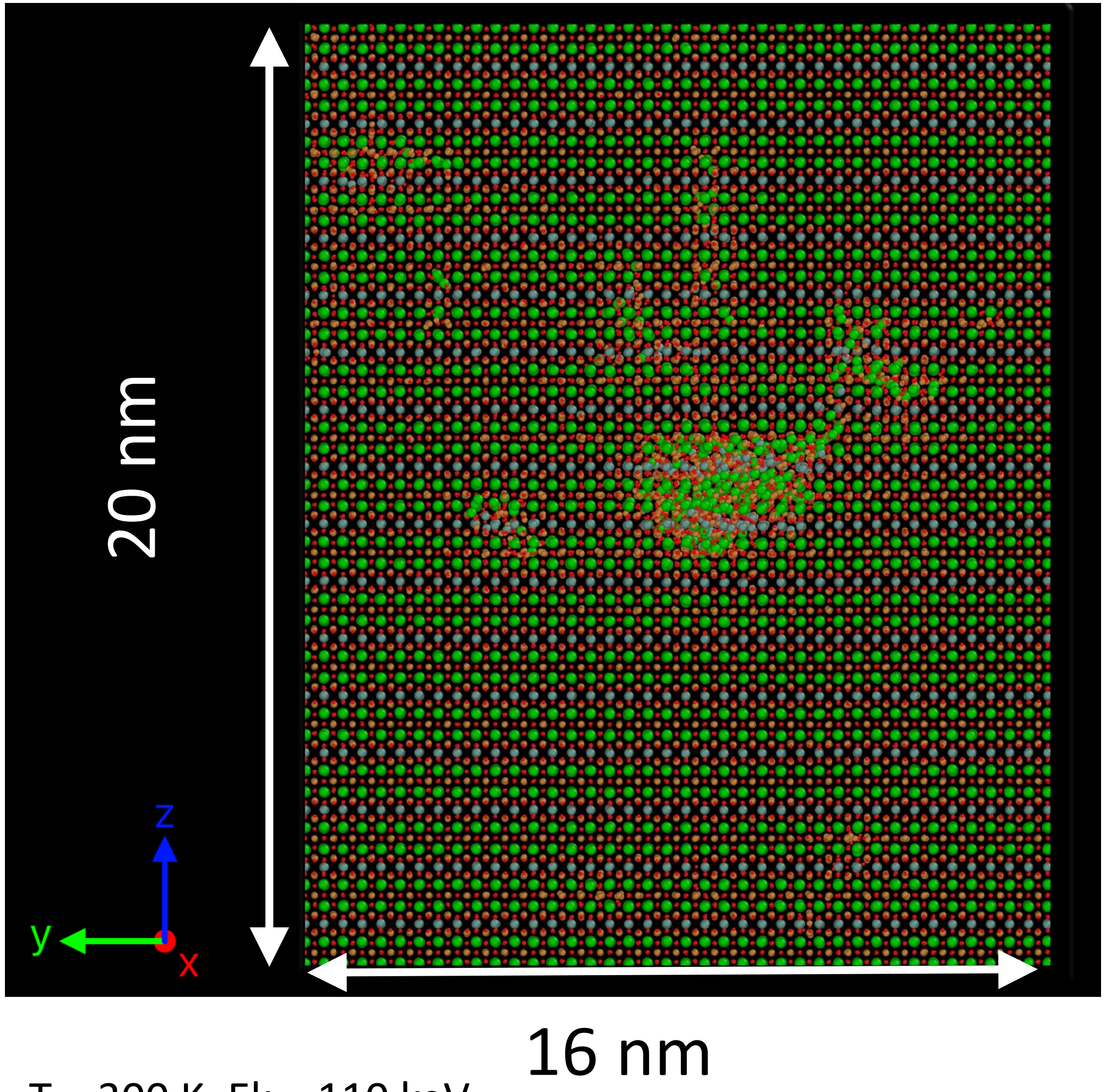
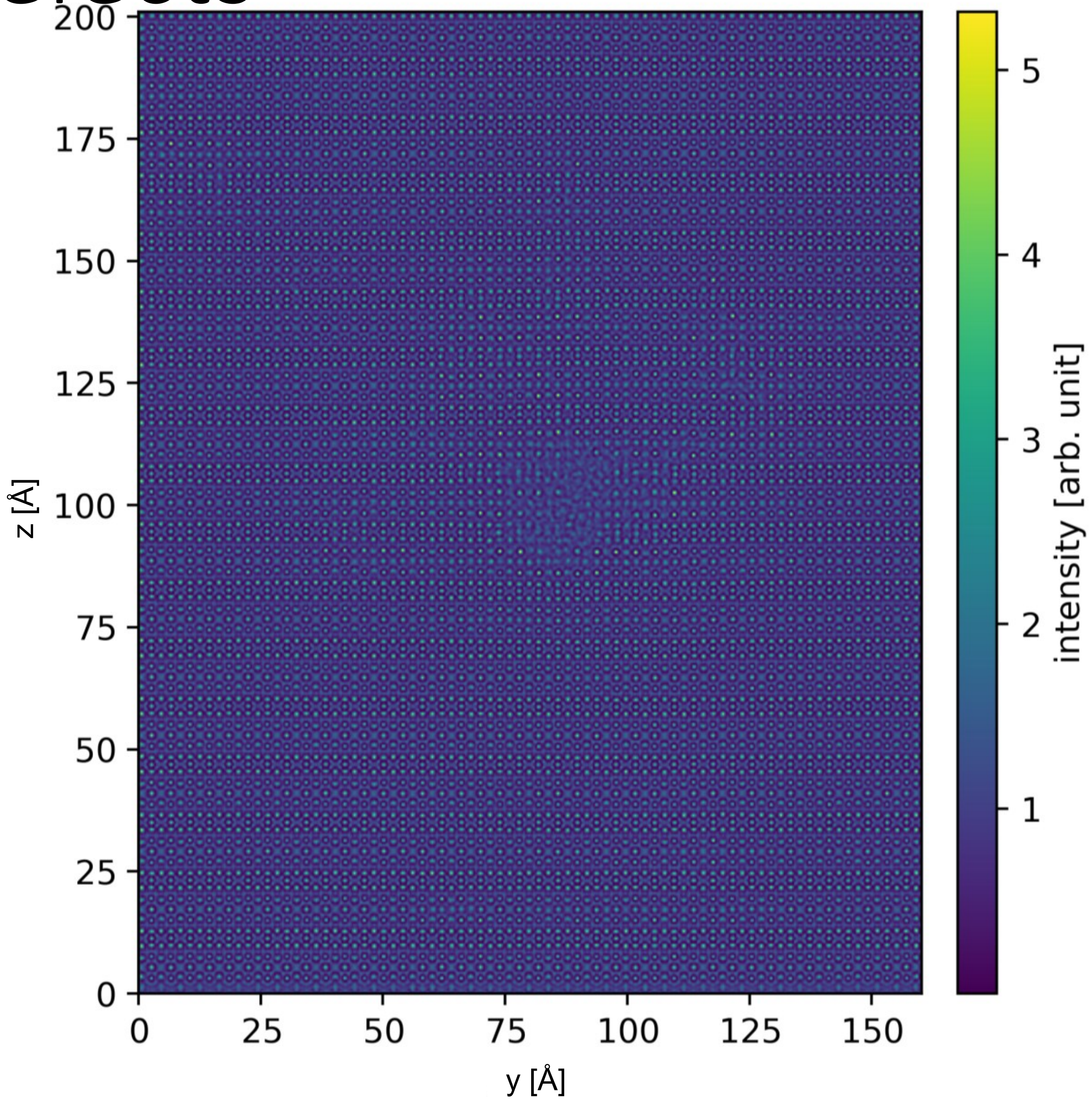


abTEM: Jacob Madsen and Toma Susi, *Open Research Europe* 1:24, 2021

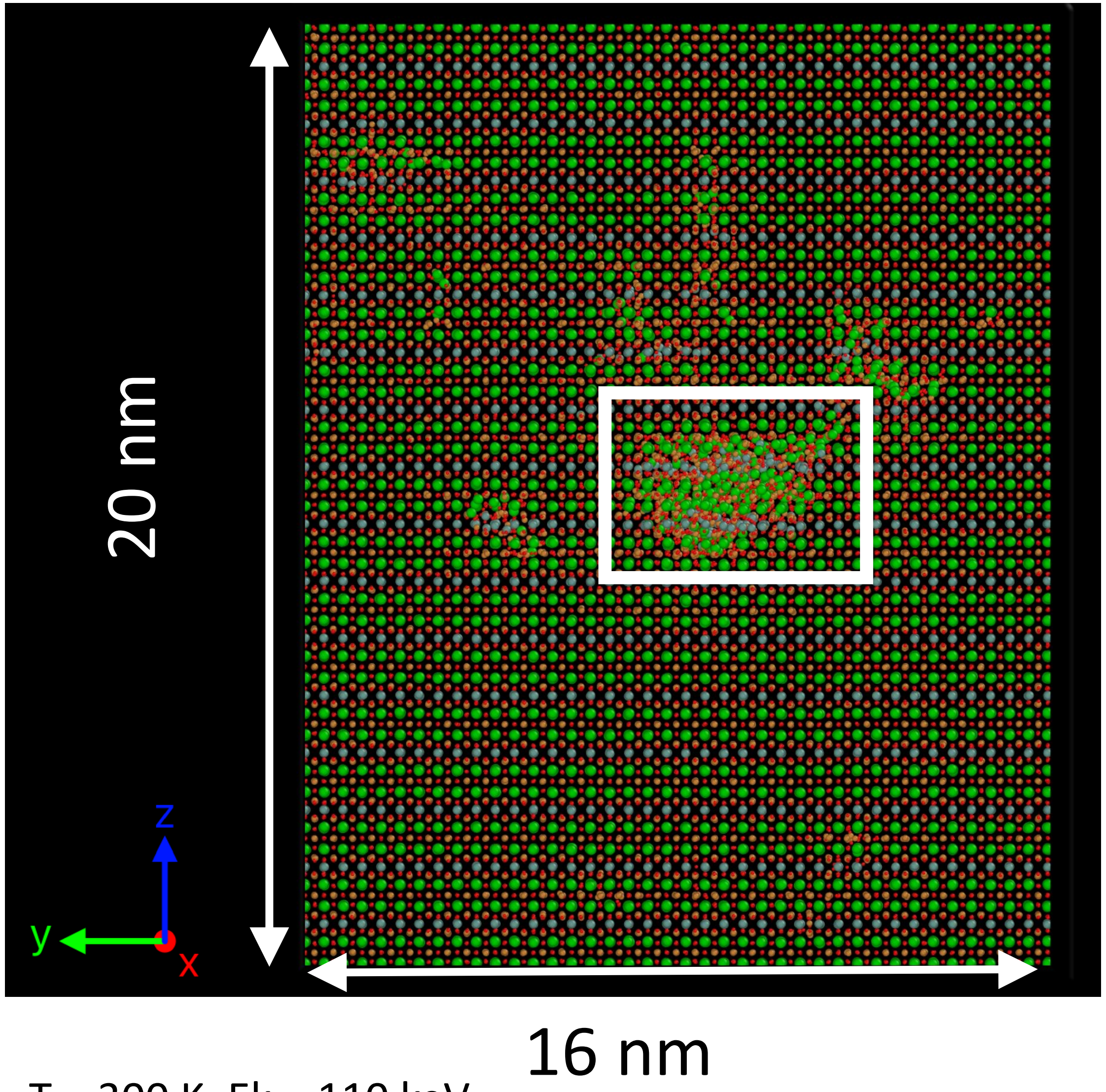
TEM reconstructions – Defects

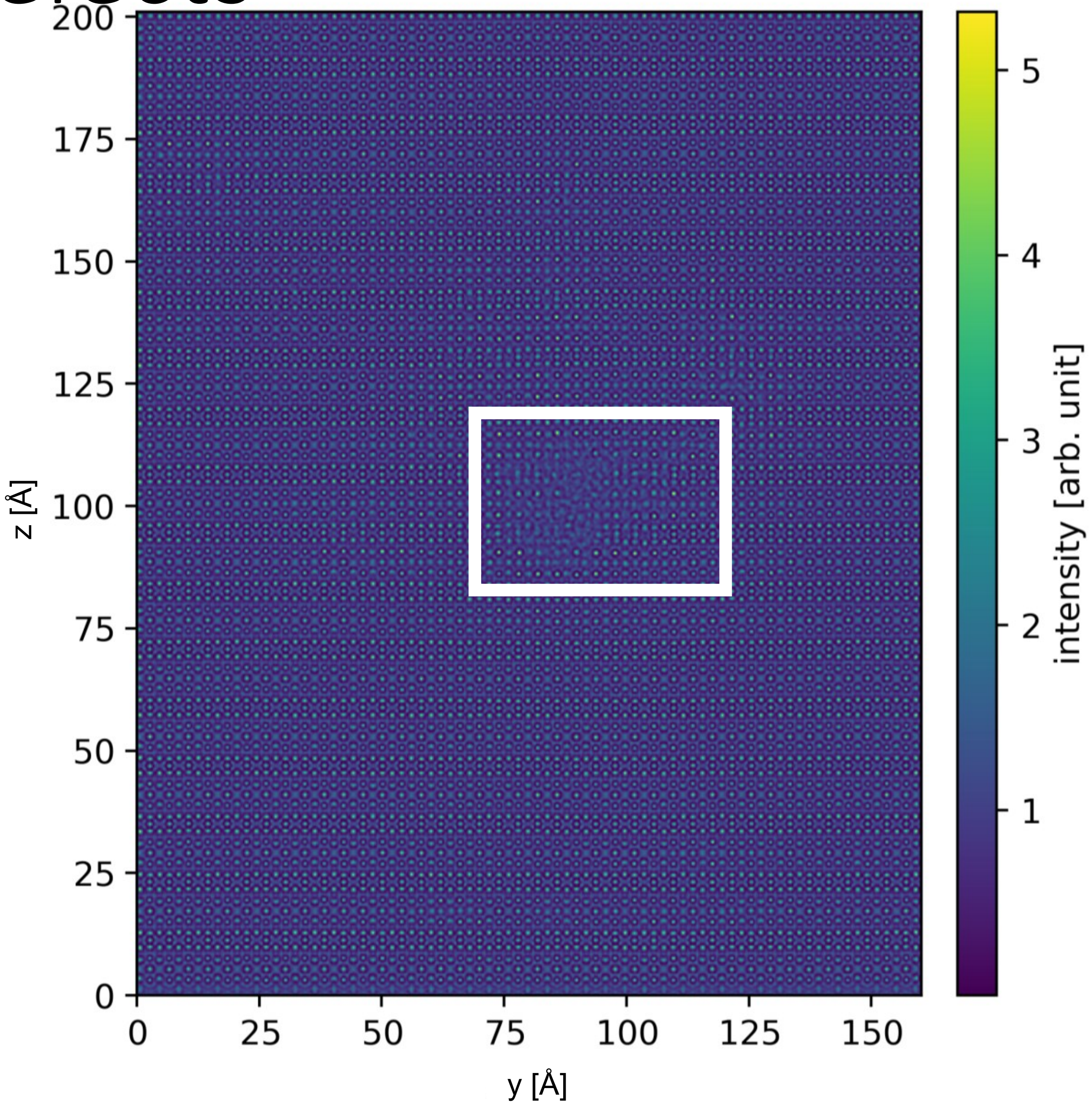




Ba PKA, T = 300 K, Ek = 110 keV

TEM reconstructions – Defects





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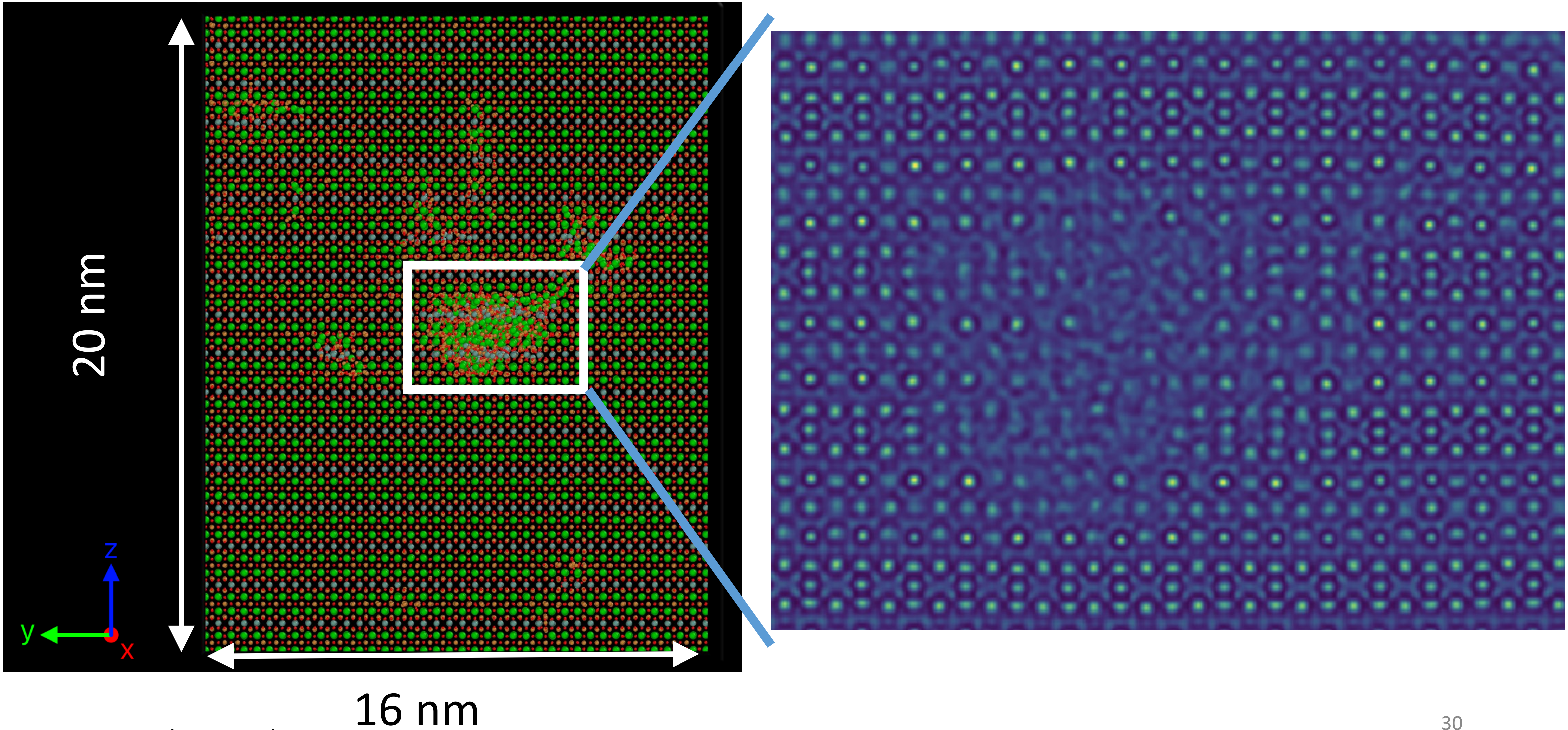

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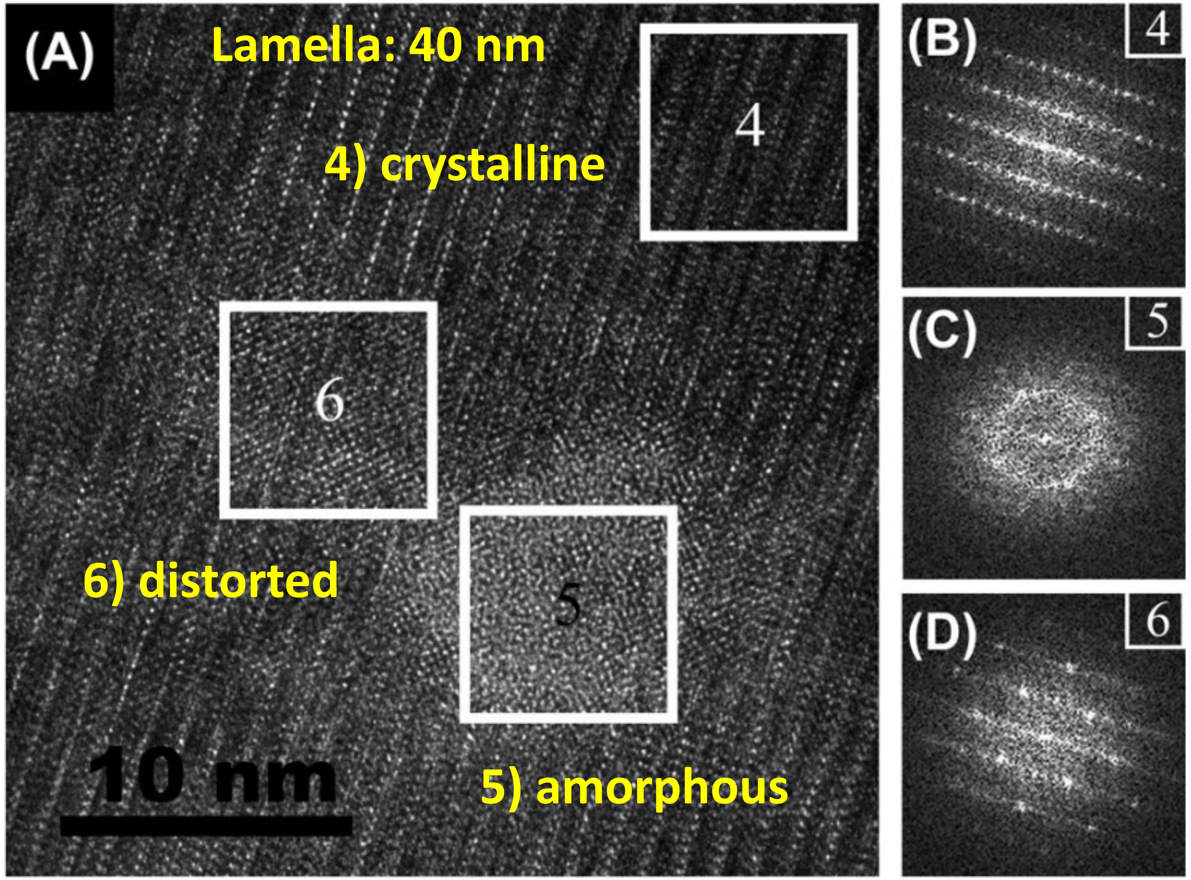

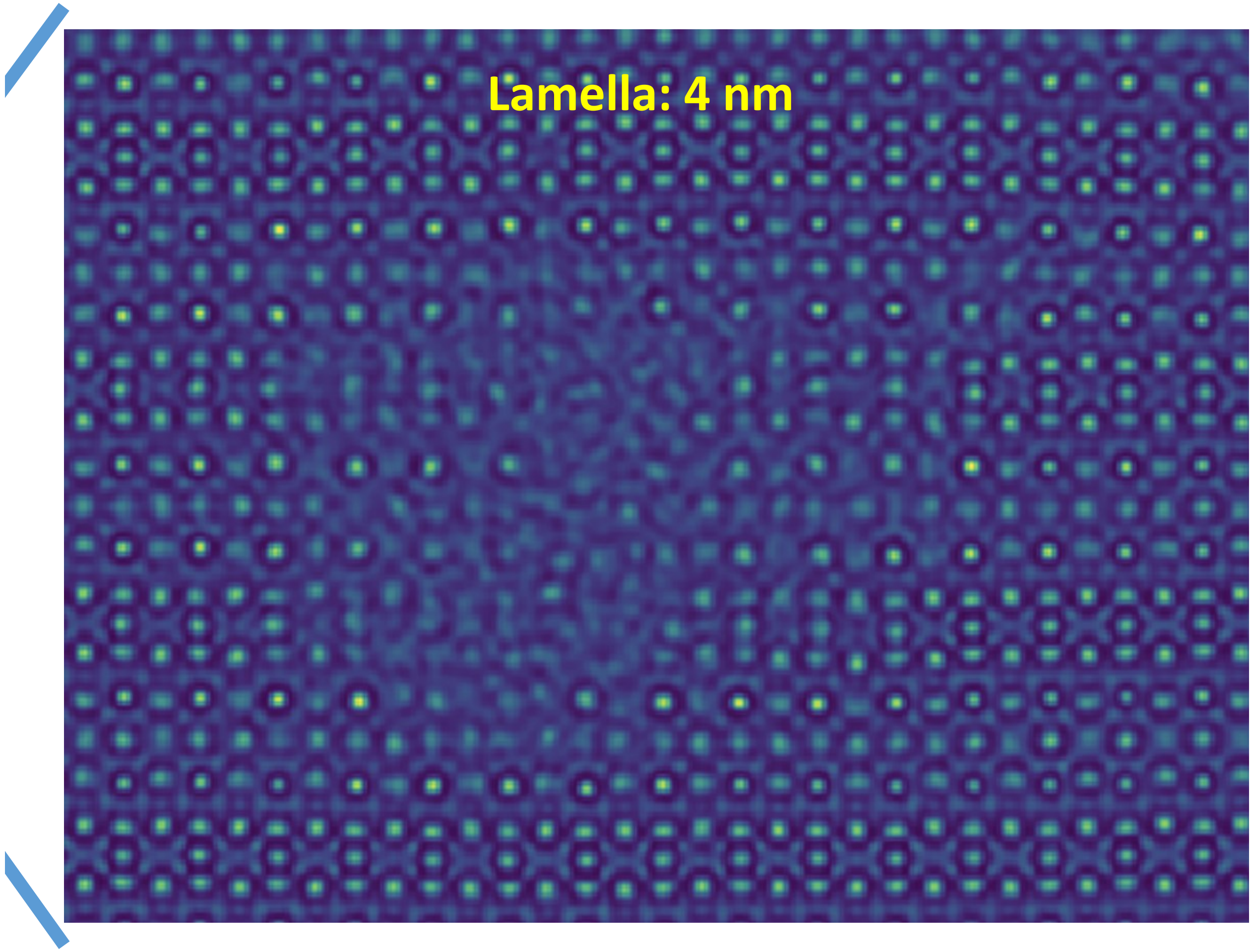

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Conclusions

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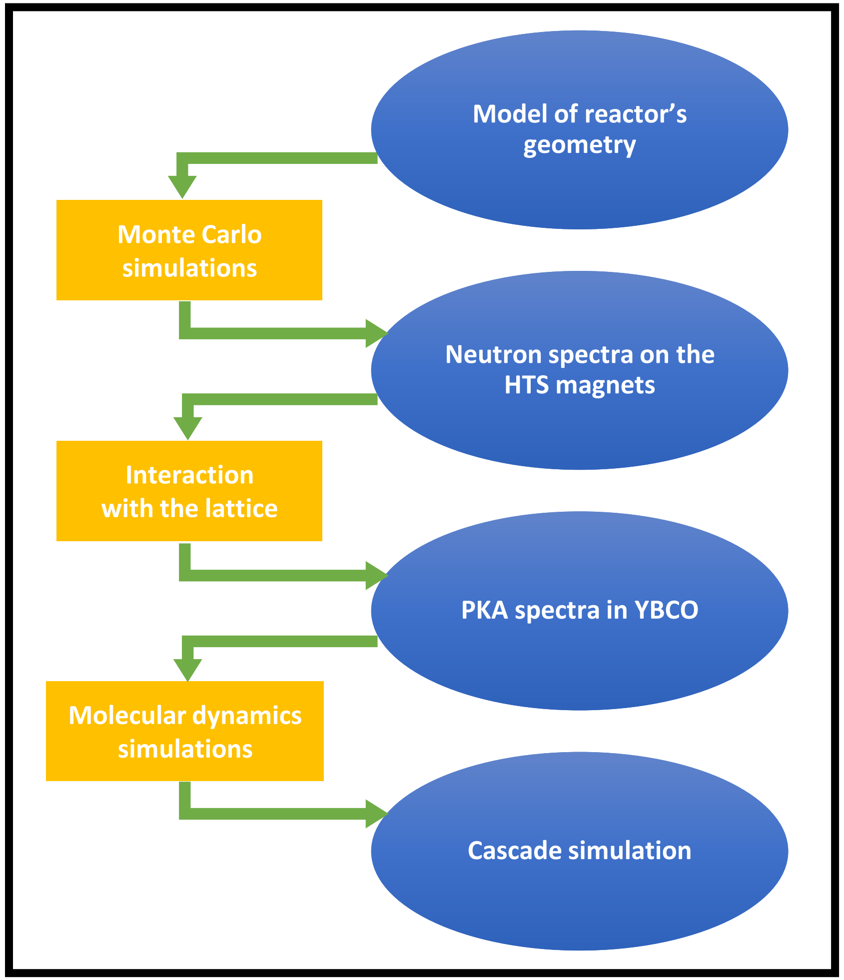
Conclusions

- Workflow for computational investigation of radiation damage of HTS for nuclear fusion – **from neutrons to damage**



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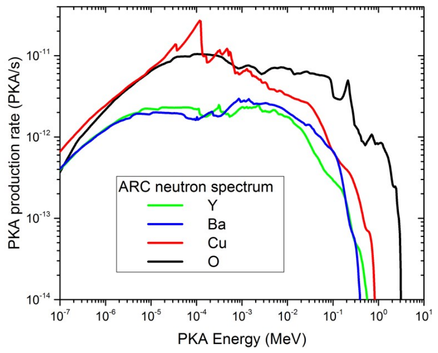

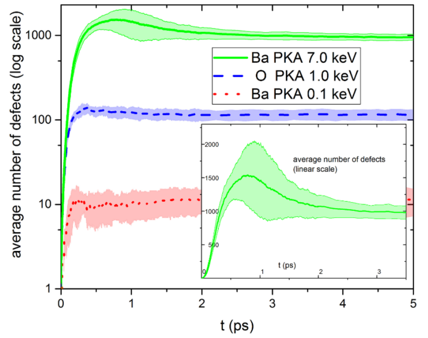

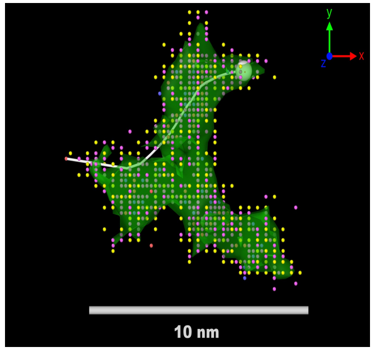

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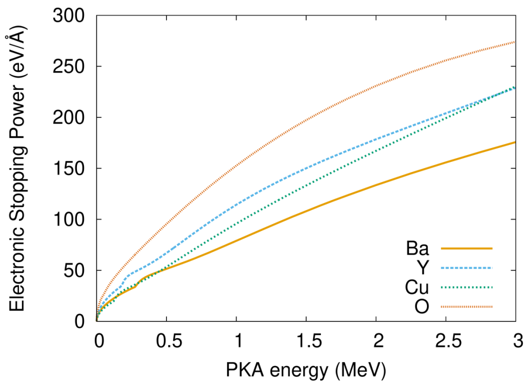

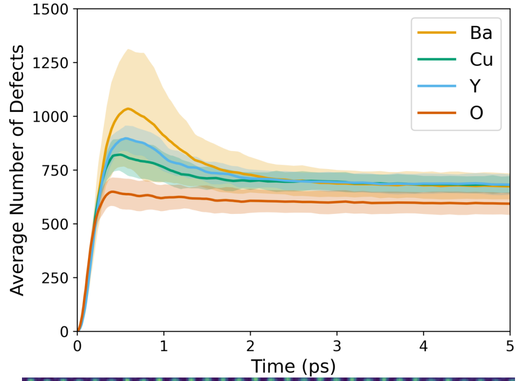

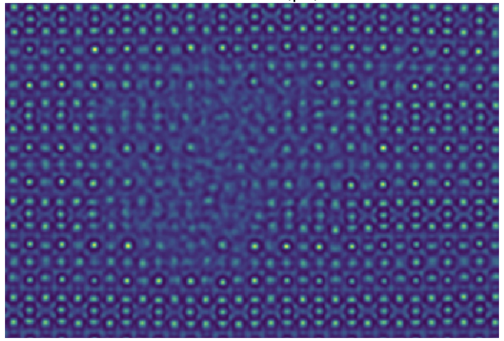

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Expected radiation environment and damage for YBCO tapes in compact fusion reactors

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