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

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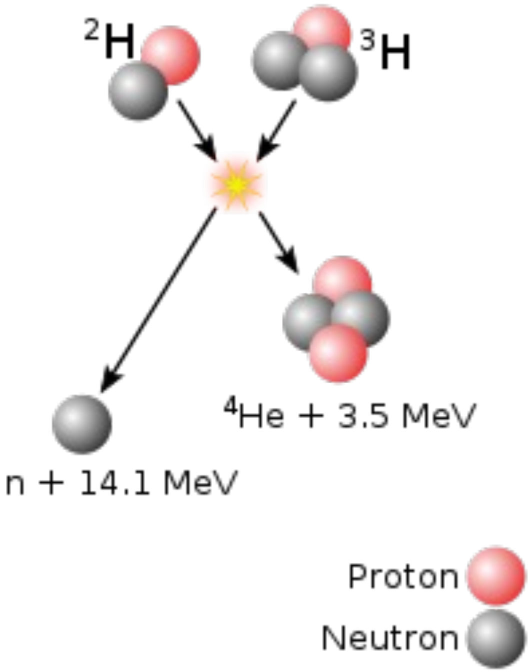
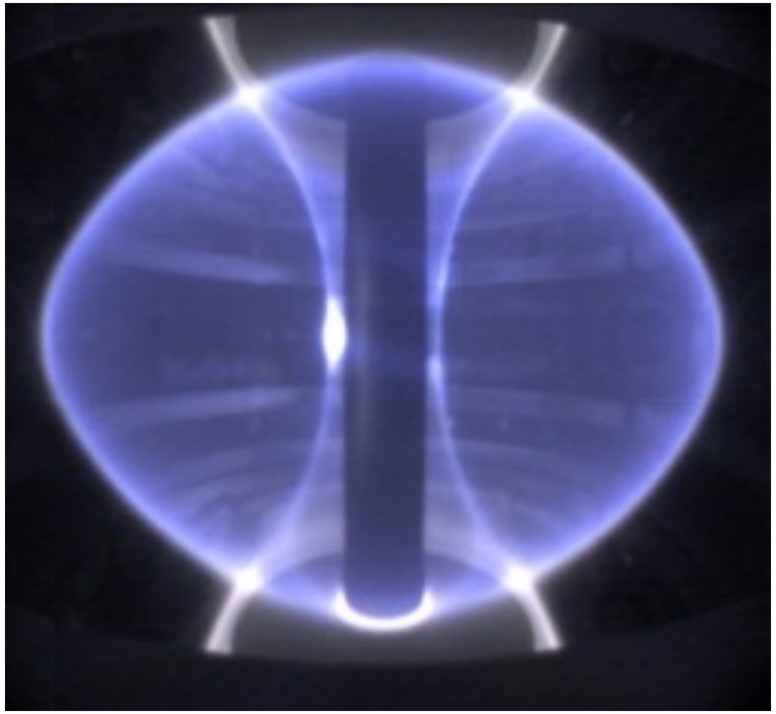
Nuclear fusion – Magnetic confinement approach

D-T fusion

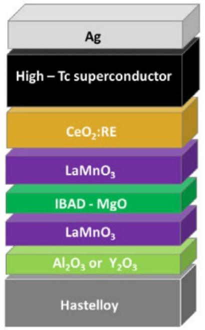


Magnetic confinement



Magnetic confinement approach – compact reactors

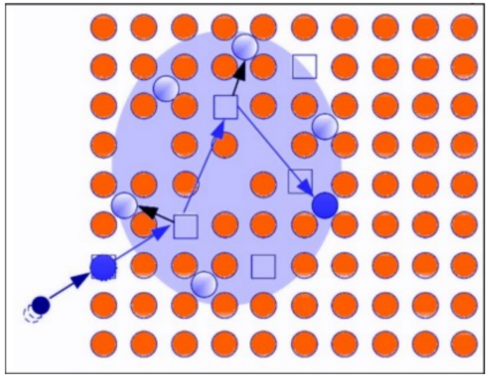
High temperature superconductors (HTS) tapes: high critical current (B = 20 T @ T=20 K)



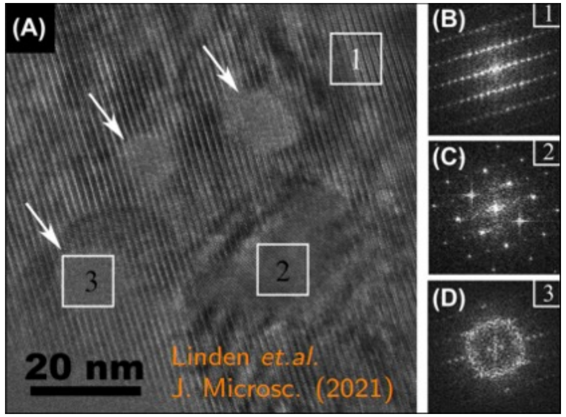
Compact reactors ($r \approx 3$ m)

But

Neutrons interact with lattice



Creating structural defects



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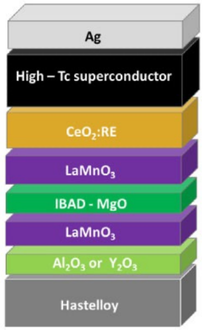
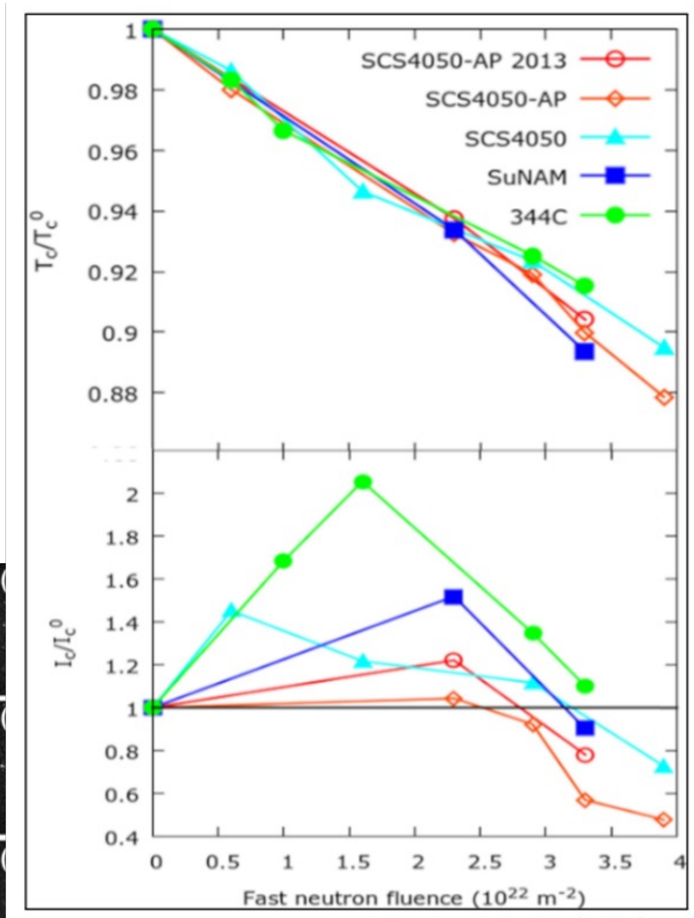


Superconducting properties vs neutron irradiation: lattice damage and vortex pinning



Fischer *et.al.* SuST (2018)

But

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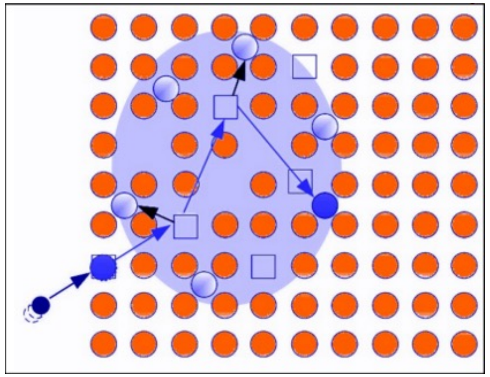
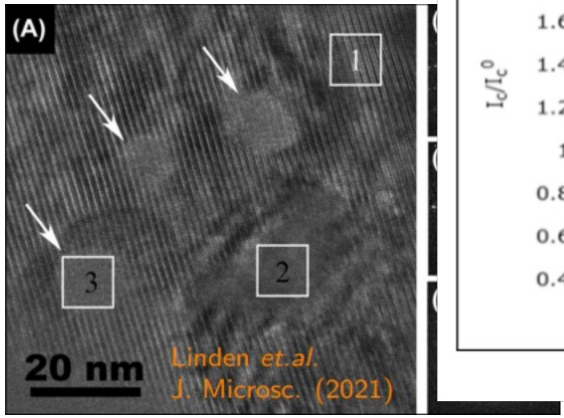


Creating structural

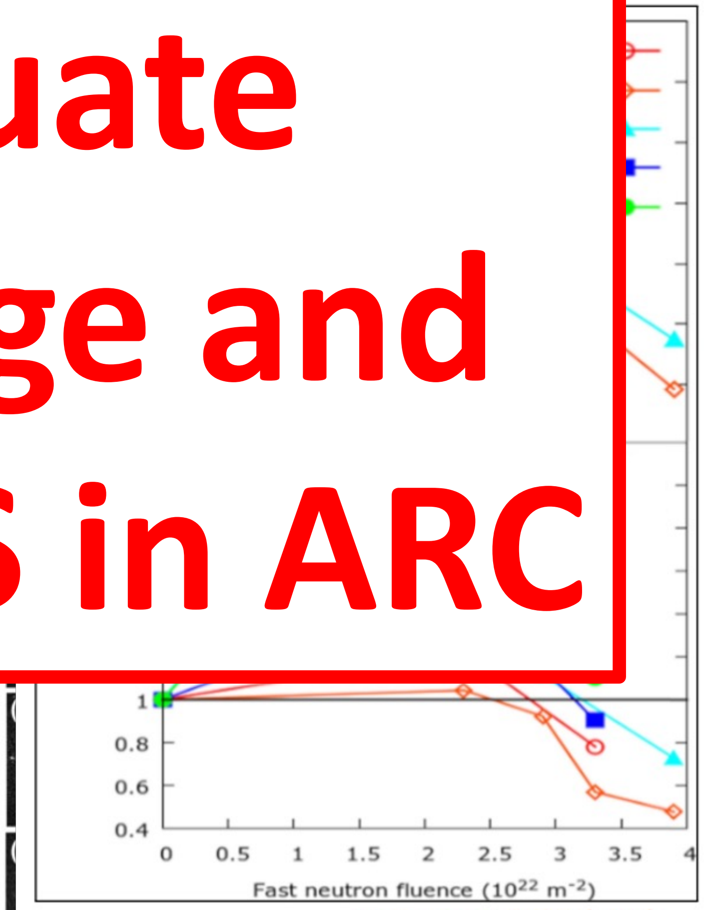


Linden *et.al.* J. Microsc. (2021)

Magnetic confinement approach – compact reactors

High temperature superconductors (HTS) tapes: hi

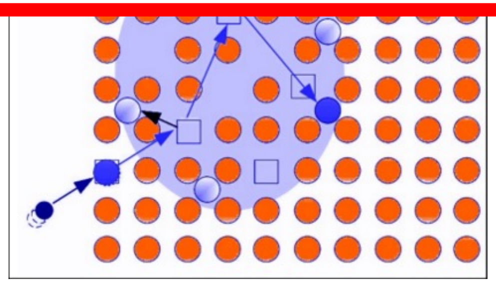
Superconducting properties vs neutron irradiation: lattice damage and vortex pinning

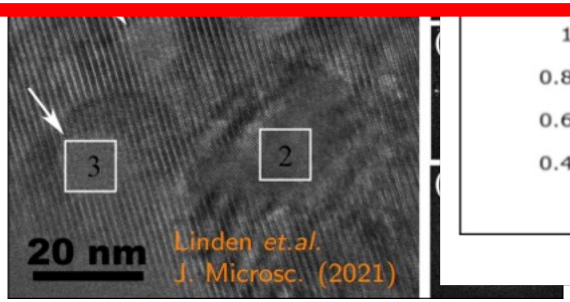


Fischer *et.al.* SuST (2018)

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

But





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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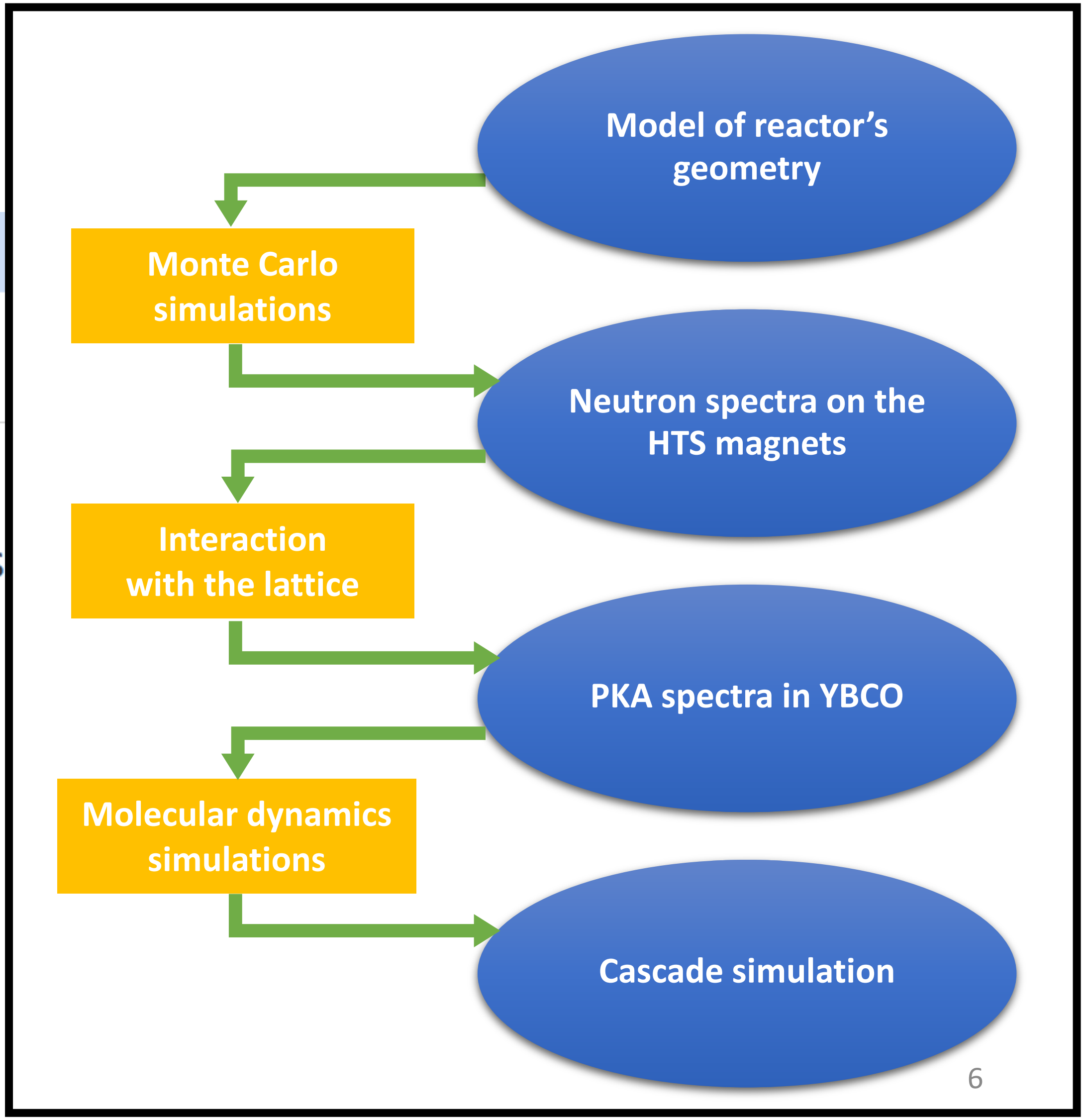
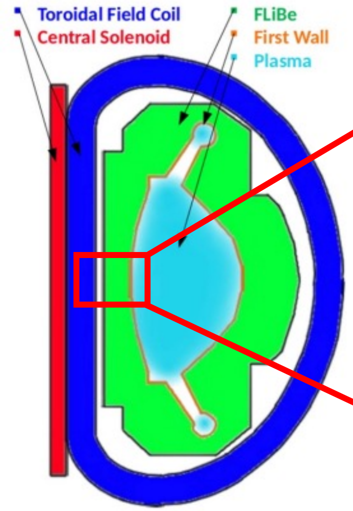


Neutron transport

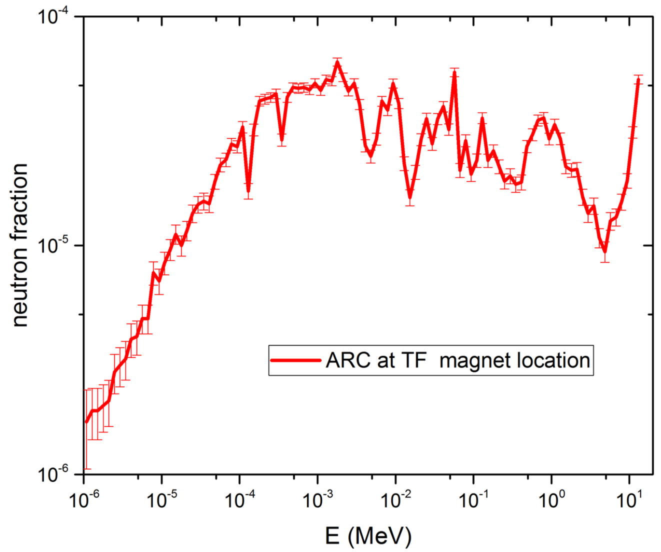
Parameter	ARC (expected in 10 years)	TRIGA (Fischer*et al* [12])
Fast neutron fluence (neutrons cm^{-2})	1.6×10^{19}	4.0×10^{18}
dpa	0.52	0.02
H yield (appm dpa^{-1})	0.5	0
He yield (appm dpa^{-1})	10.6	0

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

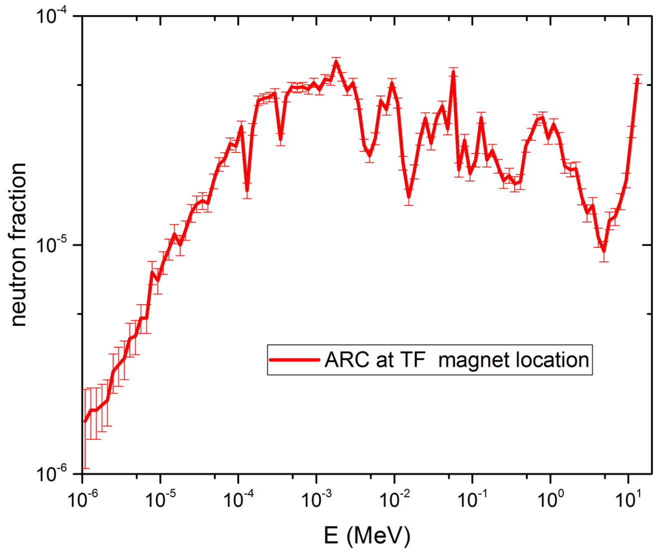


D Torsello, D Gambino, L Gozzelino, A Trotta and F Laviano, Supercond. Sci. Technol. 36, 014003 (2023)

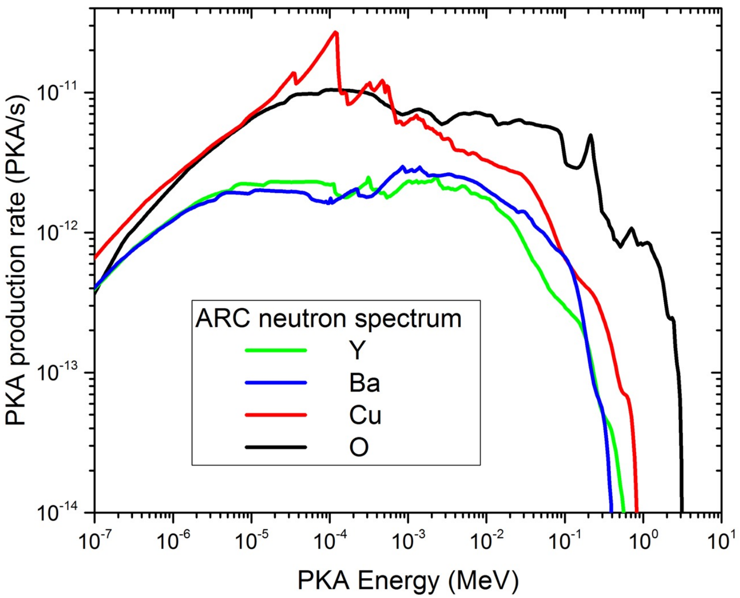
Neutron-lattice interaction

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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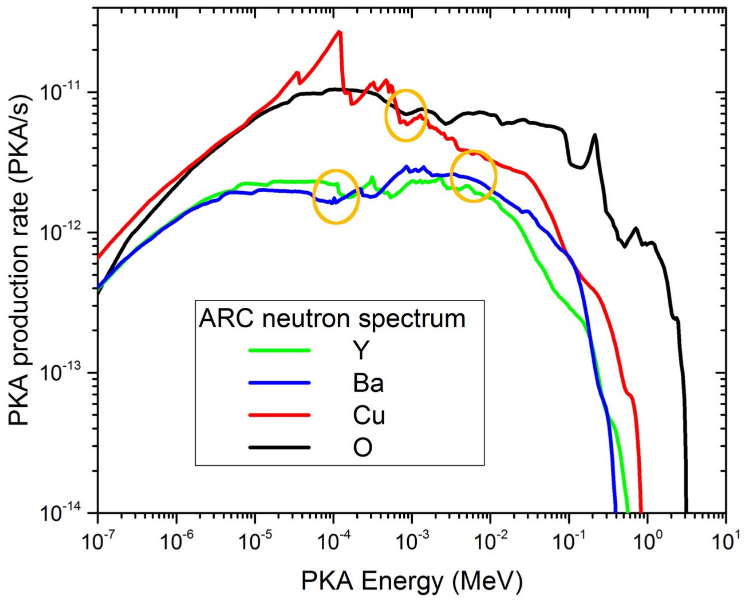
Cascade simulation

PKA spectra in YBCO → Molecular dynamics simulations → Cascade simulations



- Collision cascade simulations
- Results:
  - Defect size vs energy
  - Defect morphology
  - Defect recombination
  - Temperature transients
- Important for SC properties

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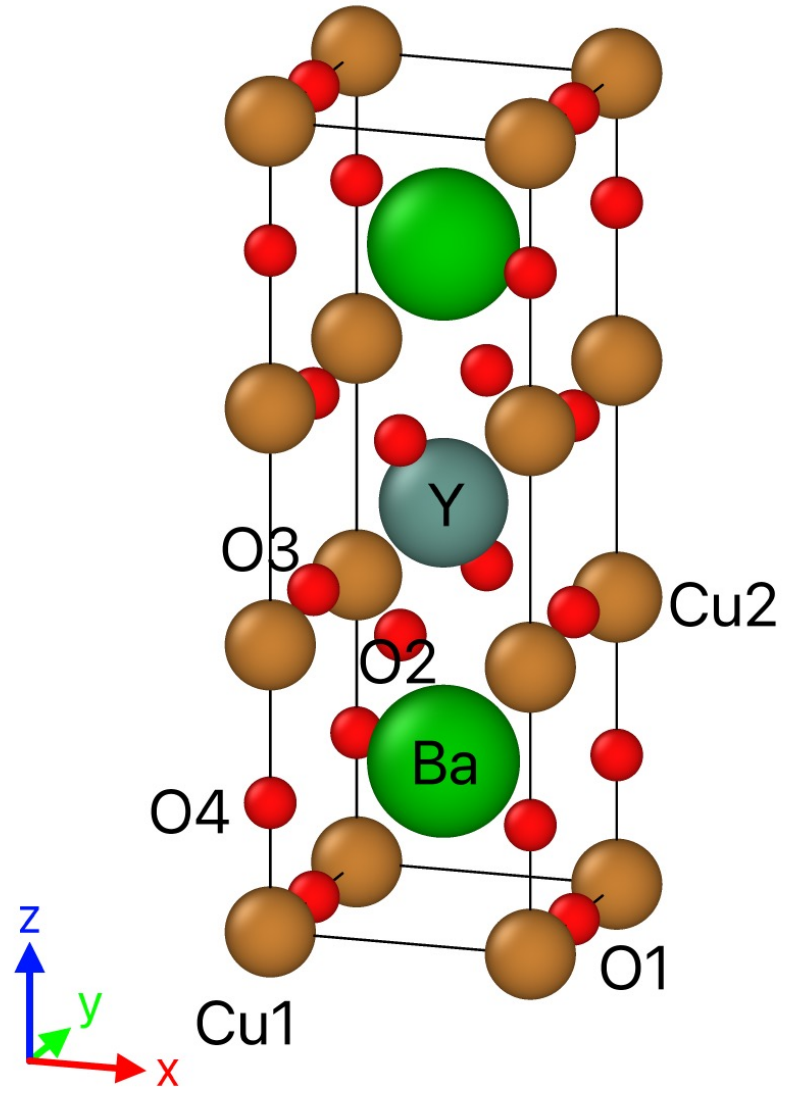
$YBa_2Cu_3O_7$ (YBCO)

- 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

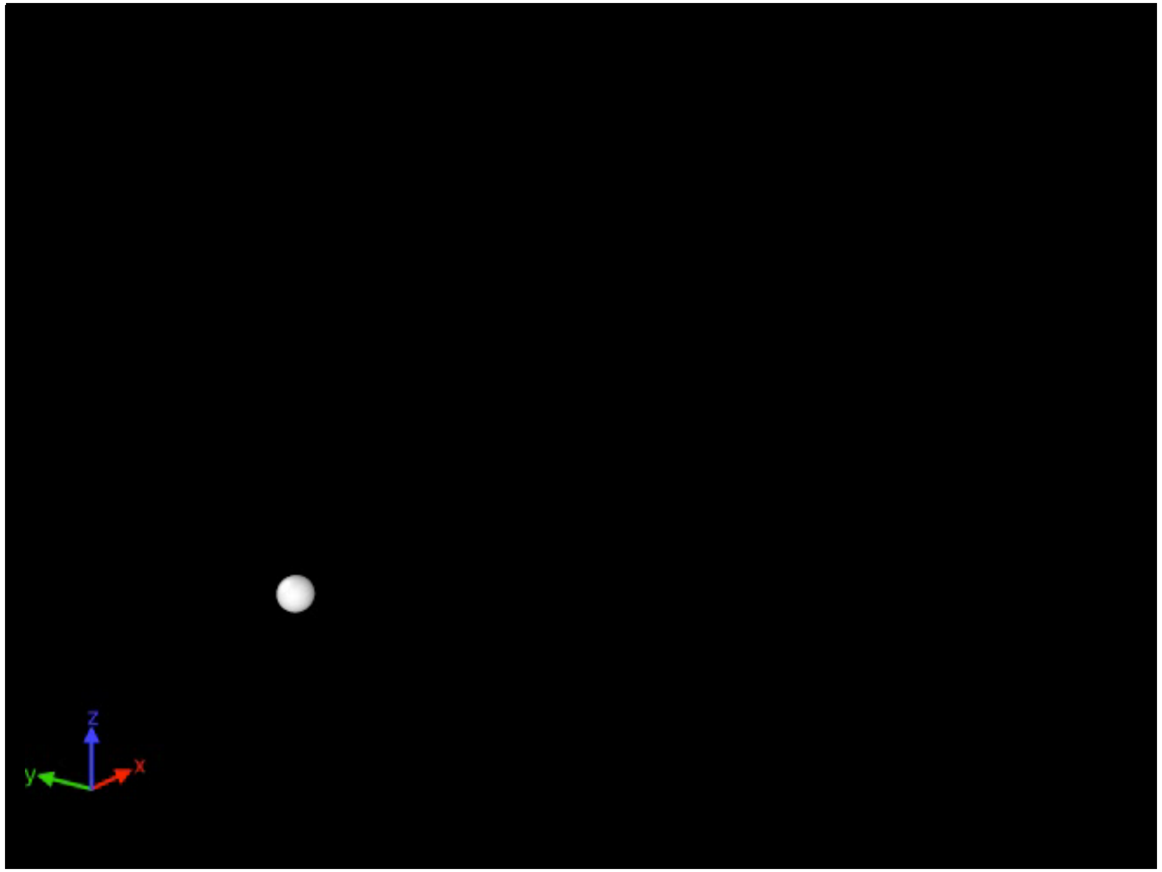


MD –collision cascade simulations

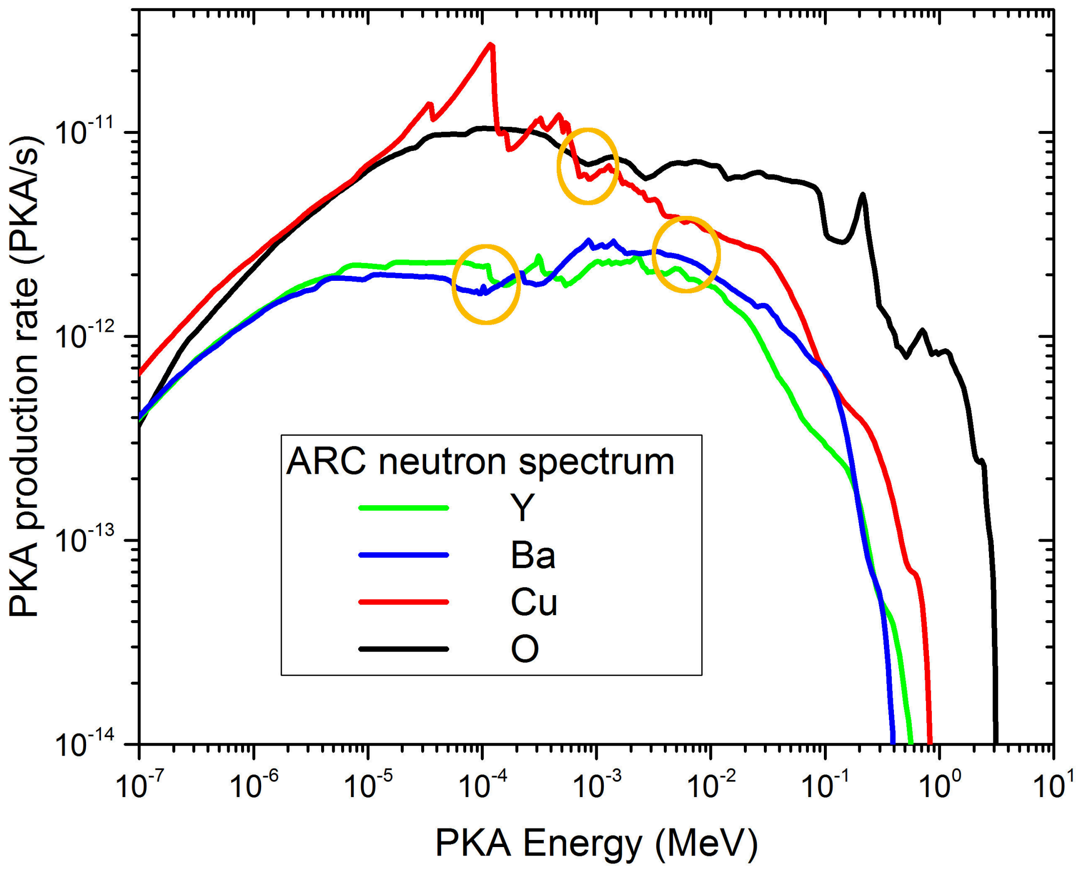
Workflow:

- 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
- Track number of defects with Wigner-Seitz analysis (Ovito)



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

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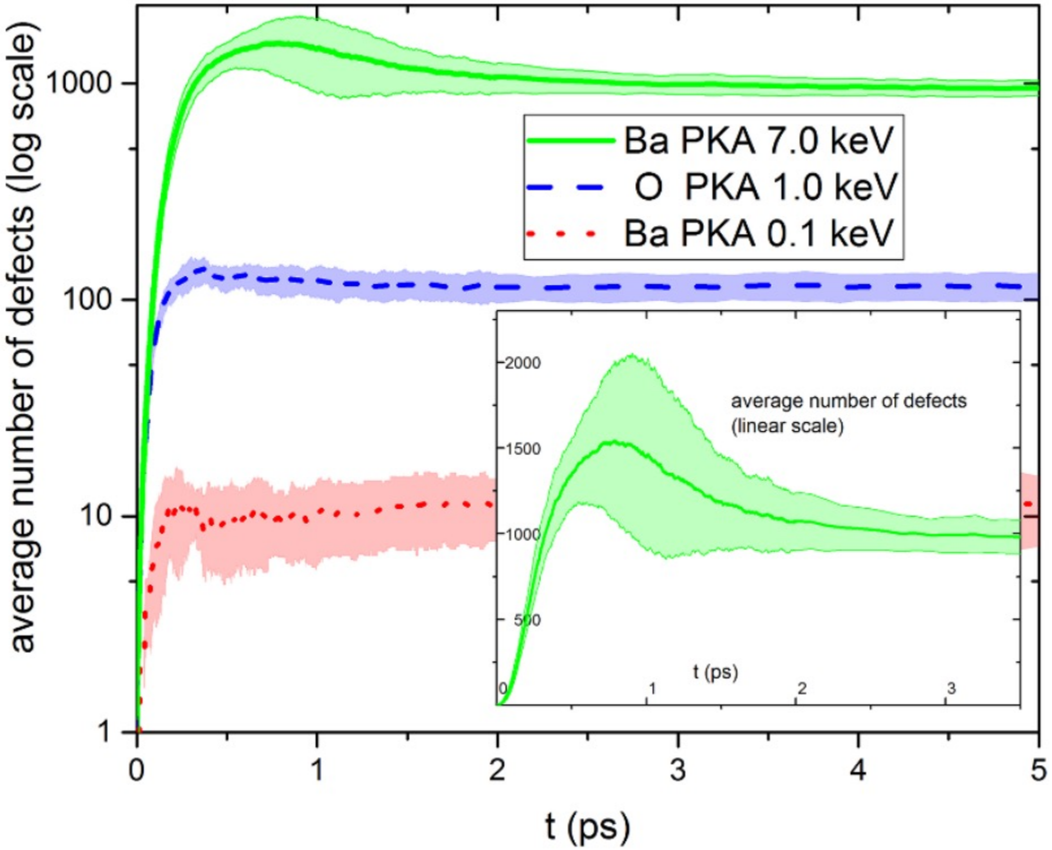
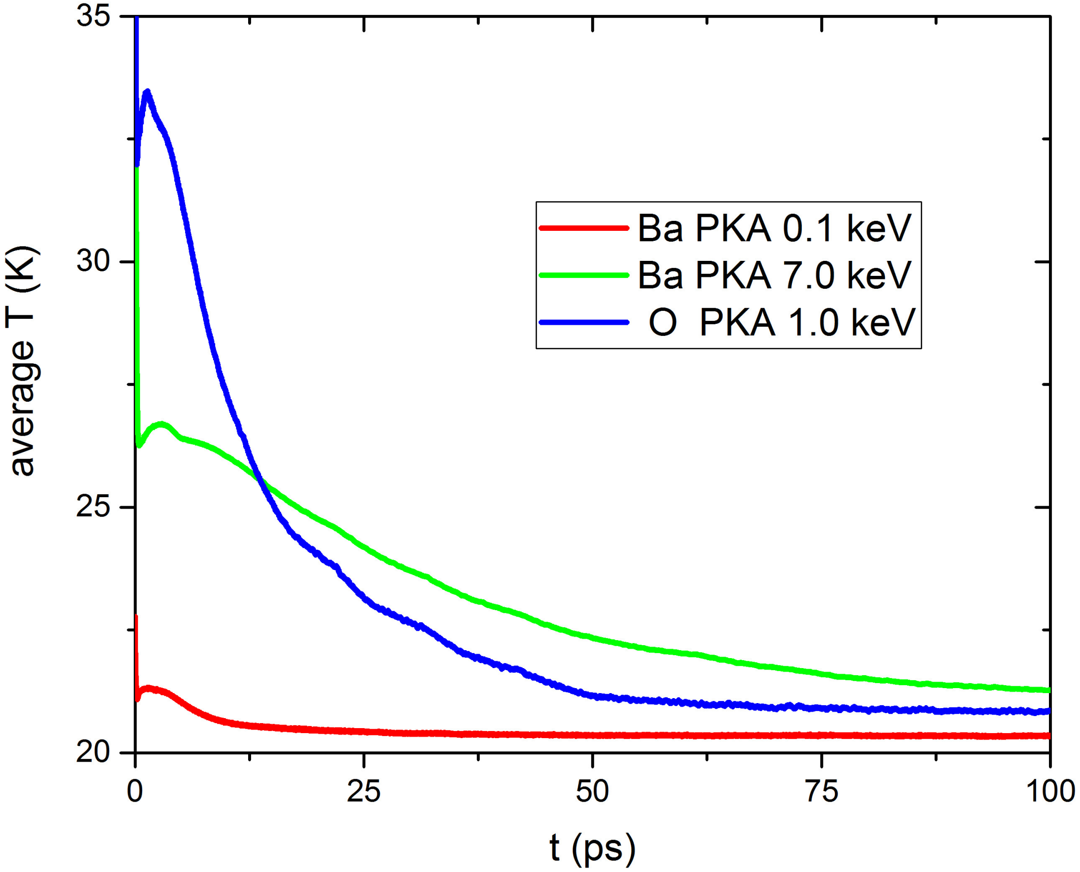
MD – Results

Average number of defect vs time



Temperature vs time



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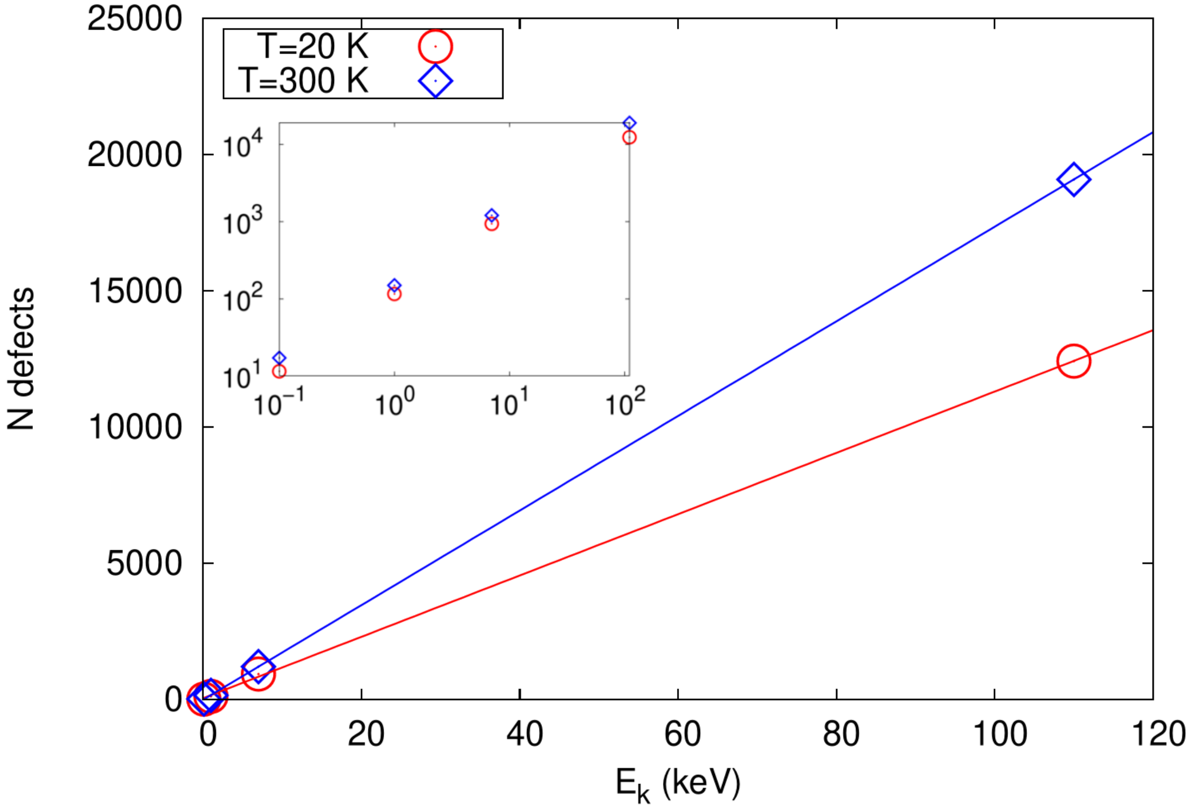
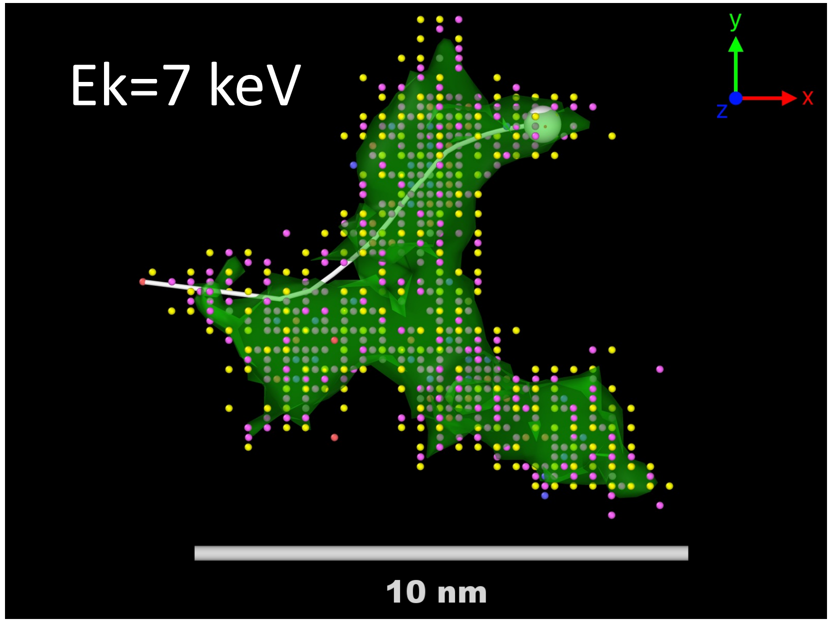
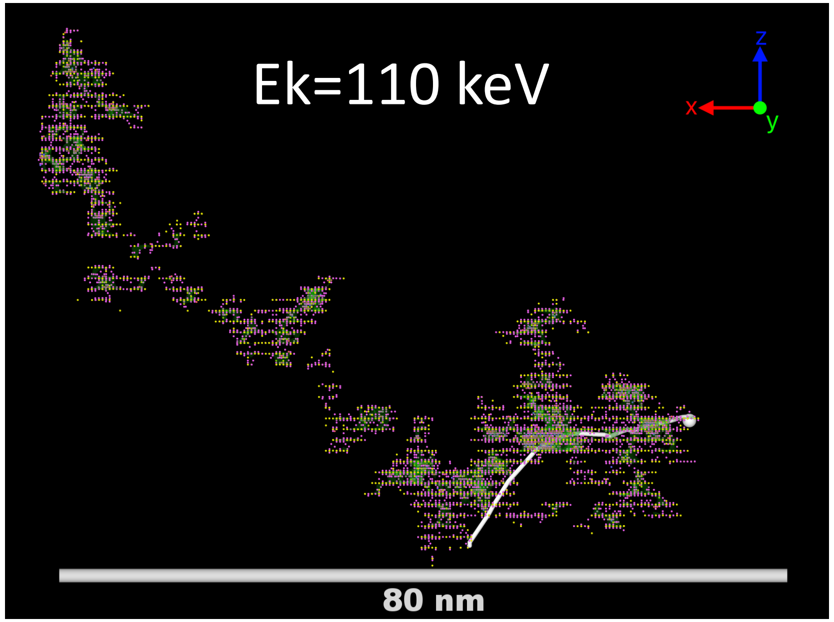
MD – Results

Average number of defect vs E_k







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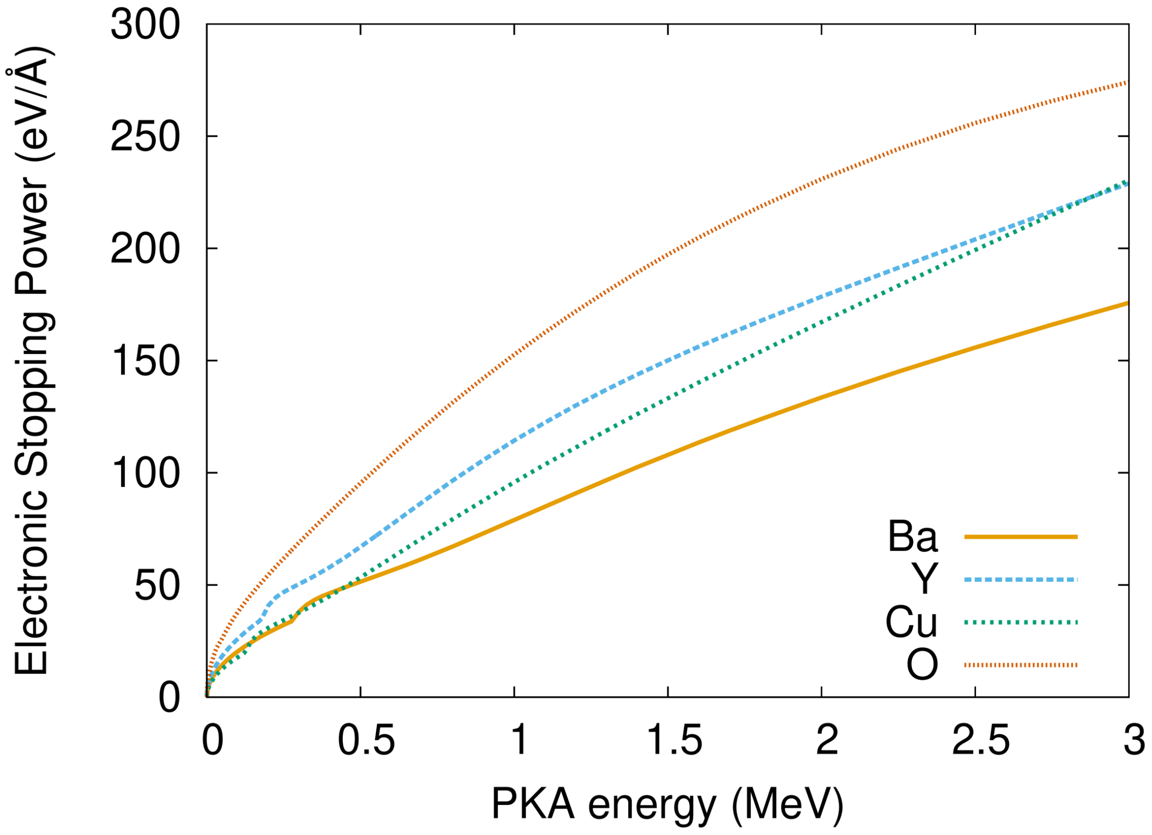
Ongoing work

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:

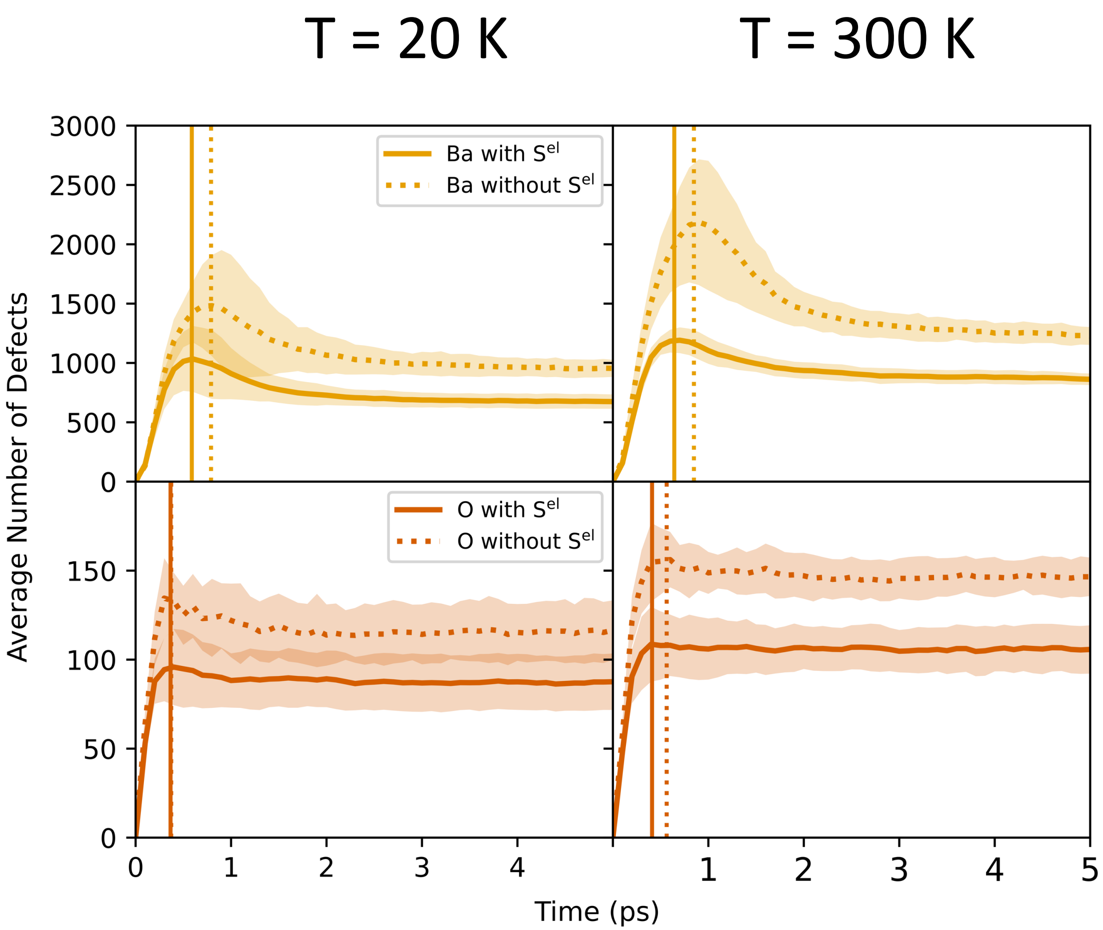
- Reduction of maximum and final number of defects
- Species and temperature dependent effect

PKA = Ba

E_k = 7 keV

PKA = O

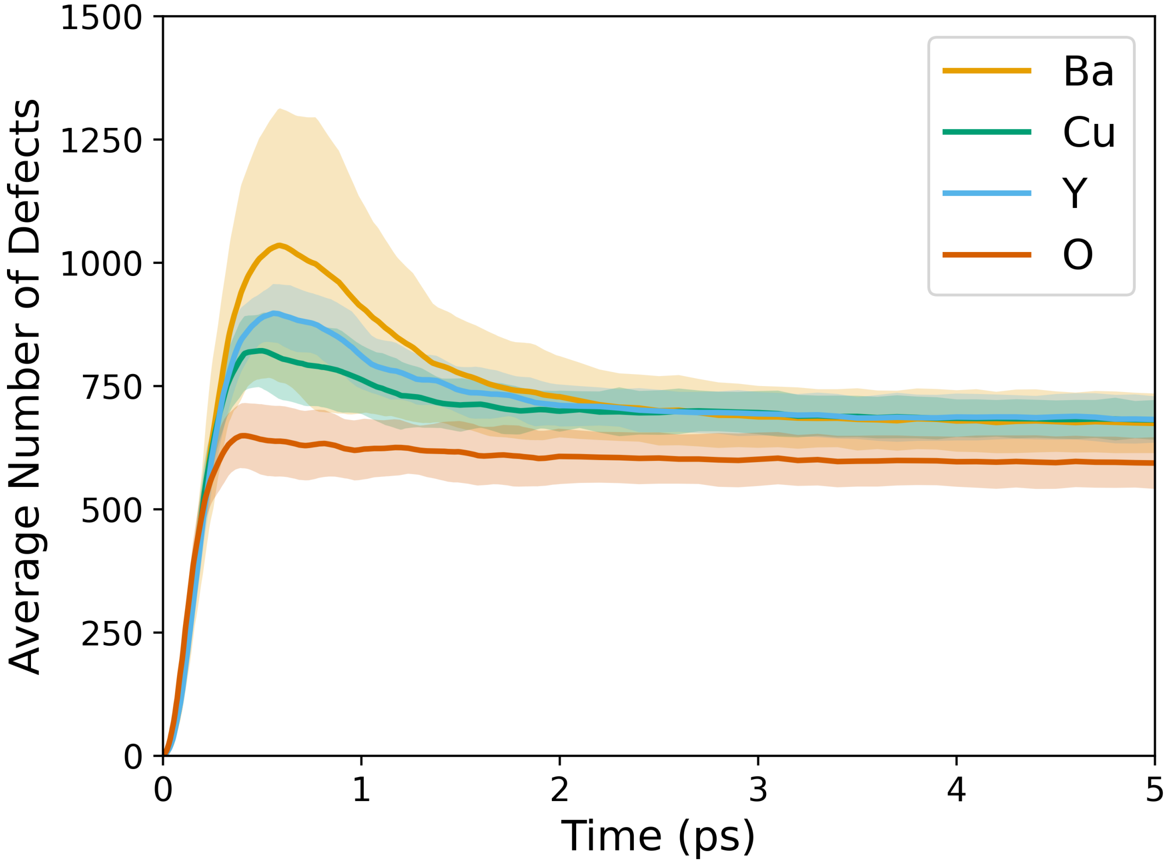
E_k = 1 keV



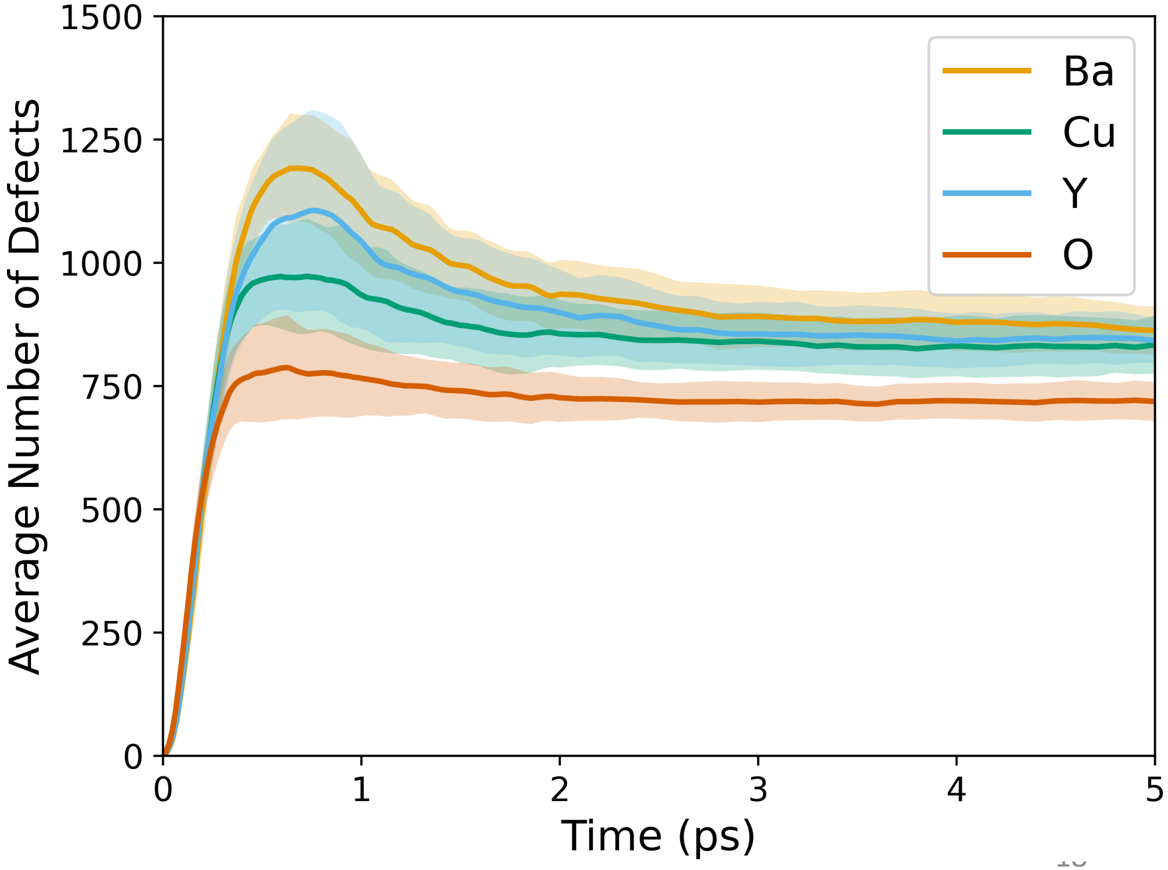
Defects vs PKA (E_k = 7 keV)

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

T = 20 K

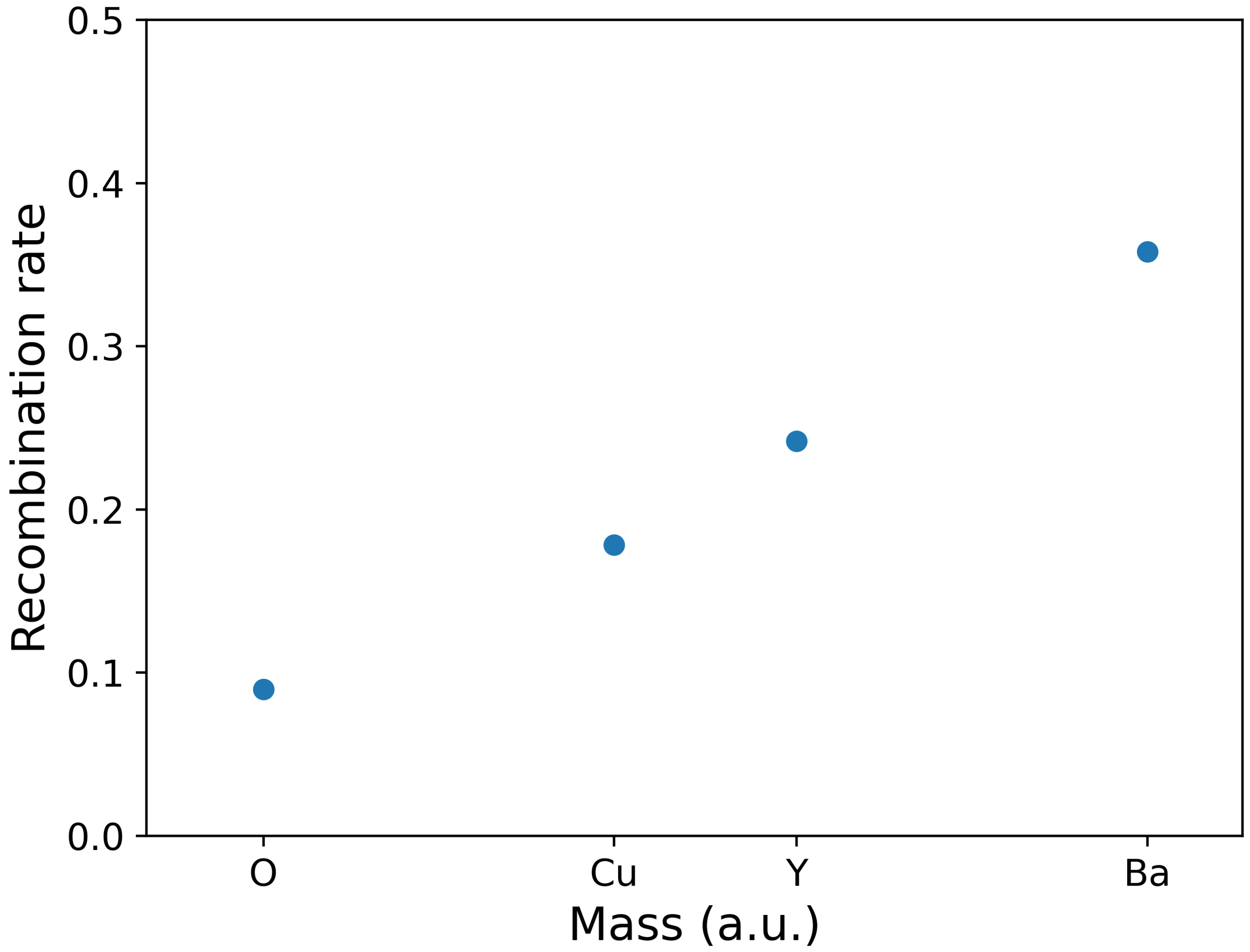


T = 300 K

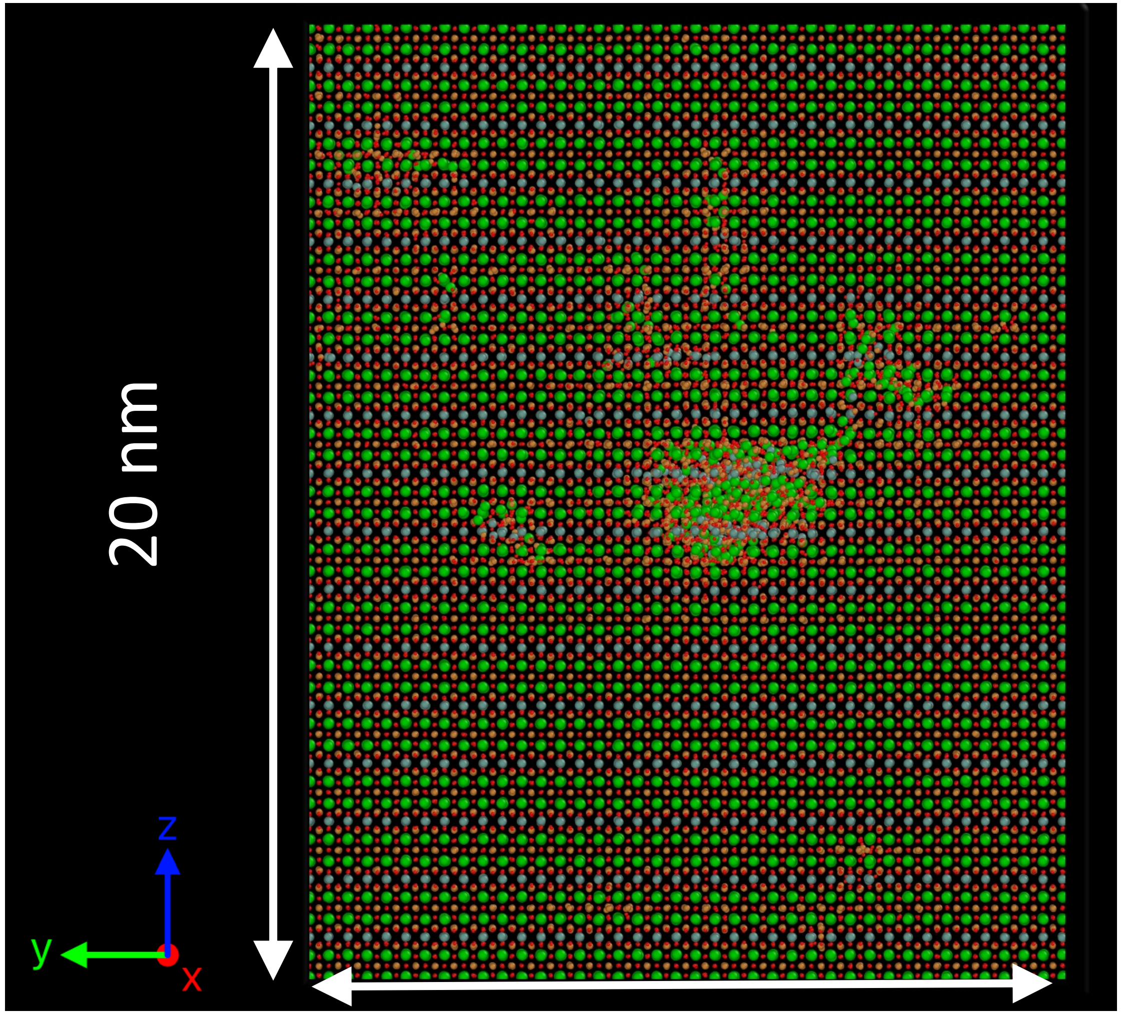


Recombination rate vs PKA (E_k = 7 keV)

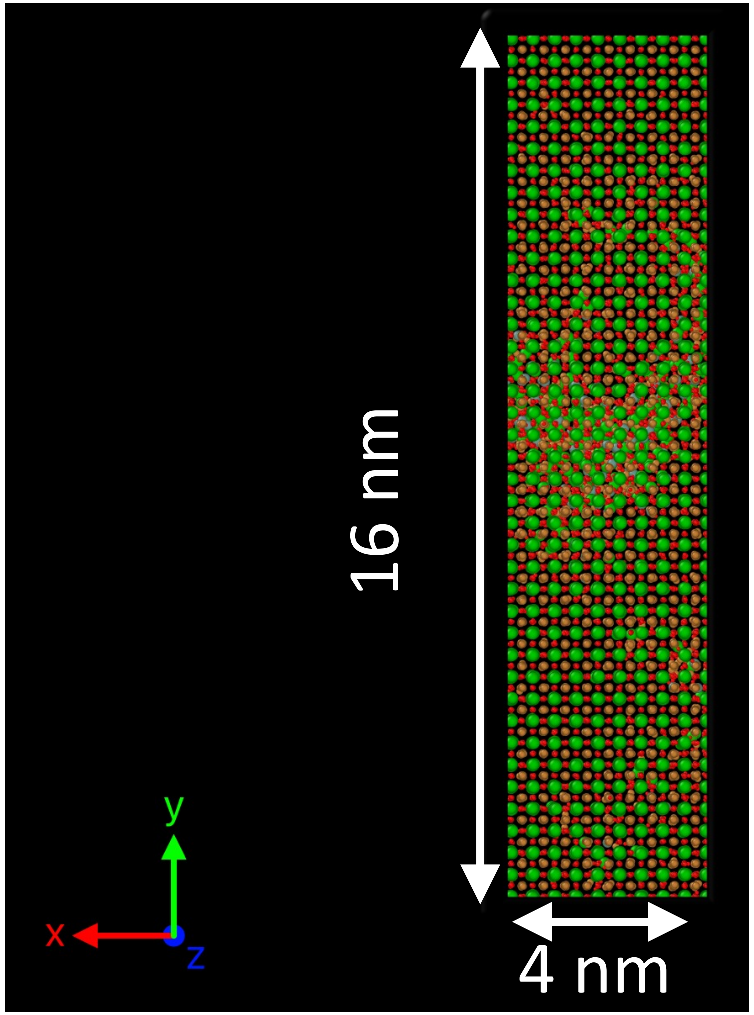
$$\text{Recombination rate} = 1 - N^{\text{final}}/N^{\text{peak}}$$



TEM reconstructions – Defects

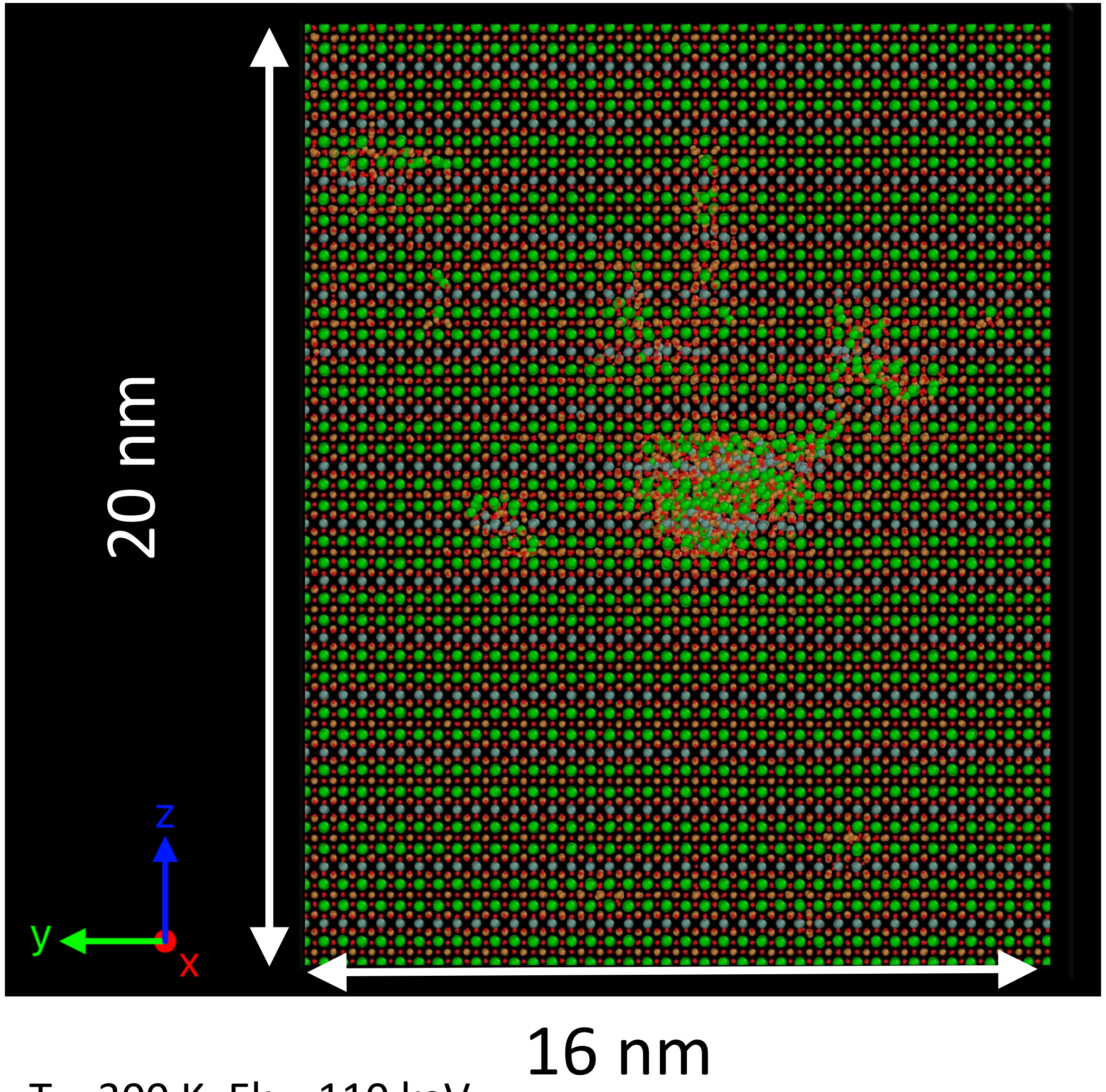


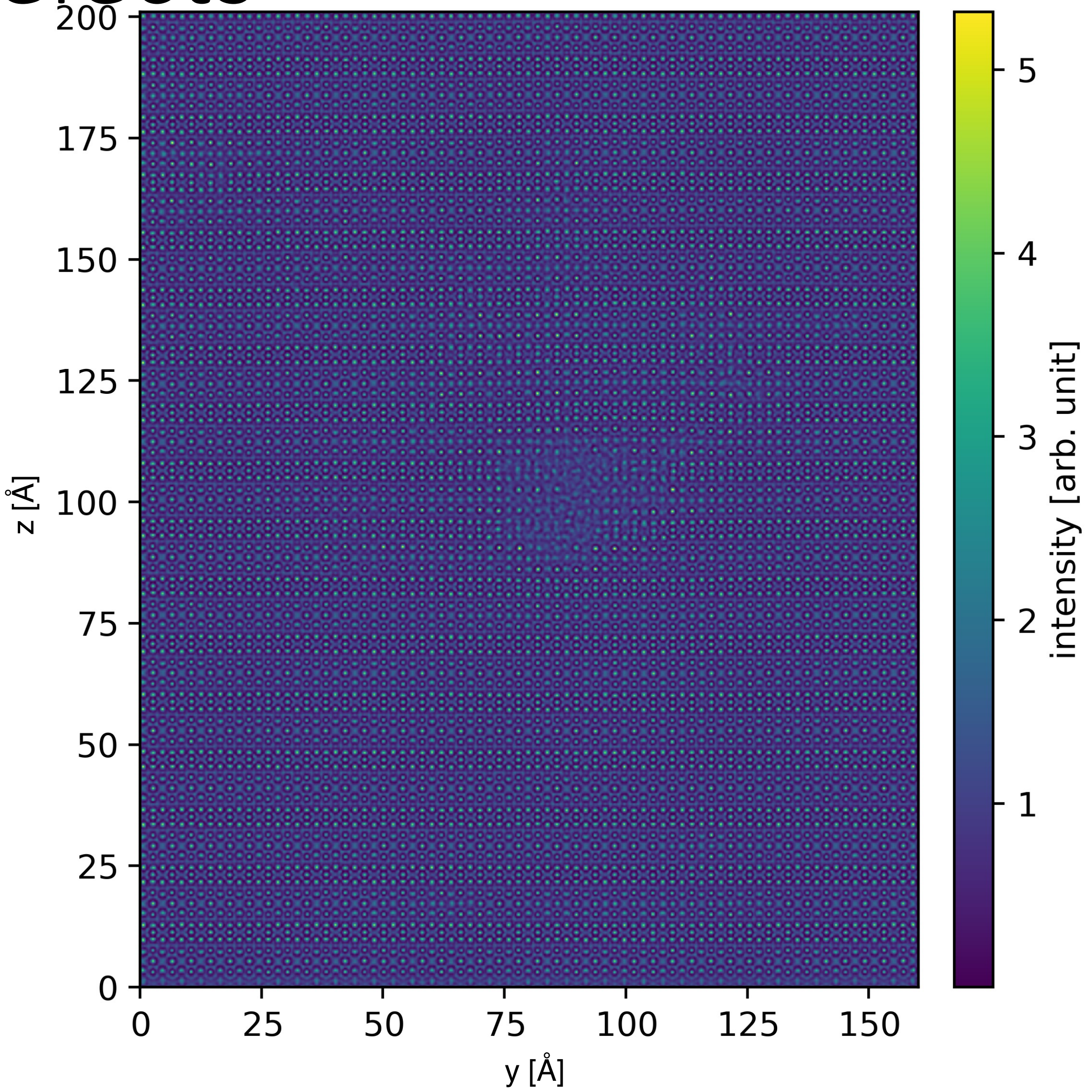
16 nm



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

TEM reconstructions – Defects





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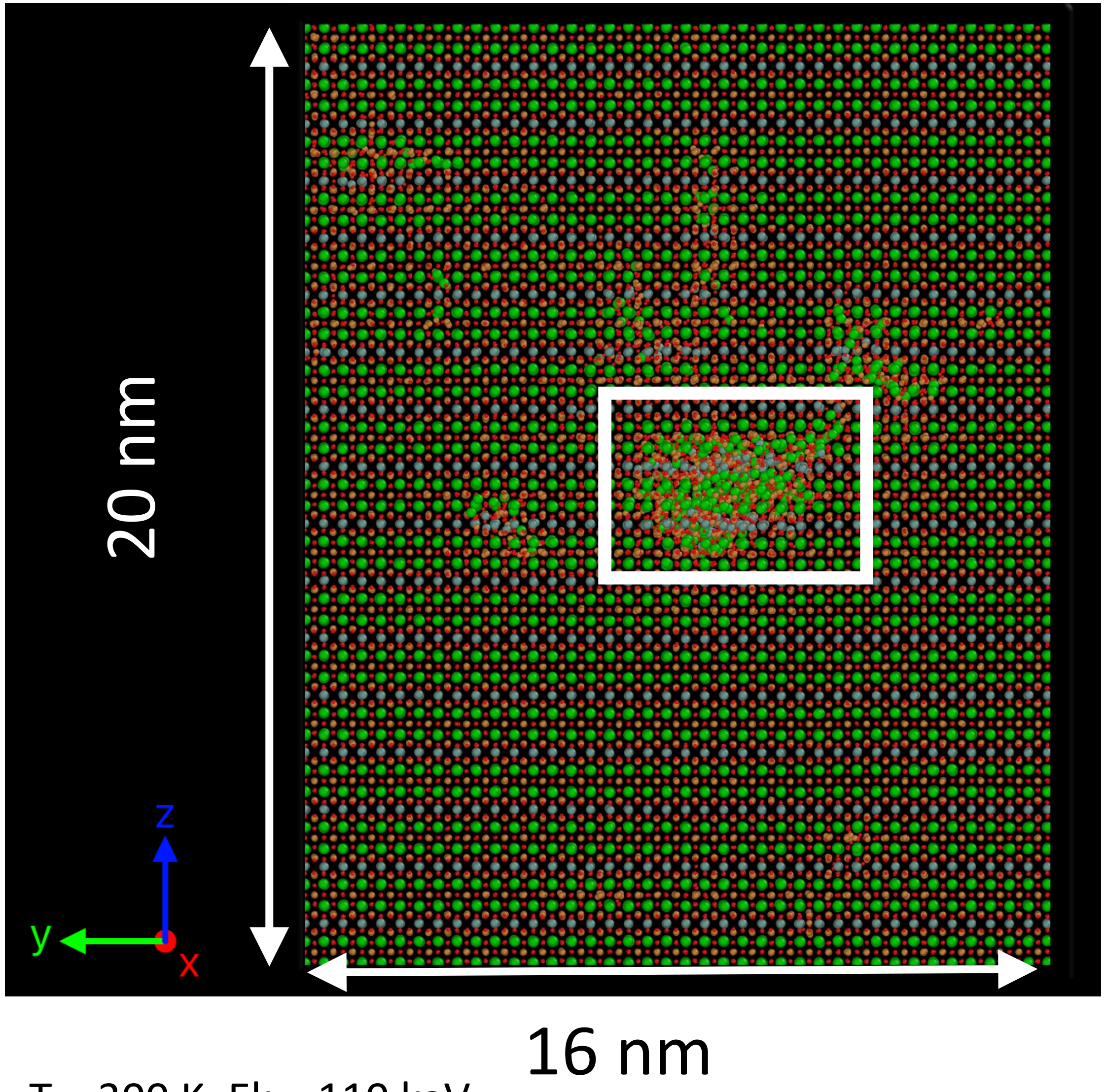

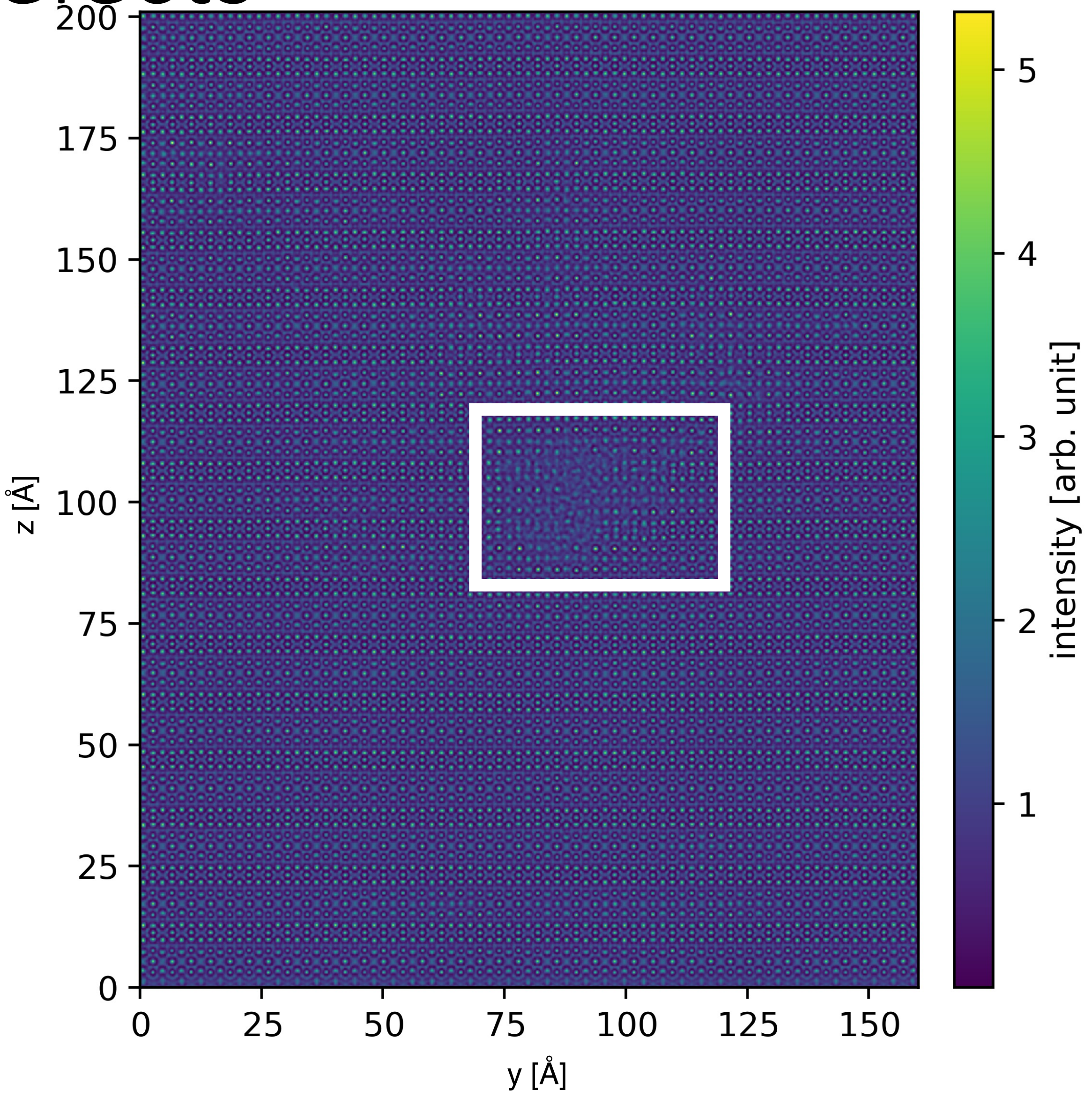

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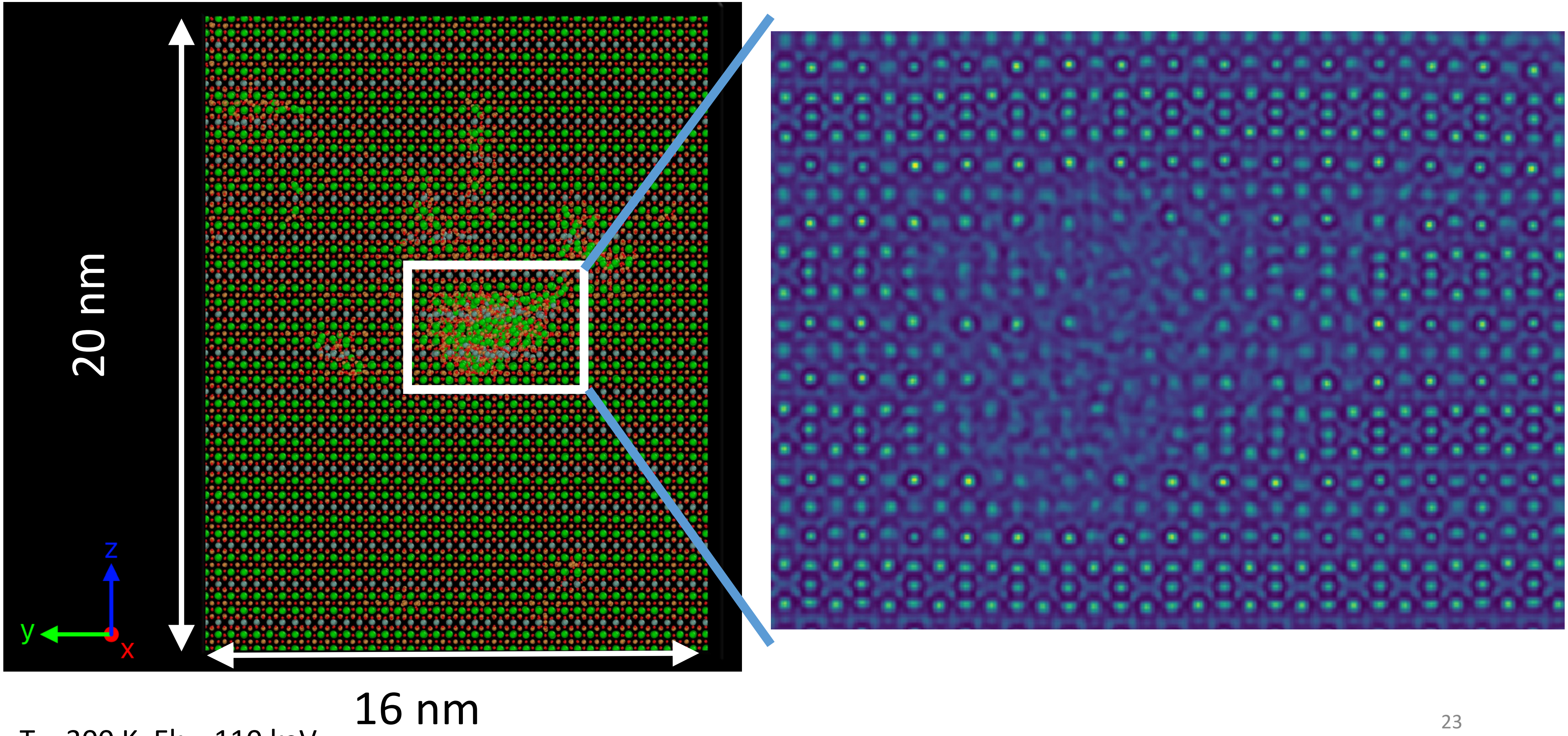

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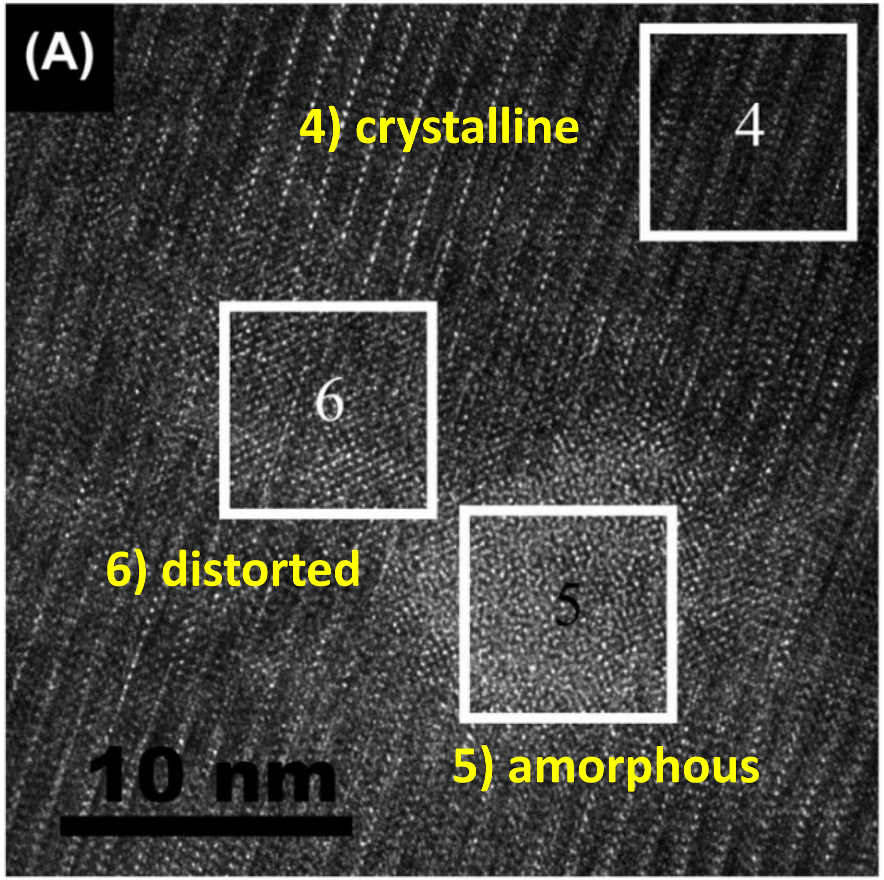

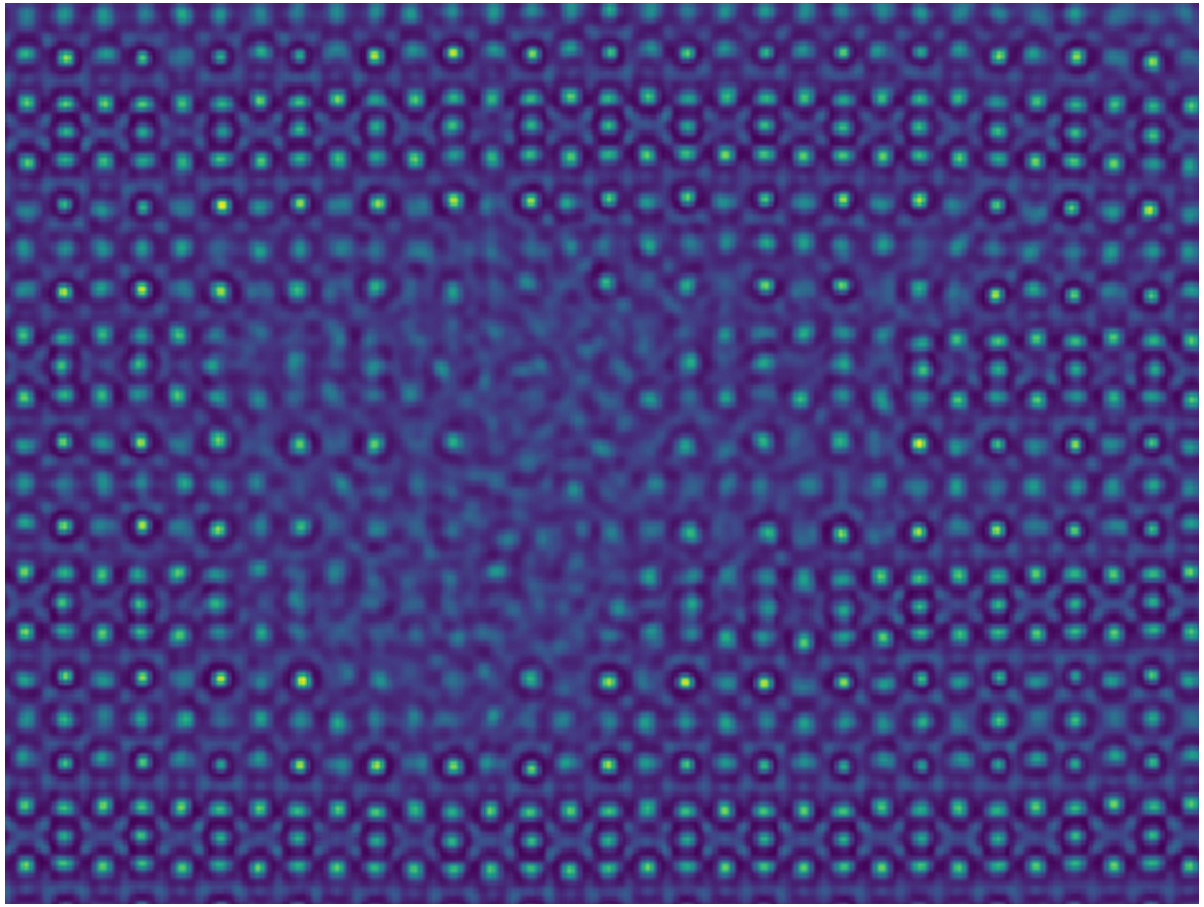

From Linden et al., Journal of Microscopy 286, 3-12 (2022), neutrons from TRIGA MARK II

Conclusions

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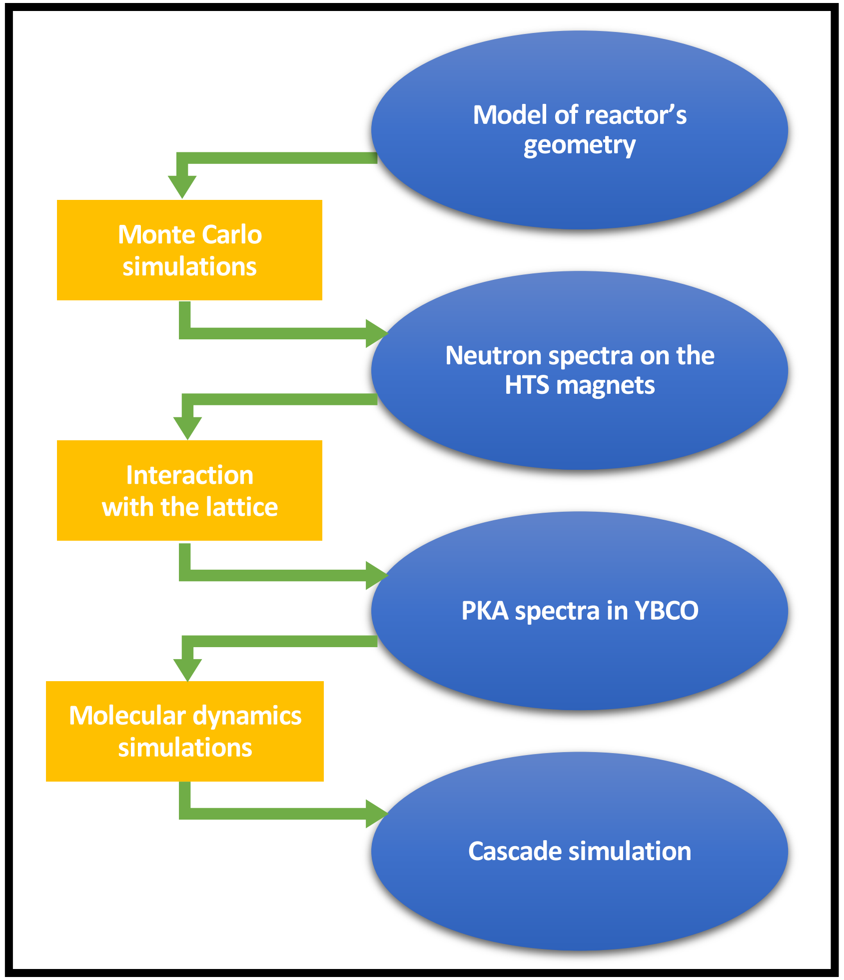
Conclusions

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



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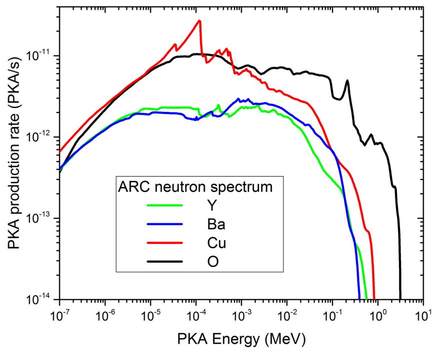

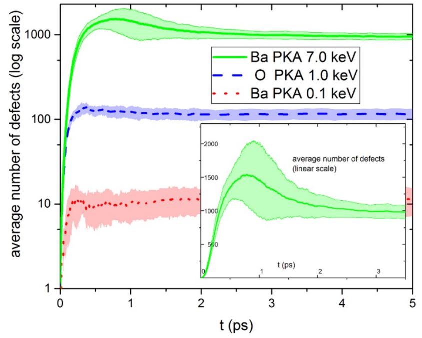

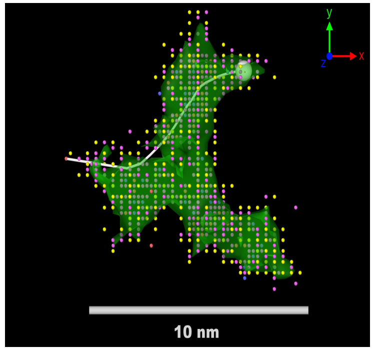

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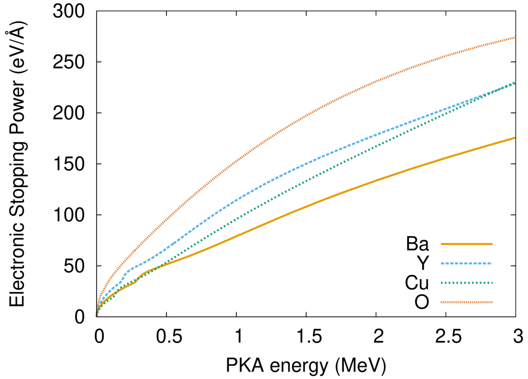
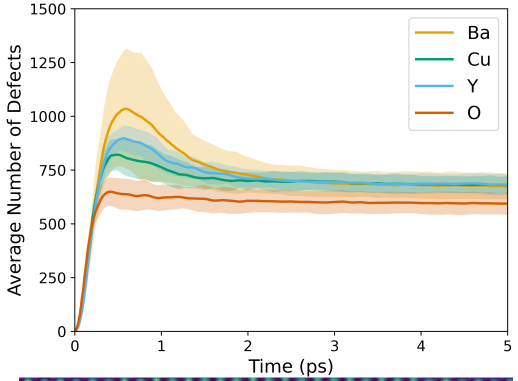
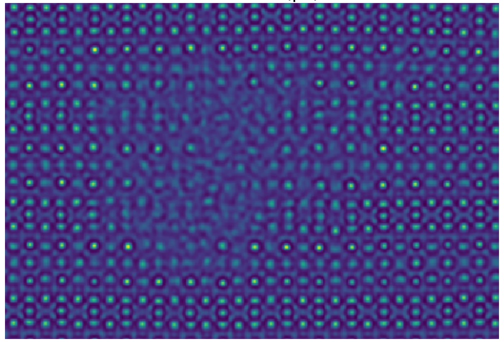
  - Electronic system
  - Defects vs PKA and energy
  - TEM







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Funding: Vetenskapsrådet

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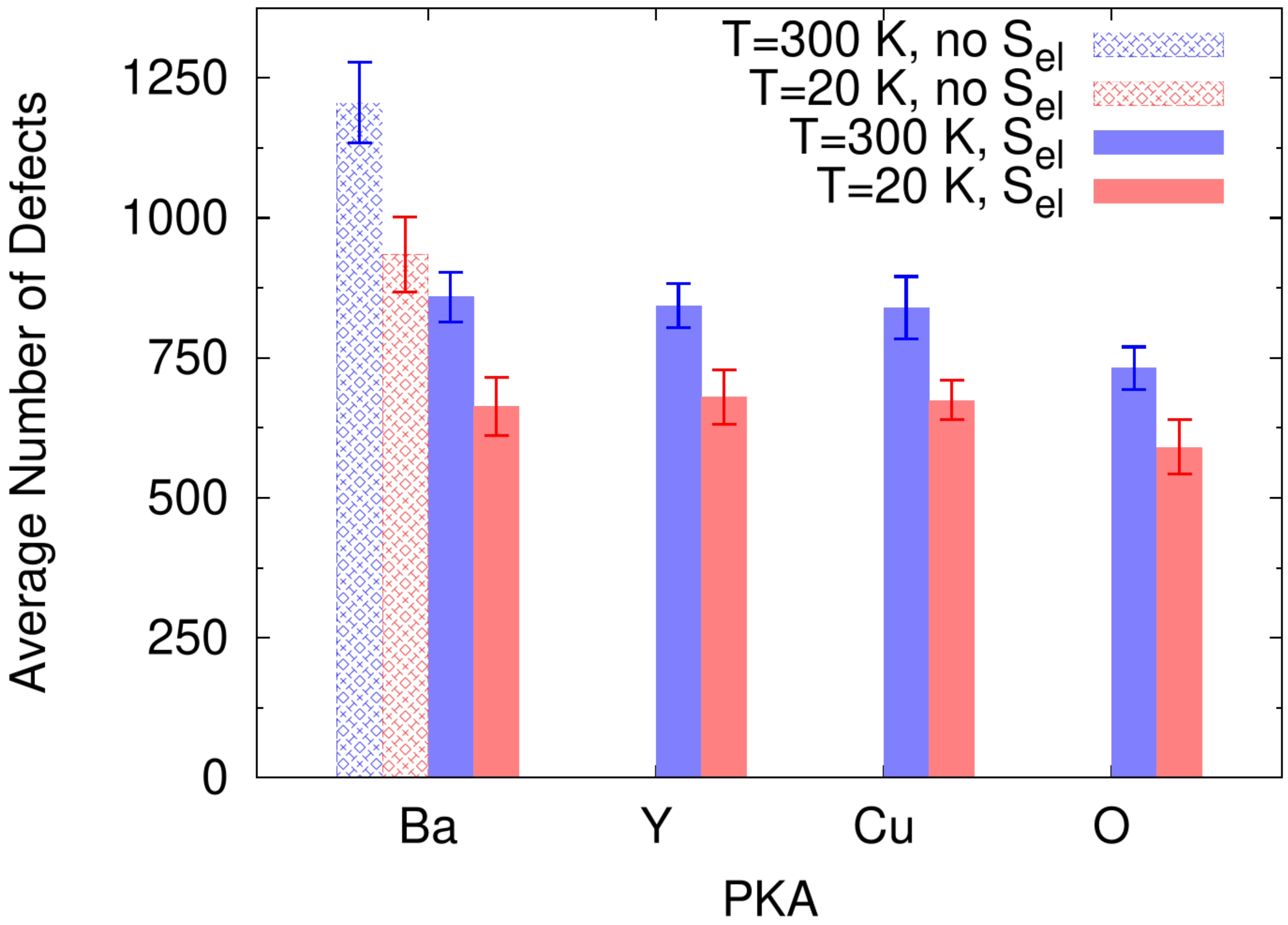
Additional slides

Defects vs PKA (E_k = 7 keV)



Number of vacancies vs PKA (E_k = 7 keV)

O vs cation vacancies