

Computer Simulation of Ion-irradiation of Tungsten: Preliminary Results

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Objectives

- To simulate the ion-induced damage in tungsten
- To study the influence of micro-structure on damage and its impact. Focus on the issues which are inaccessible for experimental investigation
- Ultimately simulate trapping and retention of hydrogen isotopes within the polycrystalline-W

Plan

- PKA spectrum due to neutrons (ITER-like scenario)
- Dynamics of cascade evolution
- Frenkel Pairs
- Defect structures
- Diffusive movement of interstitial
- Deuterium interaction with W-surface
- Grain Boundary Studies

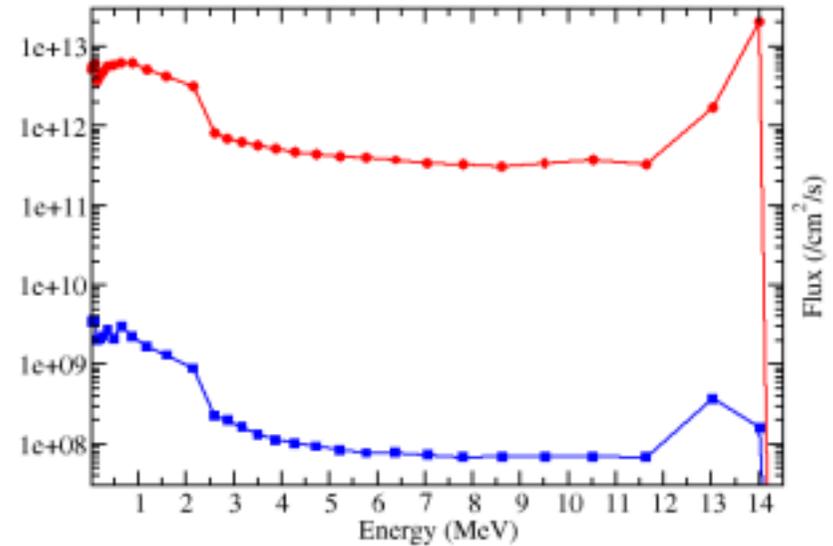
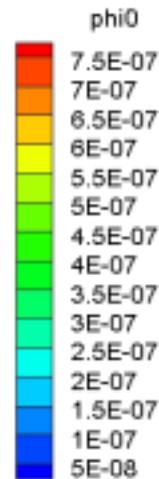
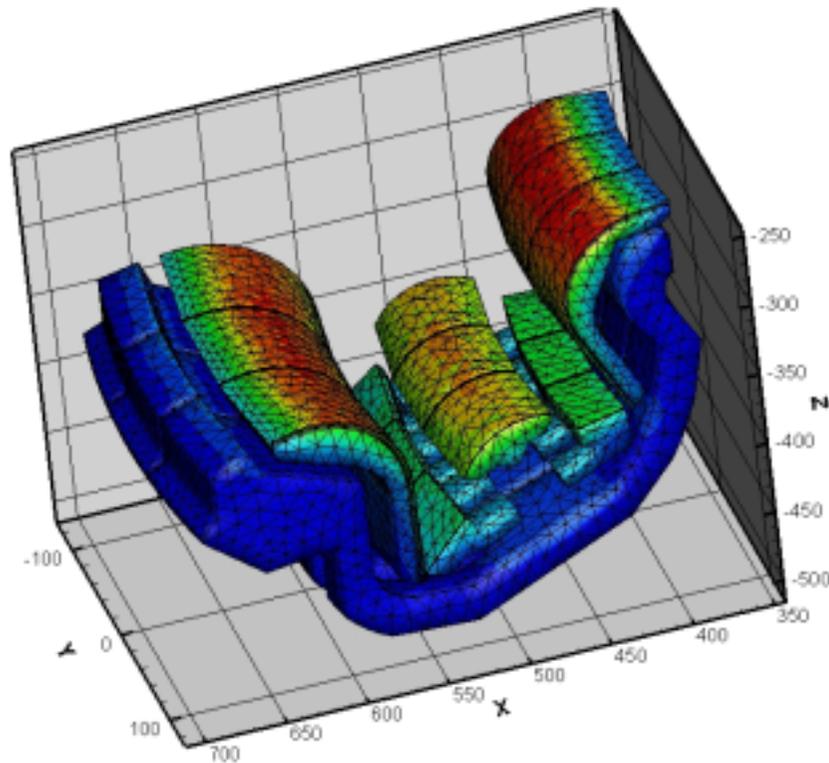
There will be a separate presentation Ion-irradiation experiments tomorrow

An ITER-like scenario

Power=500 MW

ATILA computations: Solving neutron transport equations using FEM methods

For 46 energy groups and 40017 mesh points for 500 MW H-mode D-T operations [*]



Lowest and highest neutron flux distribution

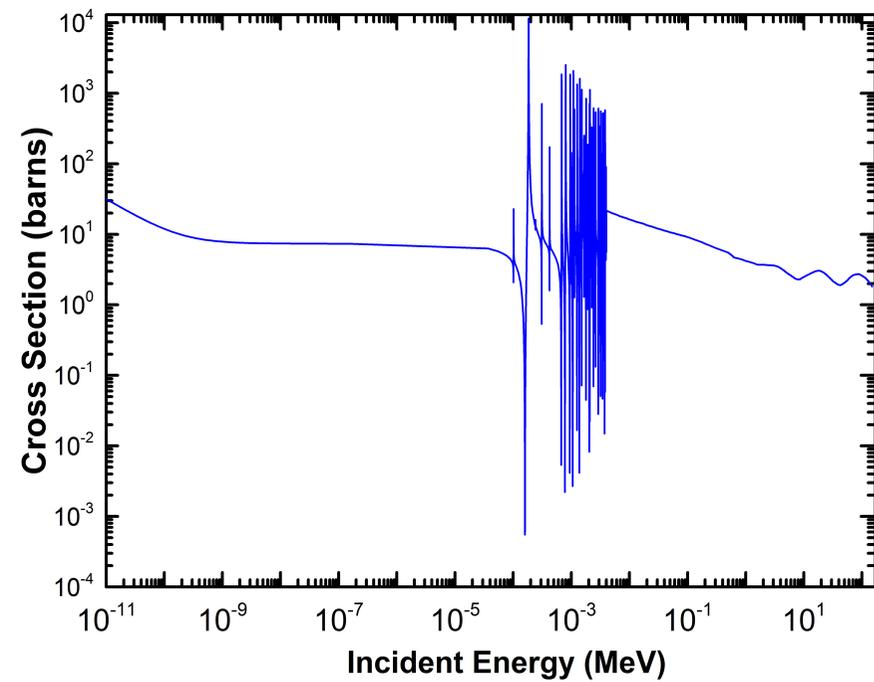
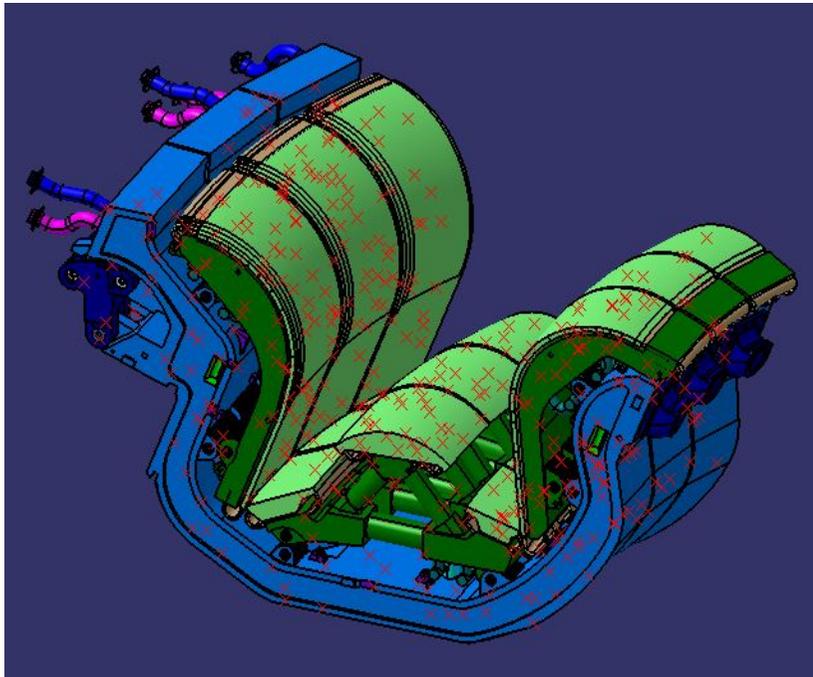
$$\Phi = \phi_0 * 1.77E20$$

[*] P.V. Subhash et.al., ITER Nuclear Calculations with ATILA Code ANST, 108 (2013)
2nd RCM of the CRP on Irradiated Tungsten, Seoul, Korea, 8-11 Sept. 2015

Primary Knock-on Atom (PKA) Energy Calculation

PKA energy was calculated at 400 selected representative points (x) using **SPECTER** code [*]. Average is about 18 keV.

Neutron cross-sections are taken from FENDL library [**]

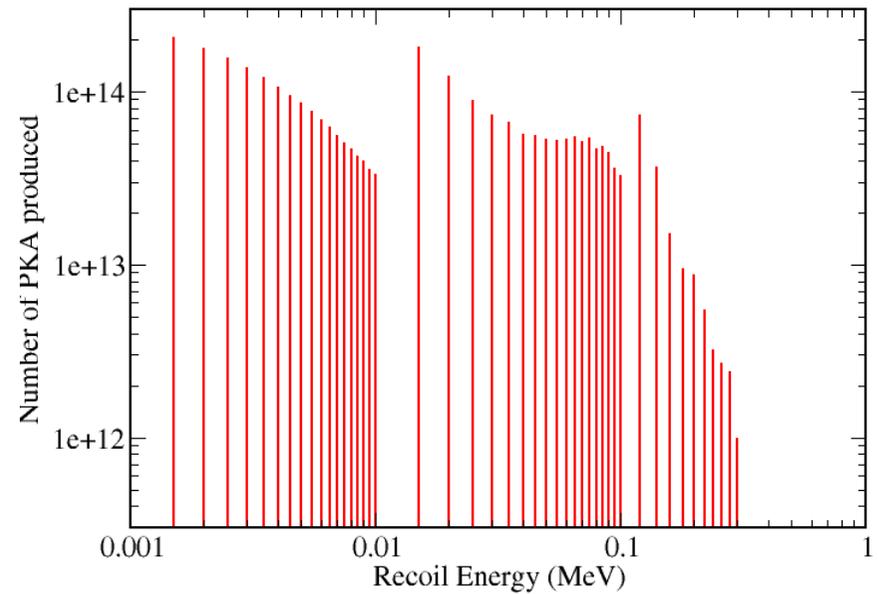
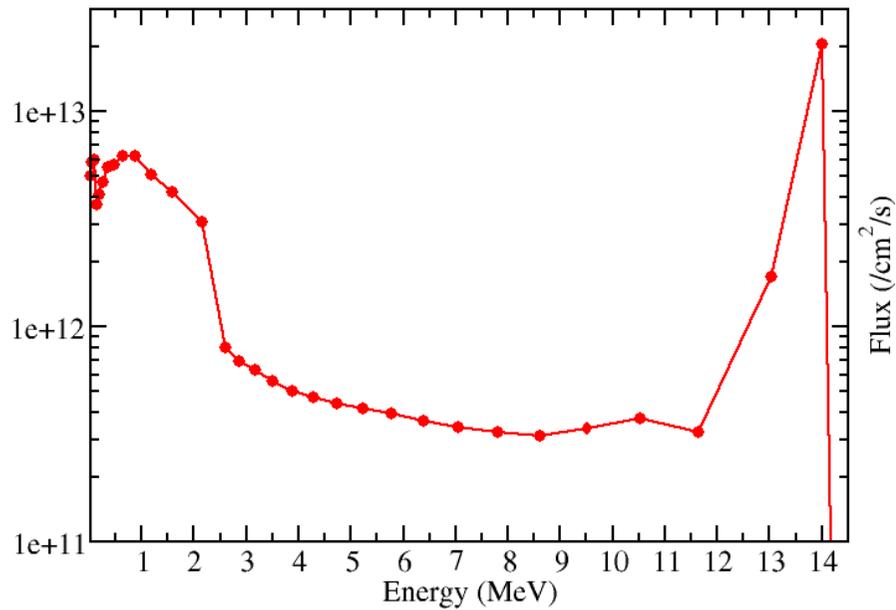


Elastic cross-section of neutrons with W184

[*] L.R. Greenwood and R.K. Smither, ANL/FPP/TM-197

[**] <https://www-nds.iaea.org/fendl30/>

PKA Energy Spectrum



PKA generated (right) within tungsten; 0.5 cm thickness, 1cm x 1cm area. One of the typical locations on outer vertical target region where n-flux is high.

Neutron flux at divertor surface on left. Fusion power 500 MW, Exposure time 400 sec.

DEMO/Next Step Tokamak: Some thoughts

- Higher flux (about 3-4 times that of ITER?)
- Higher pulse duration (about a day? ~200 times)
- Higher heat flux (3-4 times?)

- What does that translate into?
 - Damage characteristics and magnitude
 - Amount of fuel retained
 - Replacement period

Dynamics of PKA in tungsten - Ion-Irradiation Simulations

Two approaches

1. Binary Collision Monte Carlo (TRIM [*]/SRIM[#])
2. Molecular Dynamics Simulations (LAMMPS[**]/PARCAS[*#])

[* Eckstein, Computer Simulation of Ion Solid Interactions, Springer]

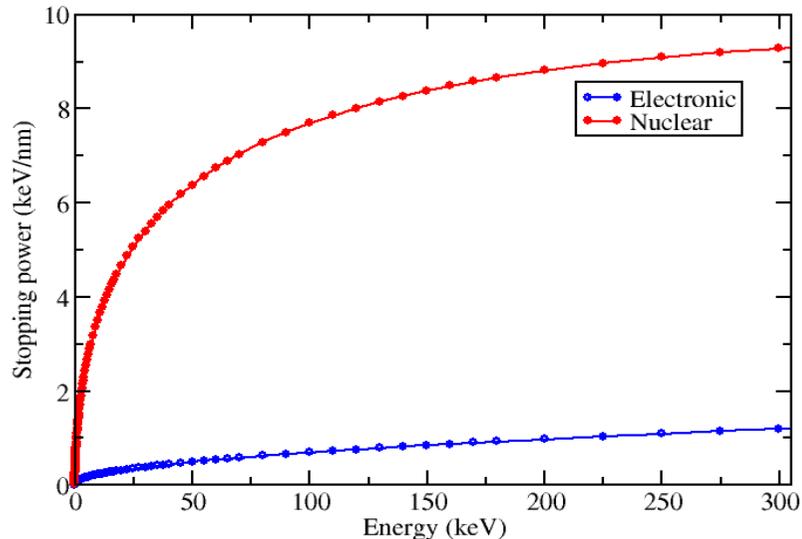
[# ZBL]

[** Plimpton]

[*# Nordlund]

2nd RCM of the CRP on Irradiated Tungsten,
Seoul, Korea, 8-11 Sept. 2015

Slowing Down of the Energetic Ions in Tungsten



Electronic loss has also been accounted for using Lindhard-Scharff Model [*].

$$S_e = \frac{8\pi e^2 a_0}{4\pi\epsilon_0} \frac{Z_1^{7/6} Z_2}{(Z_1^{2/3} + Z_2^{2/3})^{3/2}} \frac{v}{v_0}$$

The electronic stopping has been modelled as a continuous frictional loss to the electron system

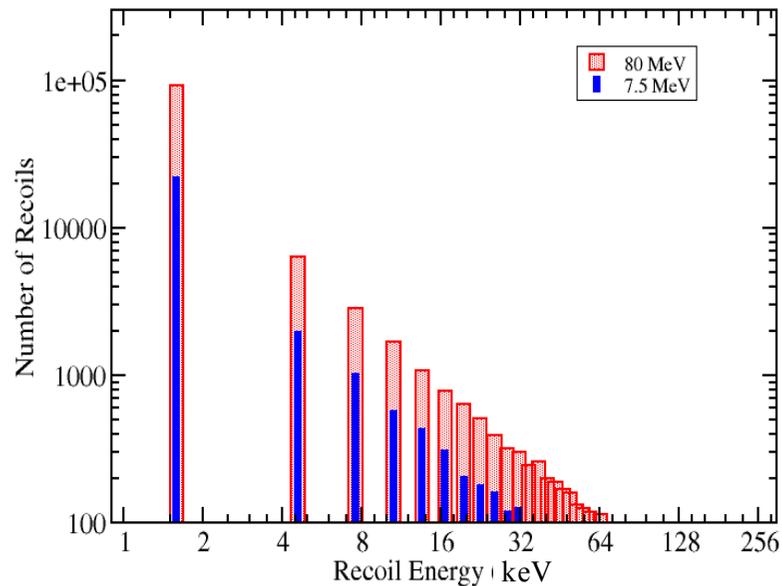
Electronic and nuclear stopping power as a function of W ion energy for neutron PKA range using ZBL formalism [**]

Both Binary Collision Monte Carlo & MD simulations and MD simulations can handle the frictional electronic losses.

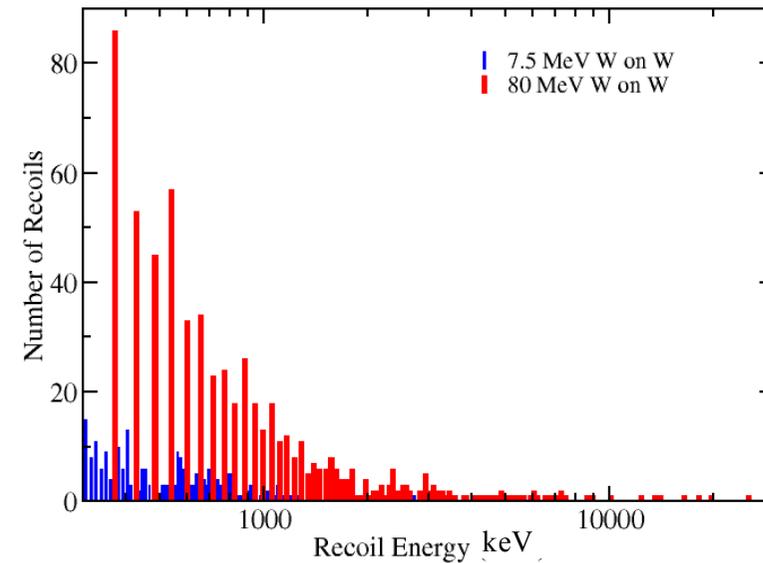
[*]Lindhard-Scharff

[**] ZBL

PKA spectrum generated by SRIM for 80 MeV and 7.5 MeV W ions in W lattice



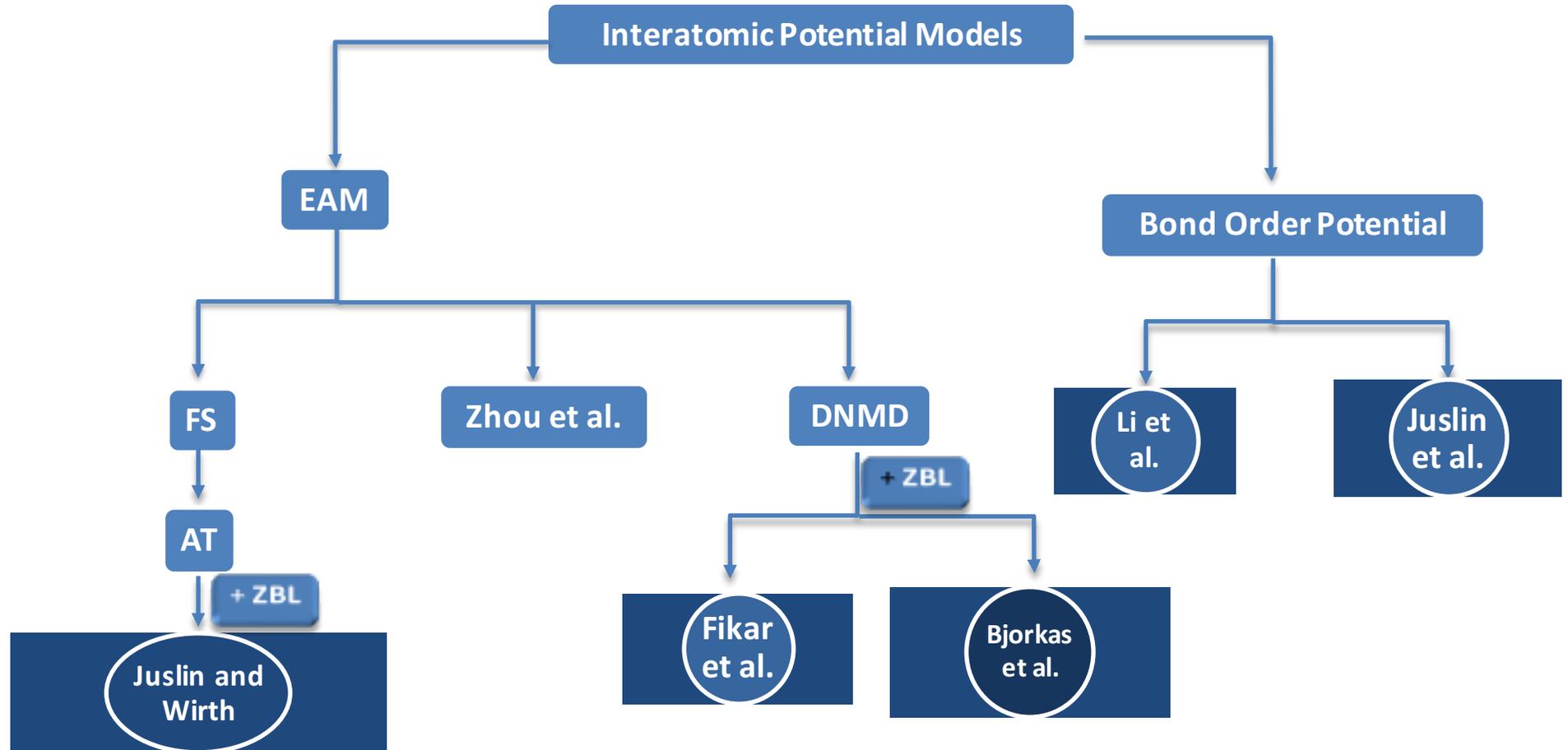
Low energy peak



High energy tail

- TRIM/SRIM can simulate collision cascades with higher incident ion energies with frictional electronic losses
- The initial ballistic phase and the PKA generation can be modelled
- The recombination in the thermal spike phase of the cascade is not implemented
- The structure of the defects created due to ion irradiation cannot be simulated
- MD simulations take care of lattice structure & thermal spike recombination
- Defect structure produced will depend on interatomic potential used for the simulations

Molecular Dynamics Simulations – W-W & W-H Potentials



| | |
|-----------------------------------|---|
| Finnis & Sinclair (FS) | <i>Philosophical Magazine A, vol. 50:1, pp. 45-55 (1984)</i> |
| Ackland & Thetford (AT) | <i>Philosophical Magazine A, vol. 56:1, pp. 15-30 (1987)</i> |
| Juslin & Wirth EAM (AT + ZBL) | <i>Journal of Nuclear Materials, vol. 432, pp.61-66 (2013)</i> |
| Derlet-Nguyen-Manh-Dudarev (DNMD) | <i>Physical Review B, 76, 054107 (2007)</i> |
| DNMD + ZBL (Bjorkas et al.) | <i>NIM B, 267, (2009) 3204-3208</i> |
| DNMD + ZBL (Fikar et al.) | <i>Journal of Nuclear Materials, vol. 386-388 (2009) pp. 97-101</i> |
| ABOP potential by Li et al. | <i>Journal of Nuclear Materials vol. 408, (2011), pp 12-17</i> |
| ABOP potential by Juslin et al. | <i>Journal of Applied Physics, vol 98, (2005) 123520</i> |
| Zhou et al (EAM) | <i>Acta Materialia Vol 49, (2001) 4005-4015</i> |

Comparison of potentials – equilibrium properties

| | E_{cohesive} | Lattice Constant | C_{11} | C_{12} | C_{44} | E_v | E_{100d} | E_{110d} | E_{111d} | E_{octa} |
|--------------------|-----------------------|------------------|----------|----------|----------|-------|------------|------------|------------|-------------------|
| | (eV) | (Å) | (GPa) | (GPa) | (GPa) | (eV) | (eV) | (eV) | (eV) | (eV) |
| Expt. | -8.90 [*] | 3.1652[#] | 522.4[#] | 204.4[#] | 160.6[#] | 3.7 | | | 9.06 | |
| DFT | | 3.18 | | | | | 11.513 | 9.84 | 9.55 | 11.7 |
| FS | -8.90 | 3.1652 | 522.44 | 204.41 | 160.61 | | 8.652 | Not stable | 7.805 | 8.524 |
| AT | -8.90 | 3.1652 | 522.43 | 204.41 | 160.61 | | 9.783 | Not stable | 8.883 | 9.968 |
| Juslin (EAM) | -8.90 | 3.1652 | 522.47 | 204.45 | 160.64 | 3.554 | 10.277 | 10.157 | 9.50 | 10.393 |
| DNMD | -8.90 | 3.1652 | 523.10 | 204.67 | 160.81 | 3.557 | 11.334 | 9.768 | 9.472 | 11.7 |
| DNMD+ZBL (Bjorkas) | -8.90 | 3.1652 | 523.10 | 204.67 | 160.81 | 3.557 | 11.332 | 9.766 | 9.472 | |
| DNMD+ZBL (Fikar) | -8.90 | 3.1652 | 523.10 | 204.67 | 160.81 | 3.557 | 11.333 | 9.768 | 9.472 | |
| Li-ABOP | -8.86 | 3.1652 | 515 | 203 | 162 | 3.52 | 12.01 | 9.53 | 9.33 | 12.05 |
| Juslin-ABOP | | 3.165 | 542 | 191 | 162 | 1.77 | 8.93 | 8.77 | 9.62 | 9.92 |
| Zhou et al | -8.757 | 3.165 | | | | 3.567 | | | | |

Displacement energy

| E_d (eV) | Expt. [**] | AT | AT+ZBL | DNMD | DNMD+Fikar | DNMD+Bjorkas |
|------------|---------------|-----|--------|----------|------------|-----------------|
| Min. | ~40-50 | 64 | 48 | 55±3 | 55 | 41±1 |
| Avg. | ~80 | 166 | 128 | 88.3±0.7 | | 84.5±0.9 |

[*] Table 3, Kittel (1976) [#] P. Bujard, Thesis, University of Geneva (1982)

[**] Maury et al. Radiat. Eff. 38 (1-2) (1978) 53-65

2nd RCM of the CRP on Irradiated Tungsten,

Seoul, Korea, 8-11 Sept. 2015

Single Crystal Studies – Cascade Simulations

Four different potentials are used for simulating cascade – DNMD, Zhu, Juslin and Li

Energy range simulated 0.5 KeV to 20 KeV

Sample temperature – 300 K

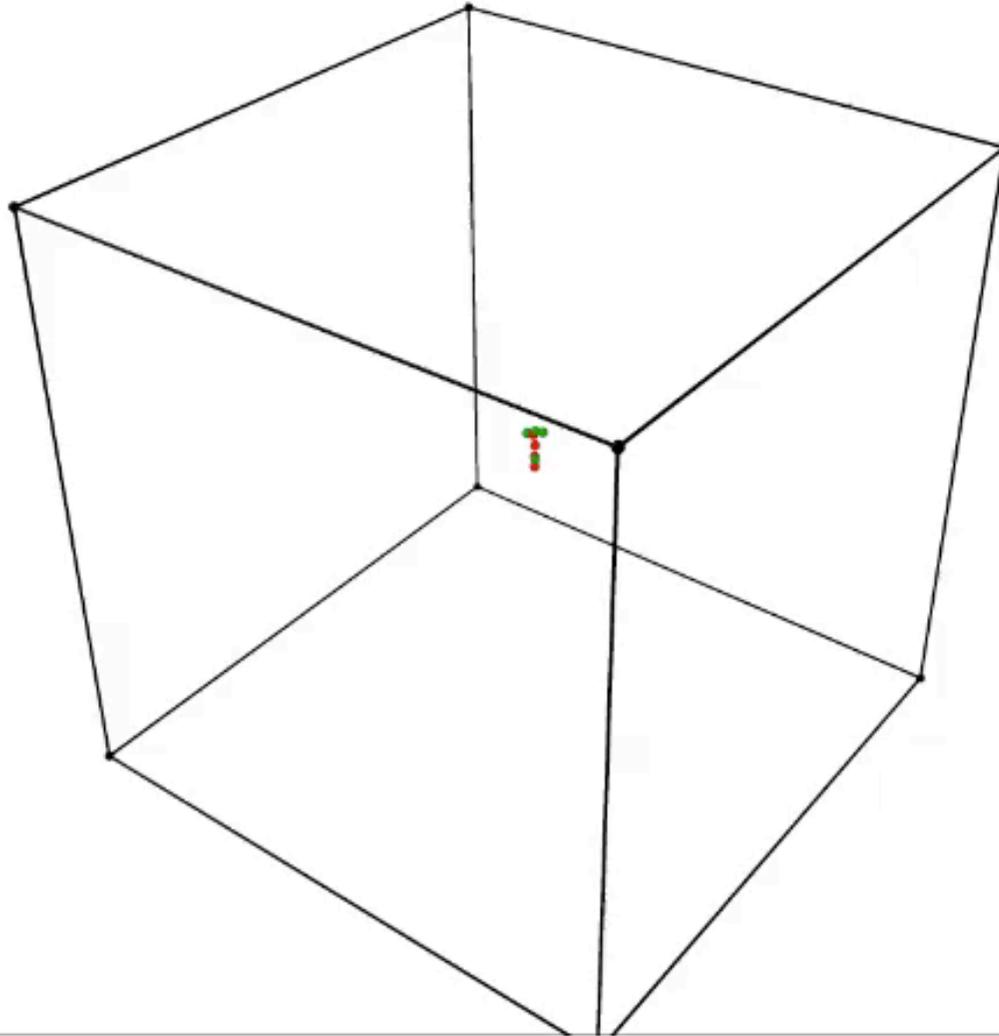
Simulation box – Cubical box with periodic boundary conditions in X, Y & Z directions

No. atoms – 54000 (500eV) 2.1×10^6 (for 20 KeV)

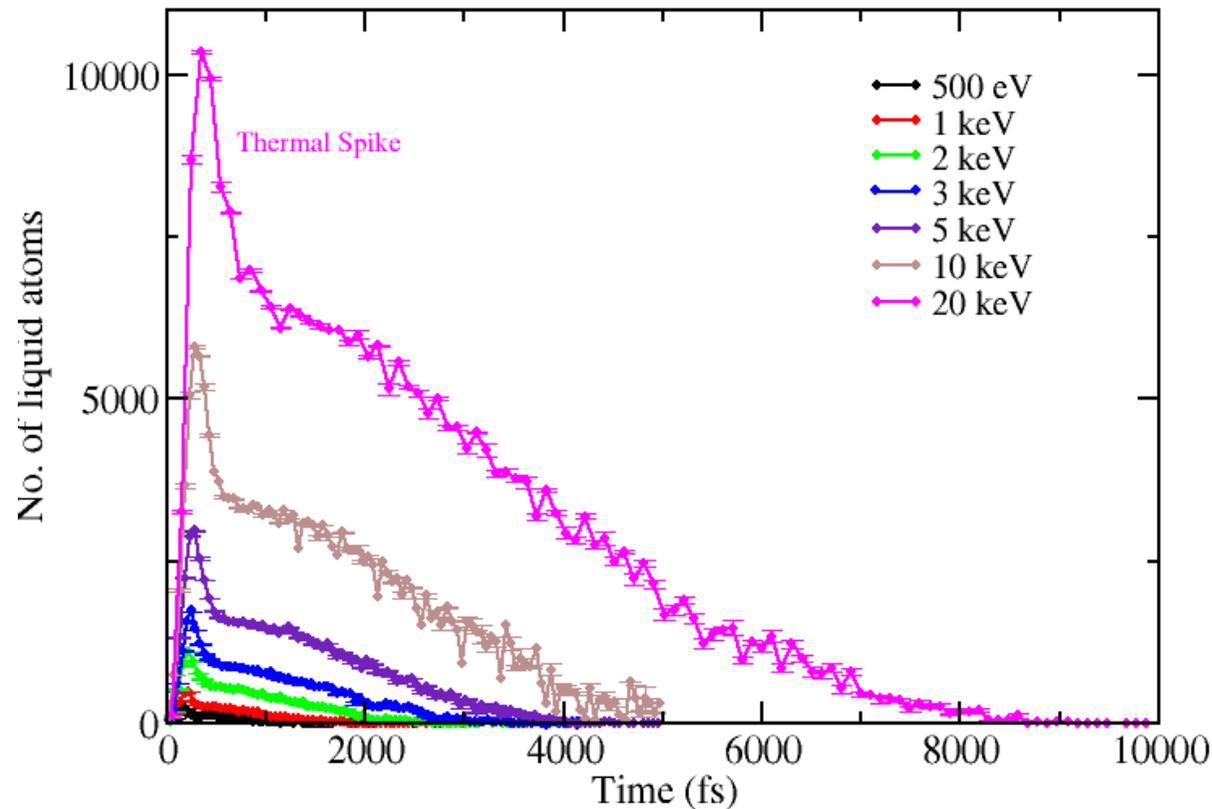
Codes used – PARCAS & LAMMPS

A minimum of 150 simulations were performed for each energy with different random directions

Evolution of a typical cascade at 5 keV (Li)



Evolution of Thermal Spike During the Cascade (Juslin BOP)

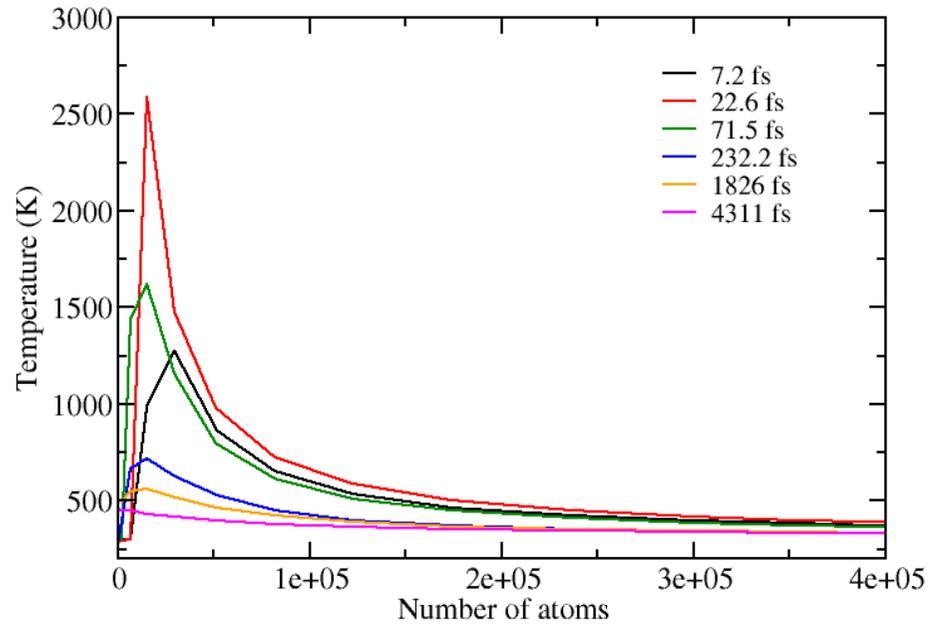


Liquid/hot atoms are those atoms where the average kinetic energy of it and its nearest neighbours were more than the melting point of the material.

It shows the extent of cascade with distinct regimes for all the energies

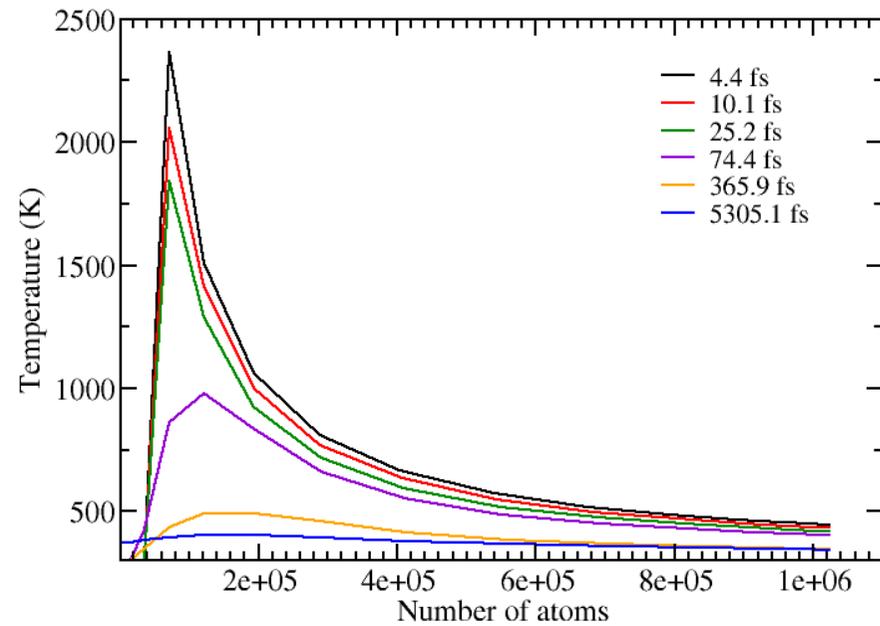
The temporal and spatial extent of thermal spike increases with the incident ion energy

Temporal evolution of cascade volume (Juslin BOP)

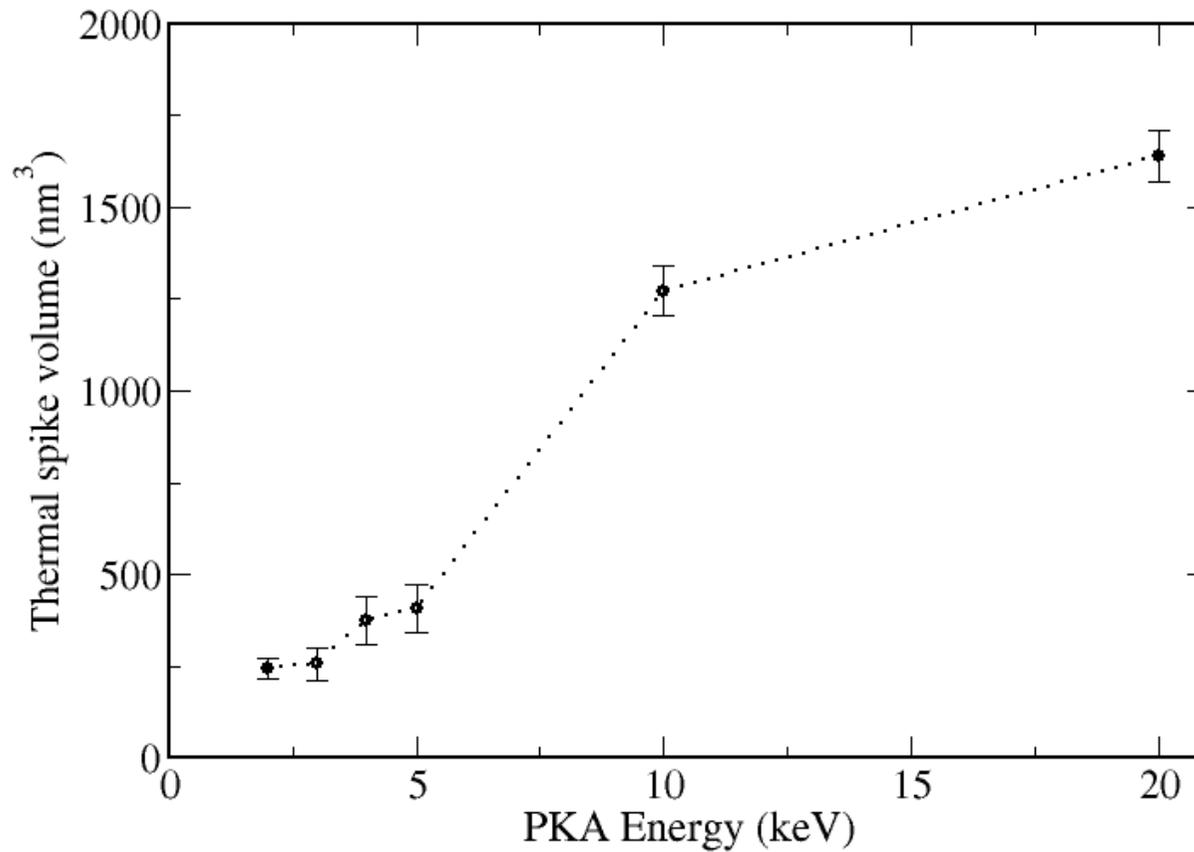


5 KeV

20 KeV



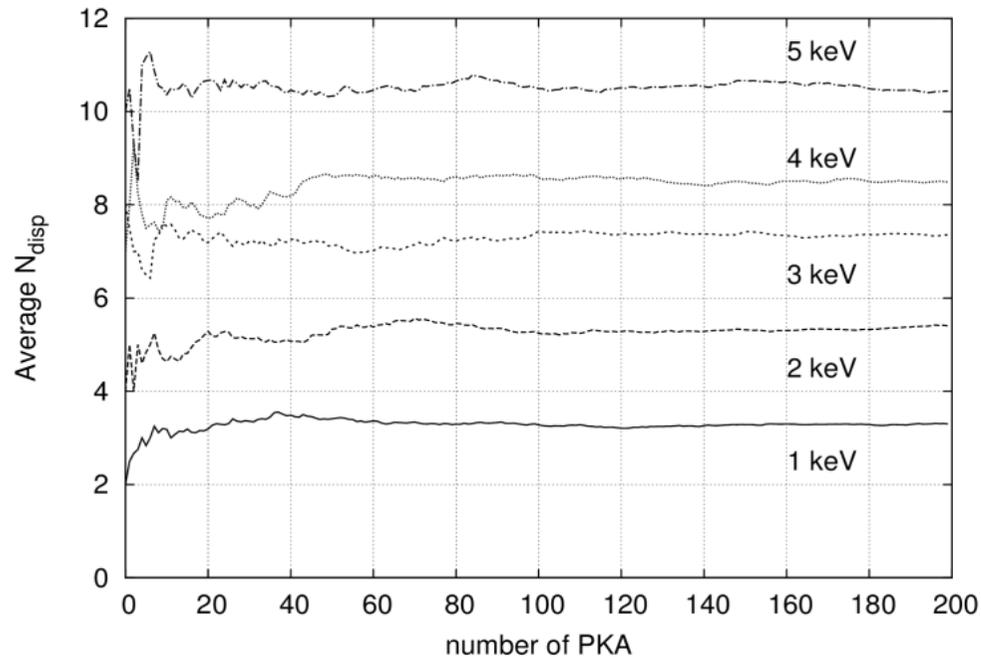
Thermal Spike Zone Increases with Incident Ion Energy



Frenkel pairs

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Requirement of Multiple Random Sampling of PKA Directions (MD with Zhou pot.)

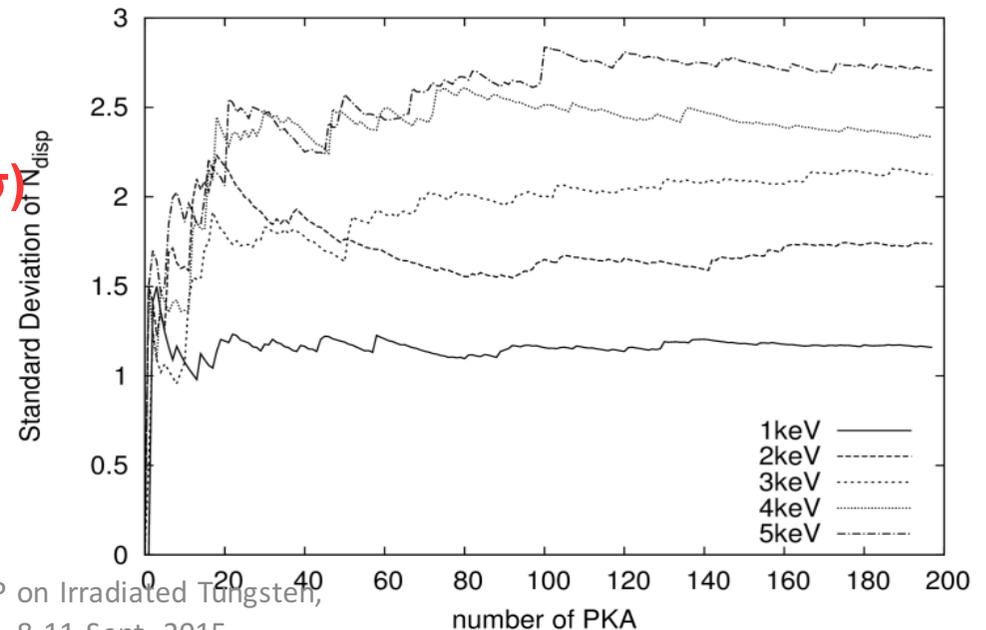


$$n_{avg,N} = \frac{1}{N} \sum_{i=1}^N n_{d,i}$$

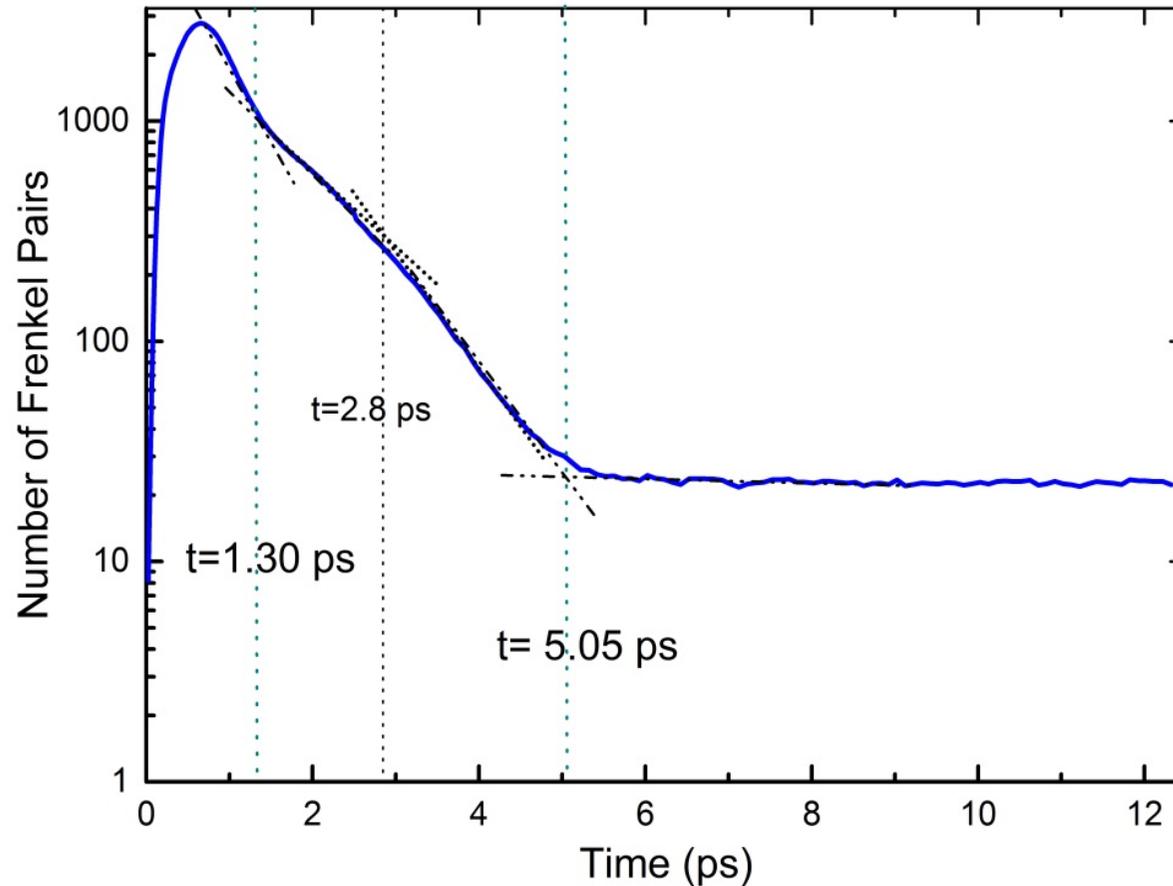
**More than 60 random directions have
To be sampled for average displacement
to level off**

**More than 100 random directions
have to be sampled for standard deviation (σ)
to level off**

$$\sigma_N = \left(\frac{1}{N} \sum_{i=1}^N (n_{d,i} - n_{avg,N})^2 \right)^{1/2}$$



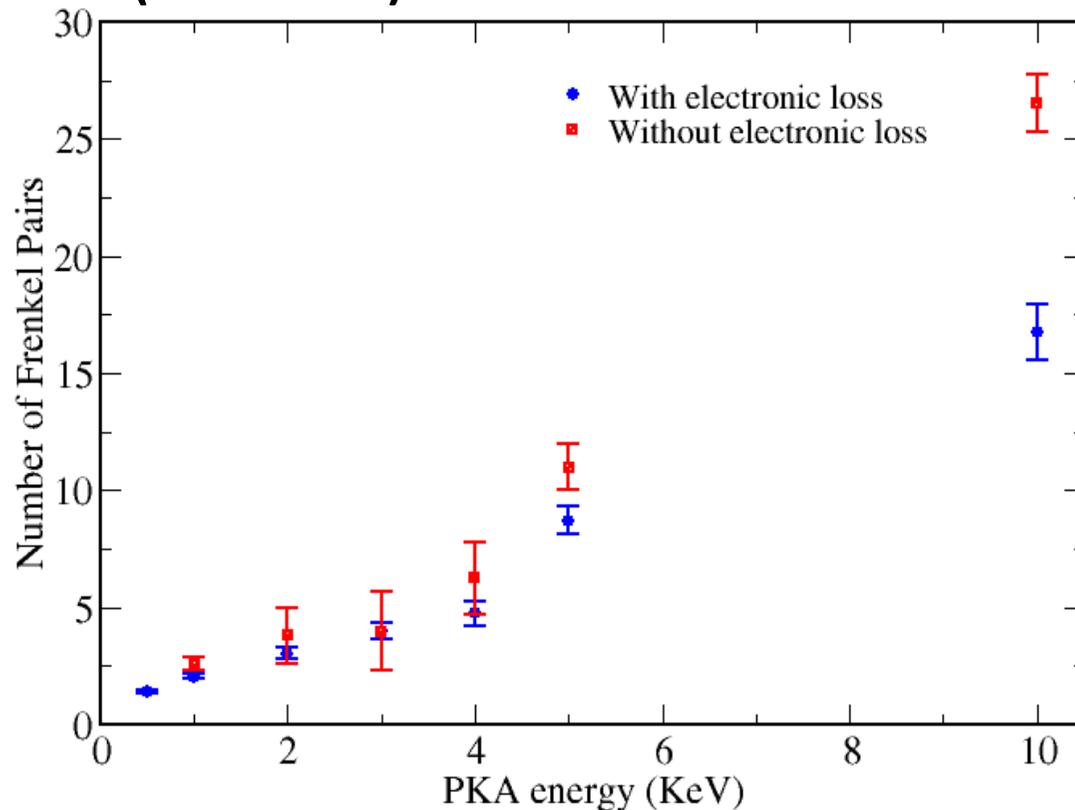
Evolution of Frenkel Pairs During Cascade (DNMD+ZBL, 10 KeV)



Most of the Frenkel Pairs (FP) are recombined during the thermal spike and there exists only a few surviving number of FP at the end of the cascade

Detailed analysis is going on for different dynamic regimes in FP evolution

Number of Stable Frenkel Pairs Obtained With & Without Electronic Loss (Juslin BOP)



Frictional electronic loss (EL) reduces the number of FP

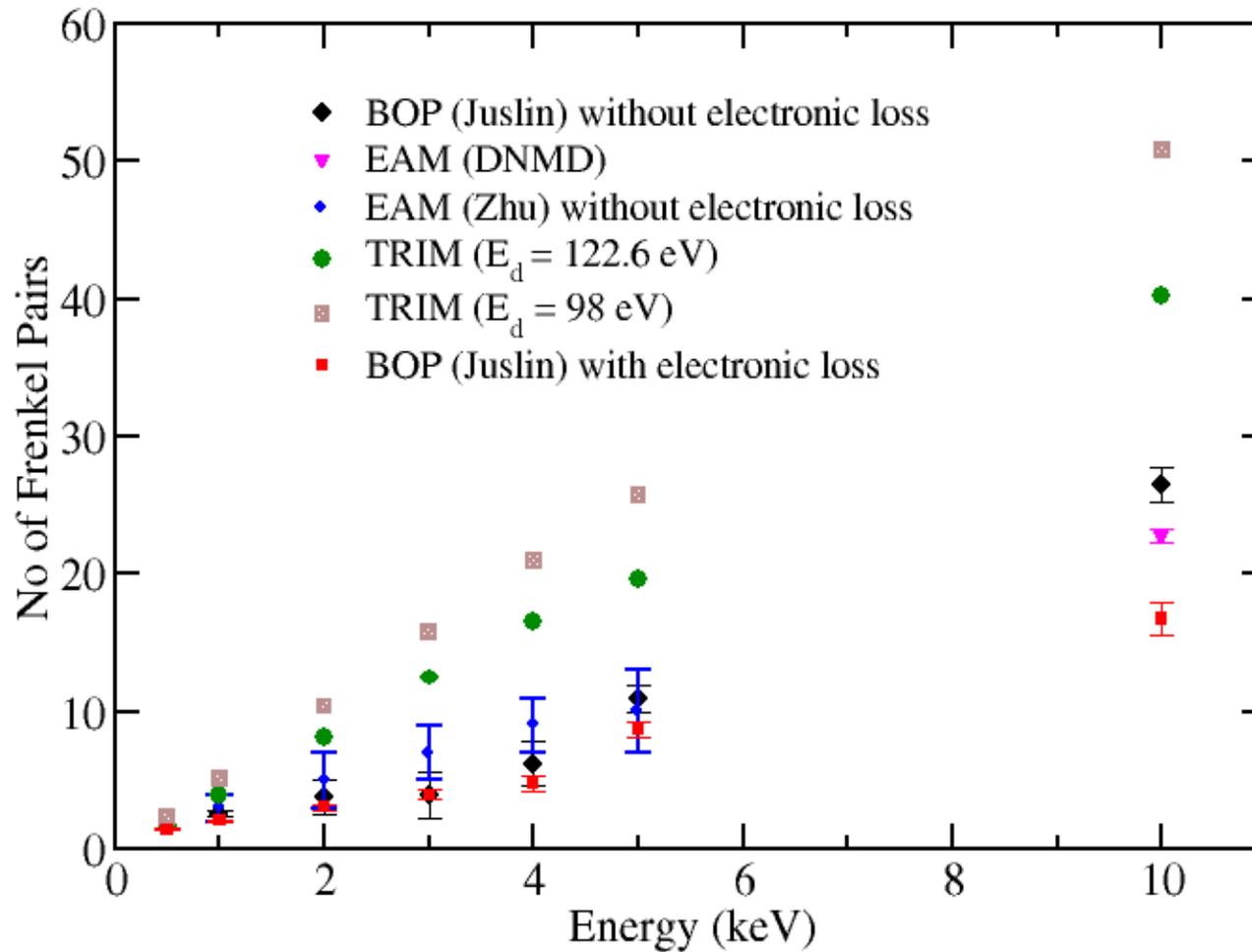
EL becomes noticeable after 5 KeV of PKA energy

It is equivalent to have an effectively lower energy for the PKA

At higher PKA energies (above 100keV), the coupling between the electrons and lattice may become significant

Simulations are on going for studying this using a two-temperature model for lattice and electronic system.

Comparison of number of FP produced using different potentials



All the studied potentials of different nature seem to show similar number of FP for the same energy in contrast to TRIM.SP data

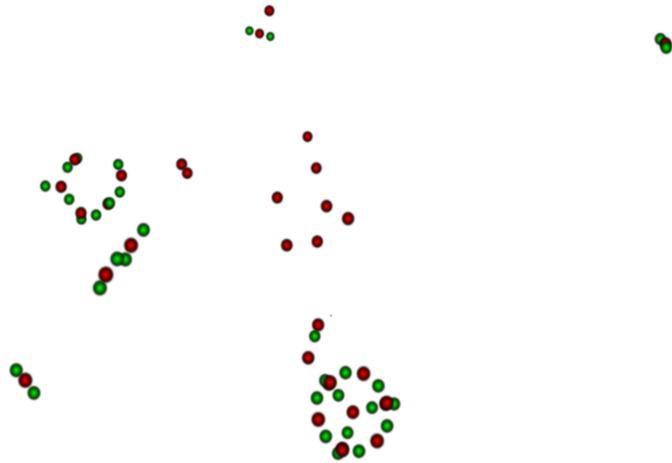
The Zhu potential data is plotted for corrected electronic loss.

Defect clusters

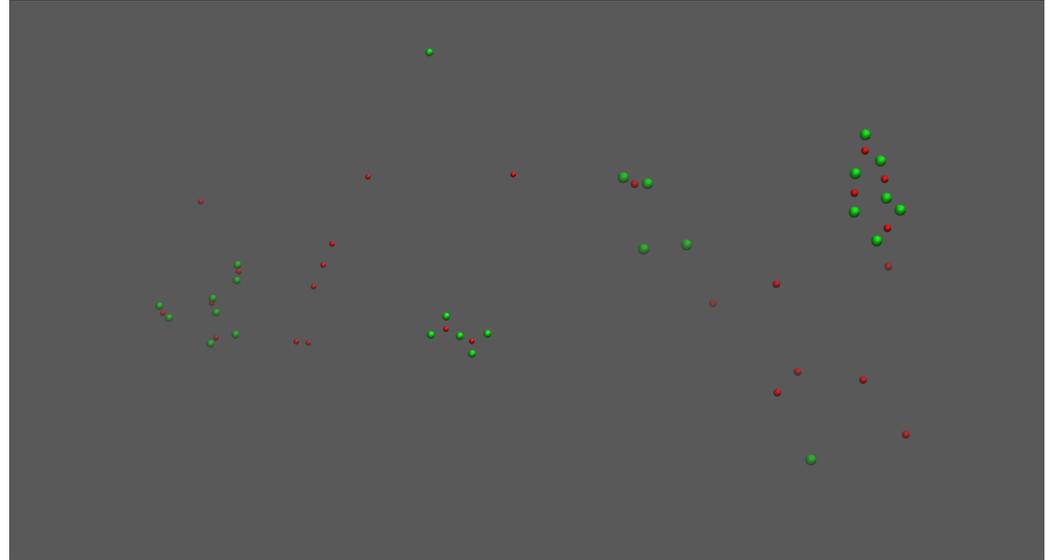
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Type of Defects Produced During the Cascade

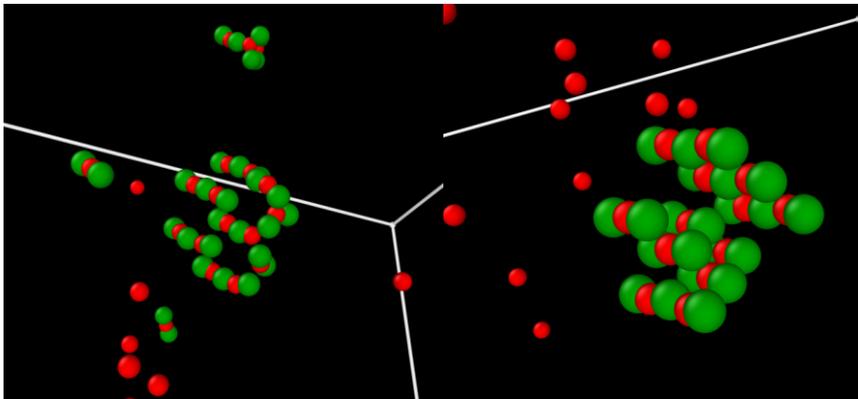
In addition to isolated vacancies & interstitials clustering of defects were observed at higher energies



Dumb bells and ring like interstitial vacancy clustering (Zhu potential)



Planar and loop-like vacancy interstitial clustering along with dumbbells (Juslin BOP)

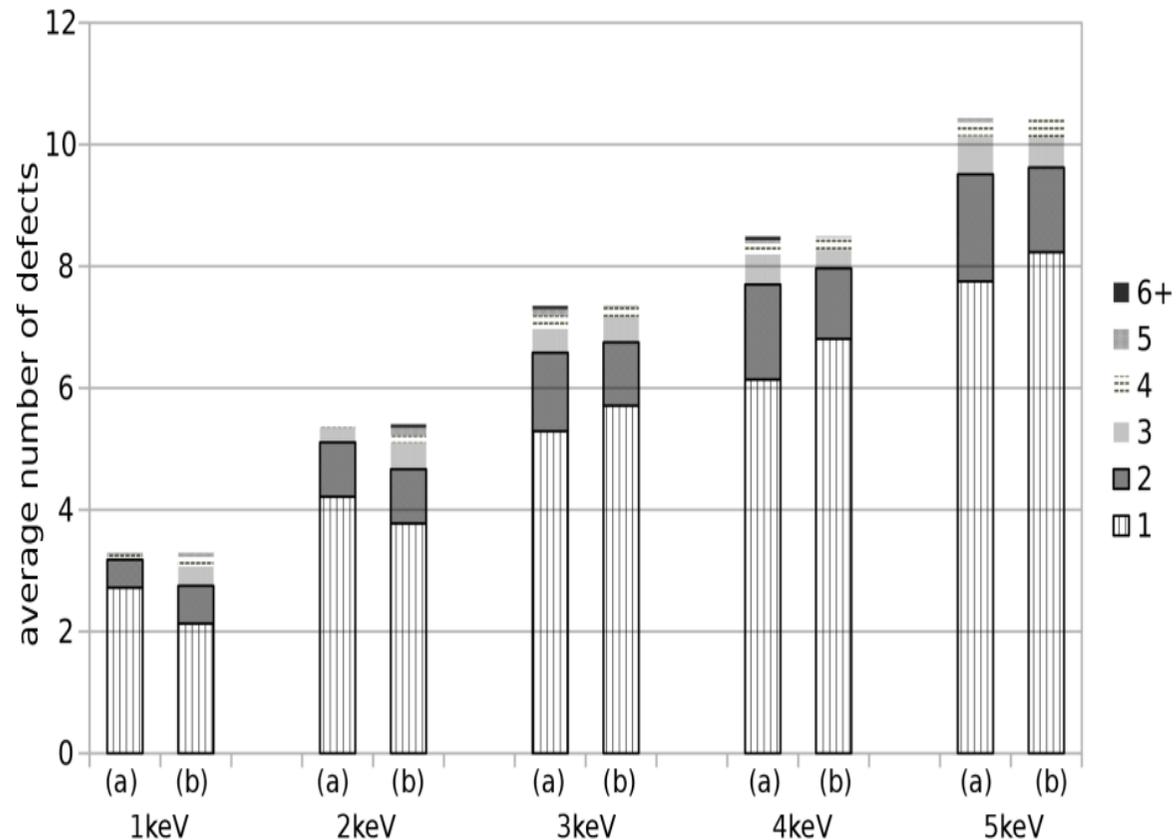


Crowdions and loop-like clustering (DNMD potential)

Although the number of FP are similar in all potentials, the type of defect produced is different

Defect Clustering – Statistics

In-cascade clustering of vacancies and interstitials are seen



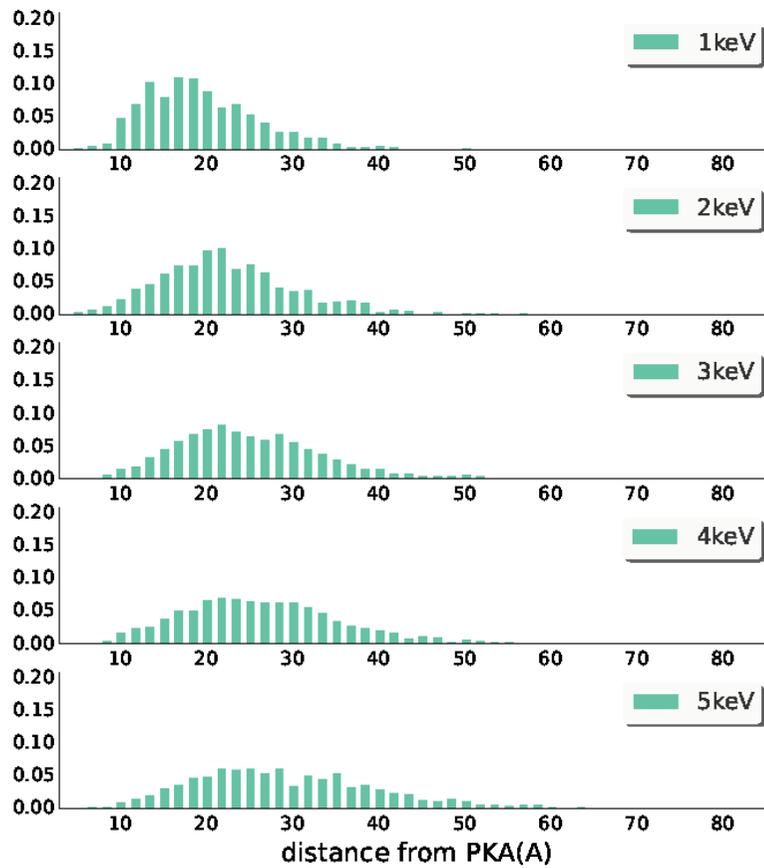
Most of the defects are single up to 5 KeV in Zhu potential.

Double and triple vacancies are observed at 10 KeV & 20 KeV in Juslin potential

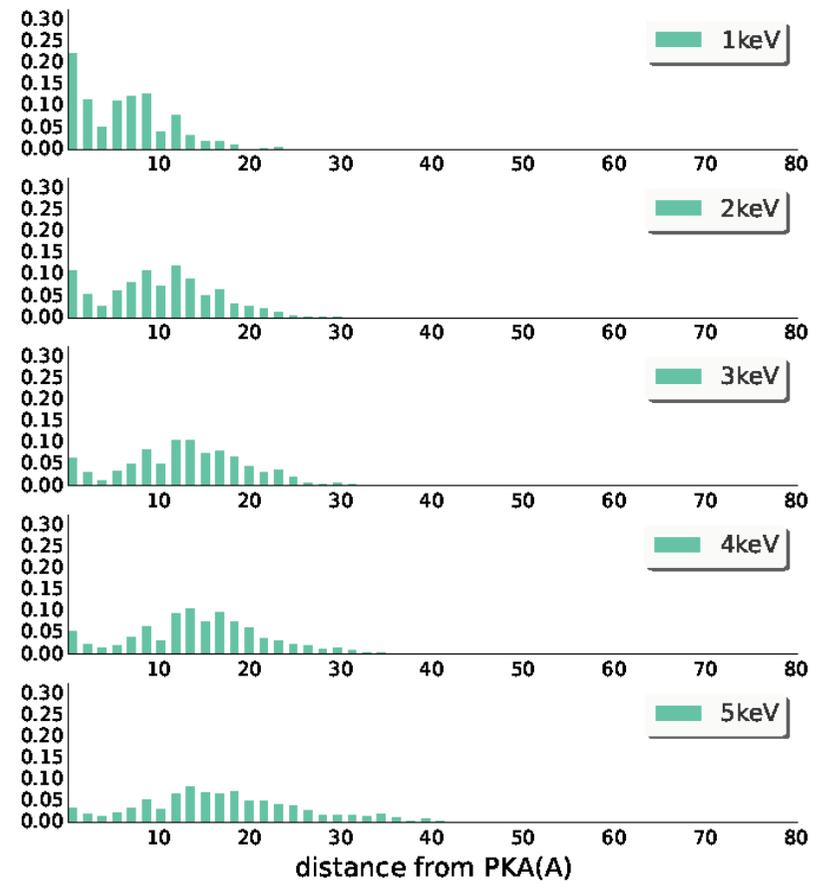
Detailed analysis of defect clustering at higher energies is ongoing

Normalized Defect Distribution

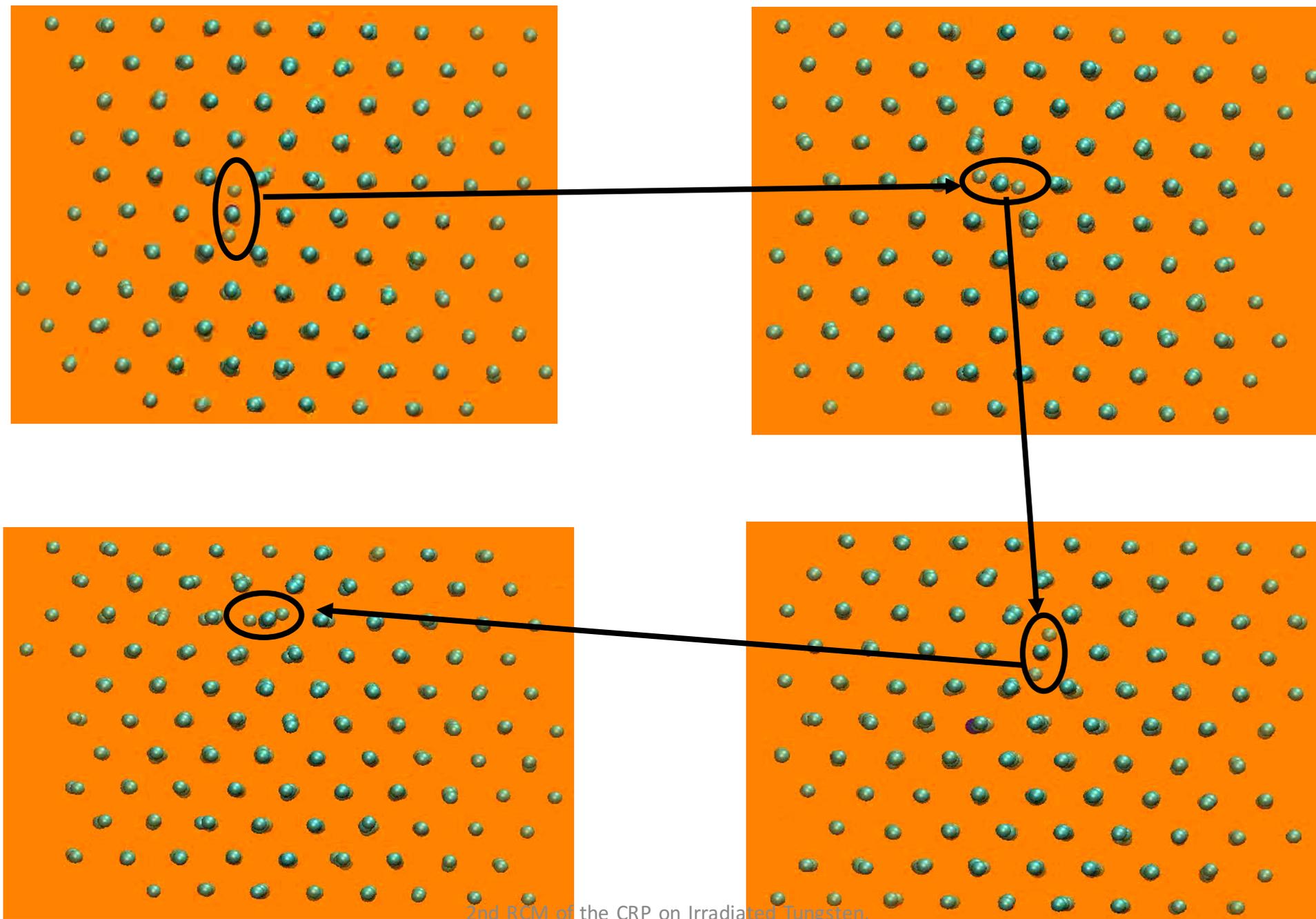
Interstitial distribution



Vacancy distribution



Diffusion of Self Interstitial Atom (SIA) in Single Crystal W – Interstitialcy diffusion

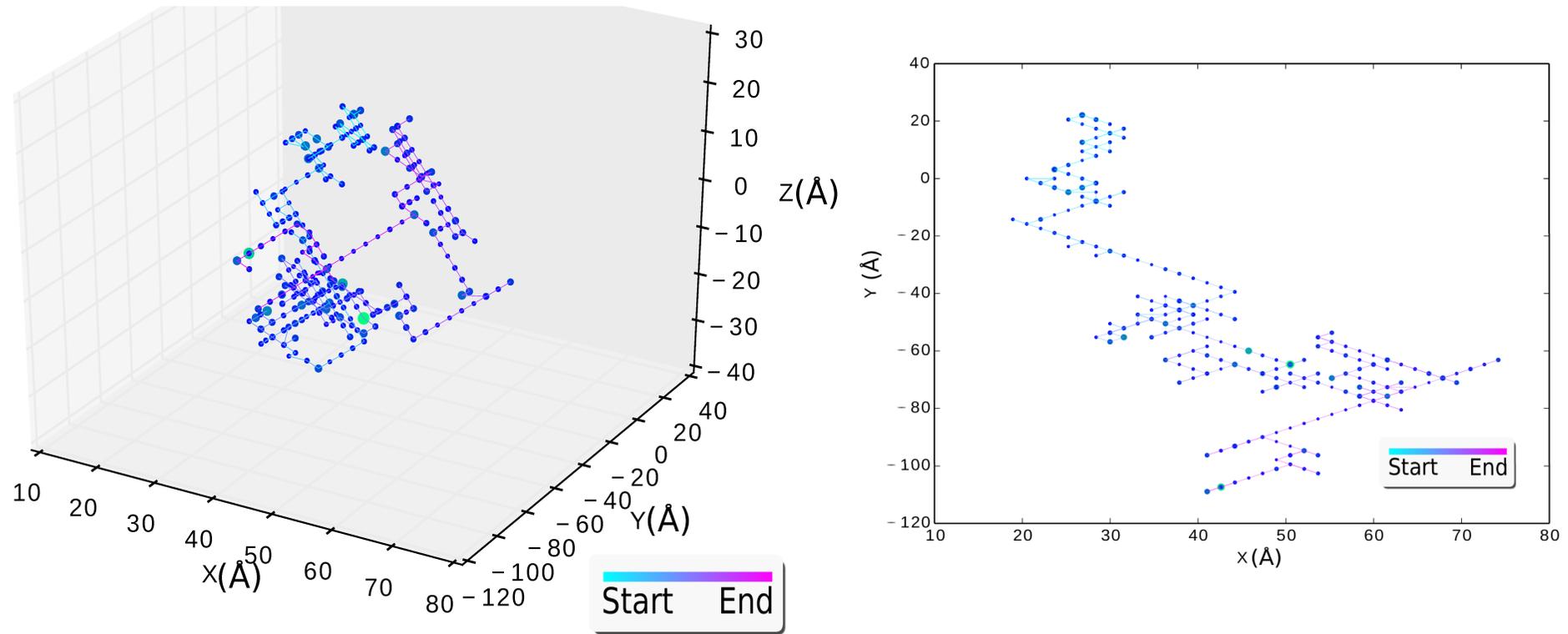


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MD simulations with a single interstitial for 10 ns at 1100 K to 2900 K

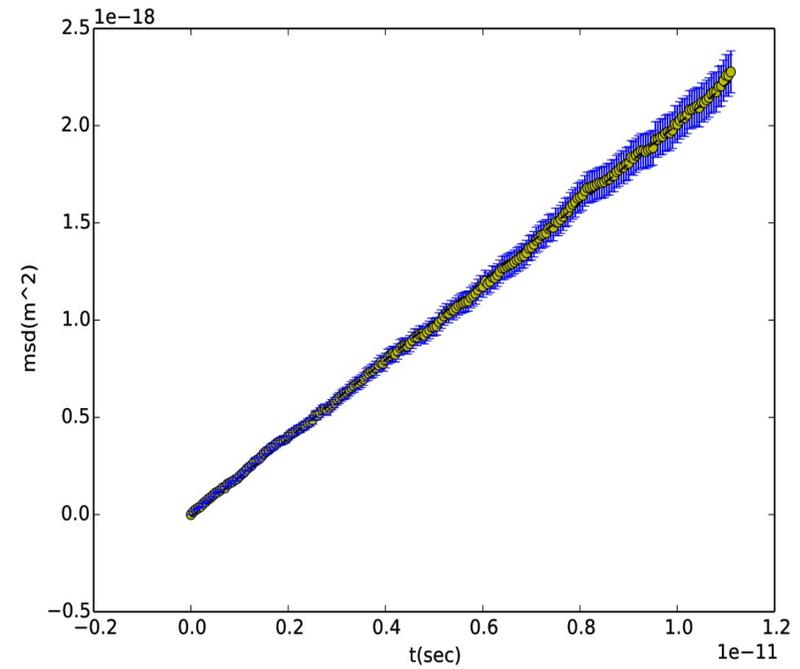
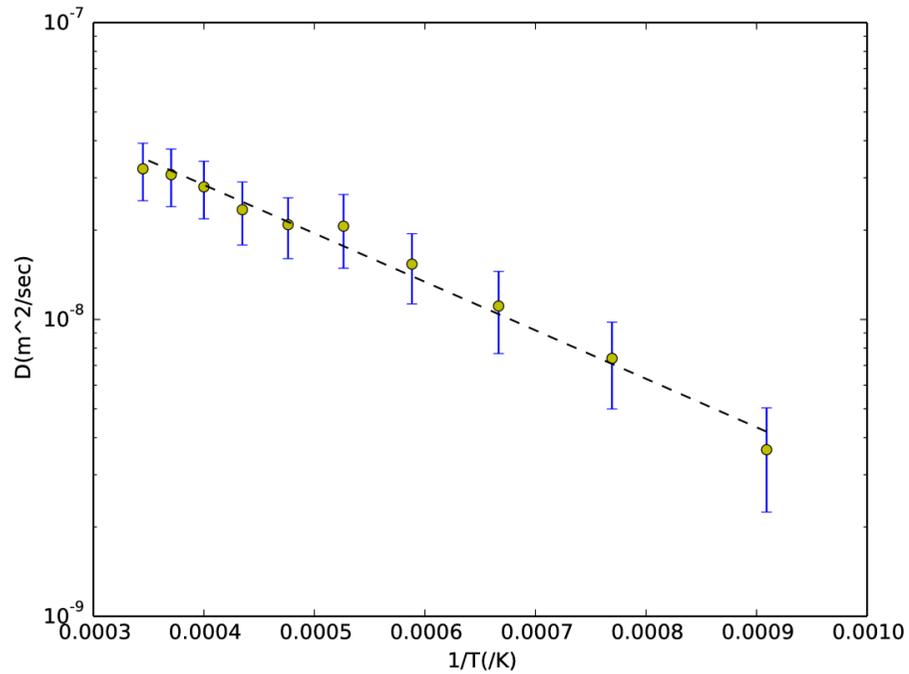
Interstitialcy Diffusion Characteristics



Most of the jumps are taking place along the diagonals of the cubic unit cells in different planes

Several jumps continue in the same direction – successive 1D jumps, else they Undergo a change in direction (rotational jumps)
Almost all jumps are 1NN (nearest neighbour)

Interstitialcy Diffusion coefficient and migration energy



$$D_0 = 2.22 \times 10^{-7} \text{ m}^2/\text{s}$$

$$E_m = 0.4 \text{ eV}$$

W Interstitialcy diffusion is Arrhenius like

Deuterium Interaction with Tungsten

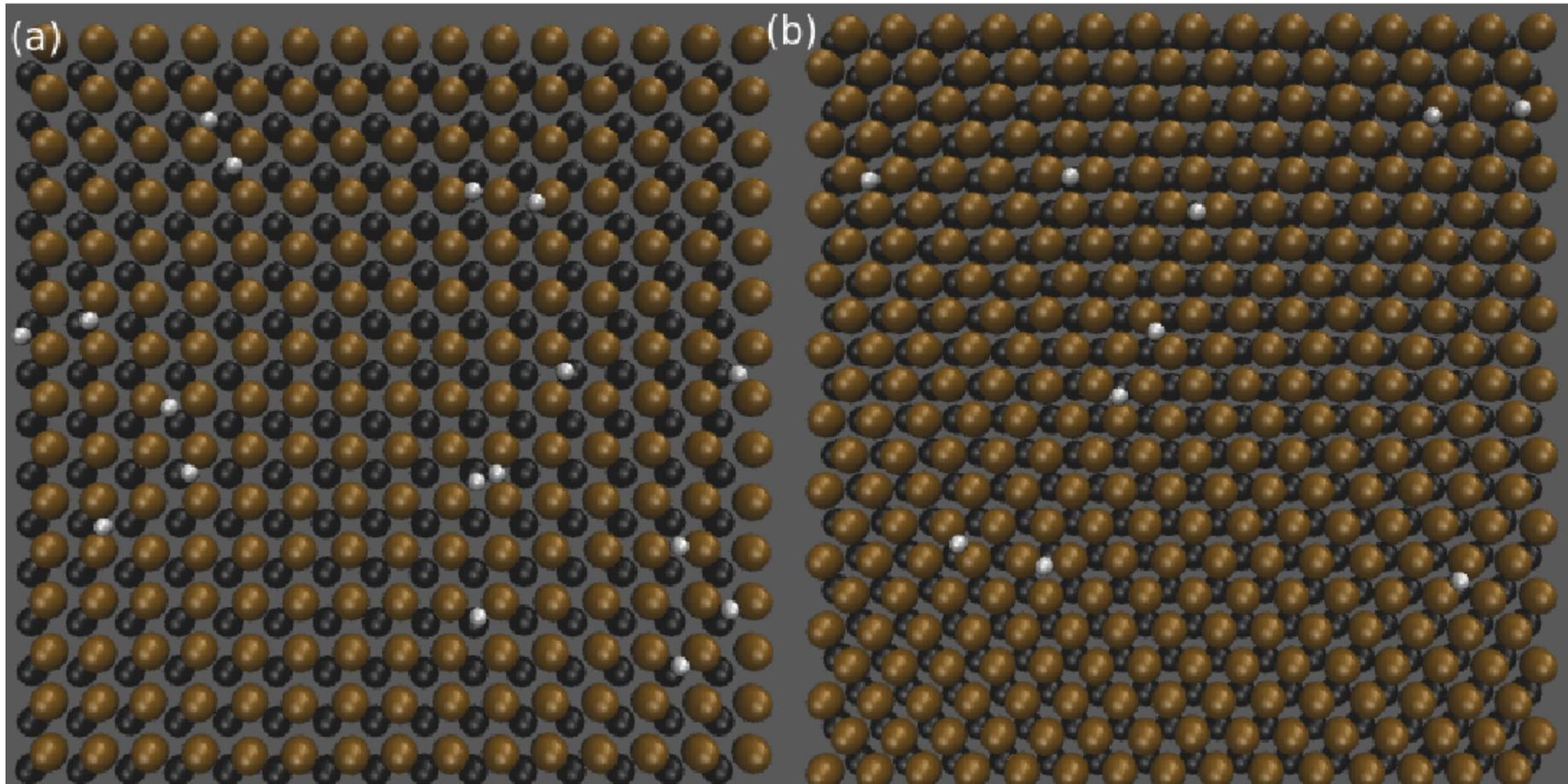
MD simulations of Deuterium sticking on single crystal tungsten (un-irradiated & irradiated W)

Two different potentials - Juslin BOP & Li BOP

Sample temperature – 300K

D energy – 0.003 eV to 100 eV, 1000 non-cumulative D bombardment on W surface

Sticking of Deuterium on W (100) & W (110) surfaces

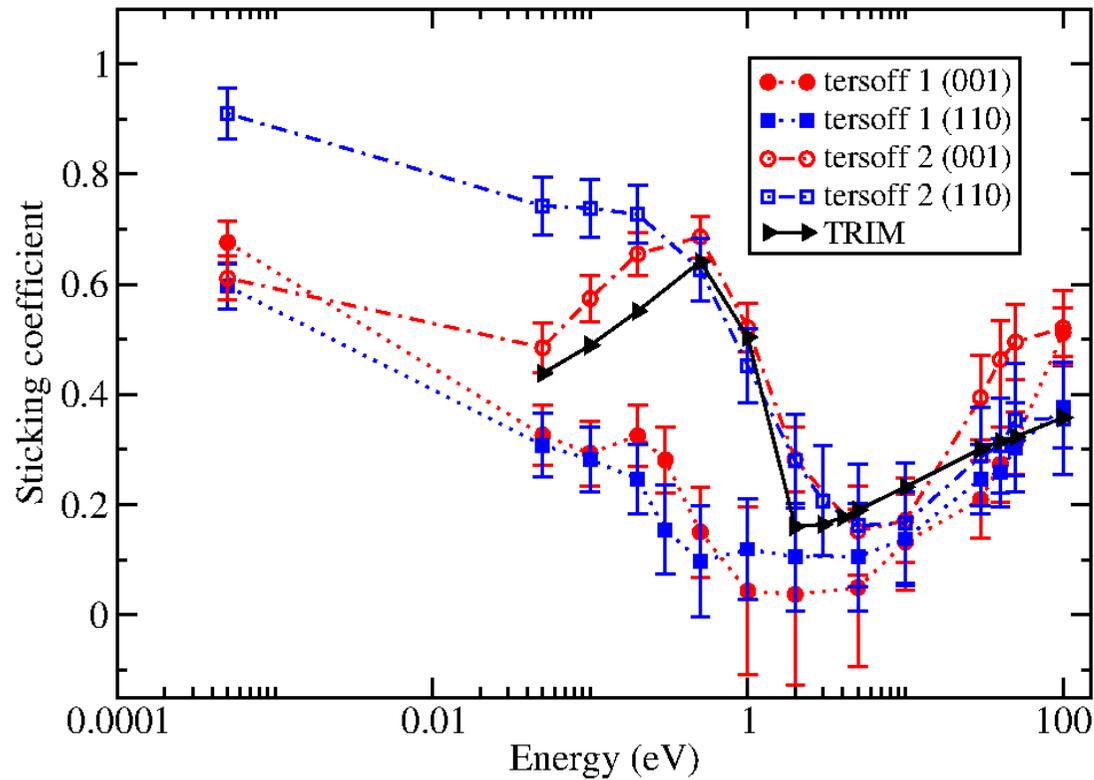


A few selected D atom locations superposed at the end of the simulations

Sticking takes place mostly on the bridge sites at the surface

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Sticking coefficient of Deuterium (un-irradiated W)

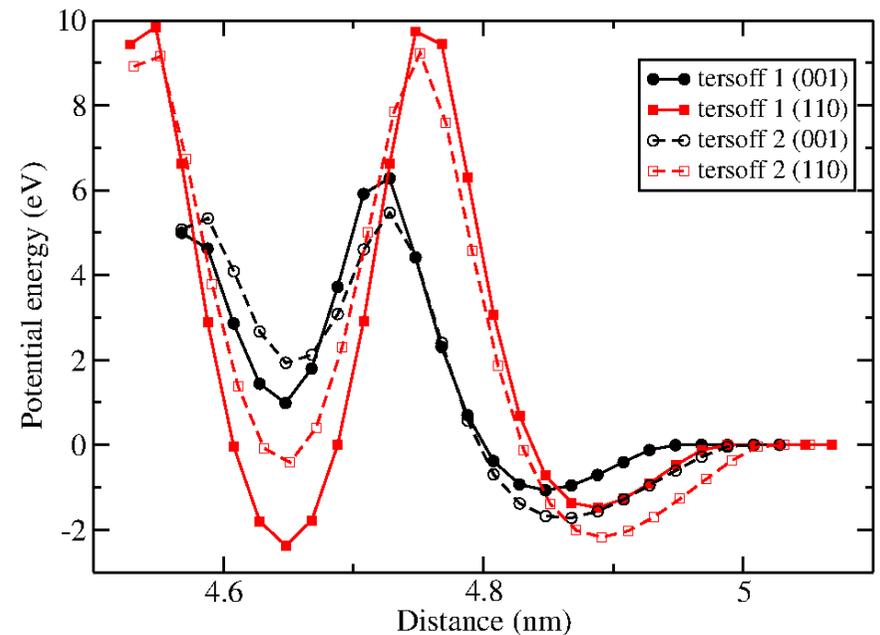


The dip in the sticking coefficient is due to the penetration barrier of the first layer of tungsten atoms

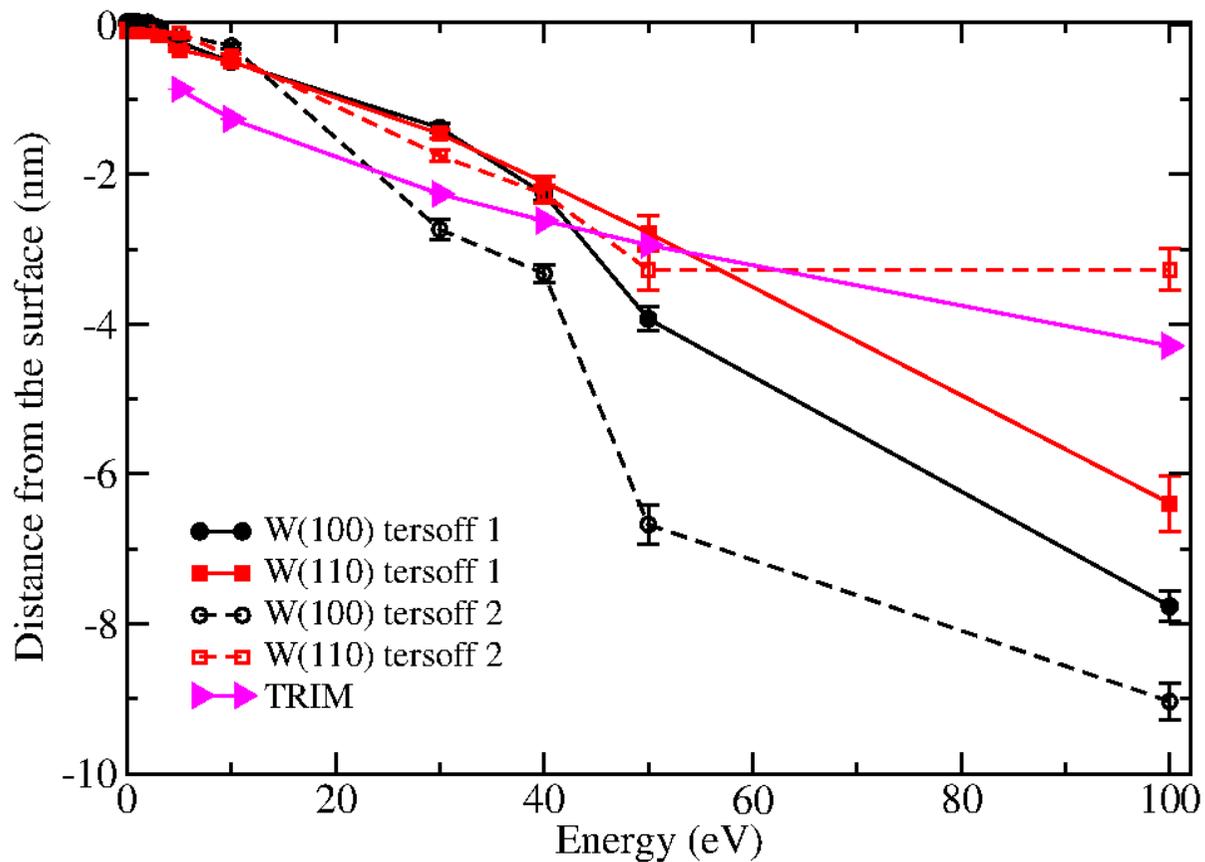
Tersoff1 – Juslin et.al

Tersoff2 – Li et.al

Plane averaged potential energy of deuterium in W from the surface (5 nm is surface)



Depth Profile of Deuterium in Tungsten



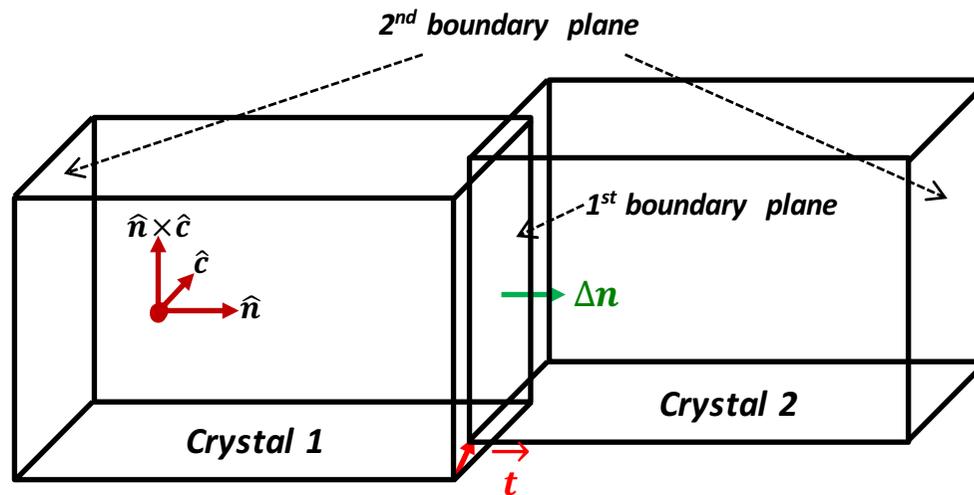
Diffusion of deuterium is not observed in the simulation time scales

Attempts for GB studies

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Search for ground state Coincidence Site Lattice configuration

The search is an involved process
Many prescriptions are available
We adopted the method outlined by Rittner and Seidman
[*Phys. Rev. B*, **54**, 6999 (1996)]



\hat{n} = normal to GB
 \hat{c} = rotation axis
 \mathbf{t} = translation in GB plane
 $\Delta \mathbf{n}$ = volume relaxation along \hat{n}

1. Atomic positions in the two grains are generated using geometrical CSL constructions
2. 3-dimensional Born-von Karman PBC applied
3. Effectively 2 identical GBs are simulated here
4. Overlapped atoms are removed
5. Crystal 1 and Crystal 2 are translated by \mathbf{t} to sample the entire DSC lattice space
6. Volume relaxation is allowed only along \mathbf{n}

As an example, for $\Sigma 13$ CSL in W, we analysed almost 40,000 initial structures and zeroed down to ground state configurations !

Defect Formation Energy

Once the ground state CSL is identified, we introduced defects in and around the GB plane and computed the impact of the specific GB on defect formation energies

FLOWCHART



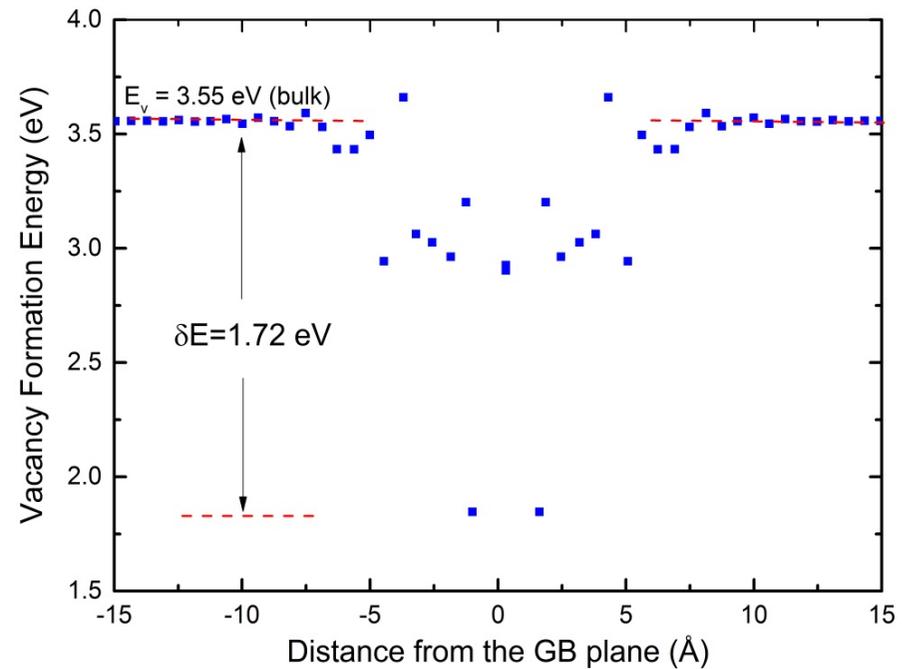
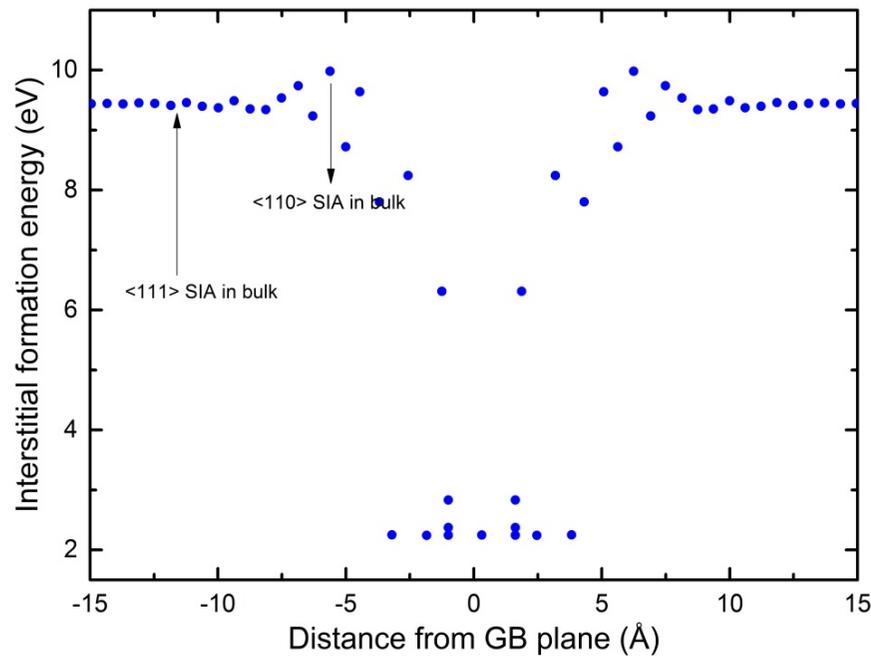
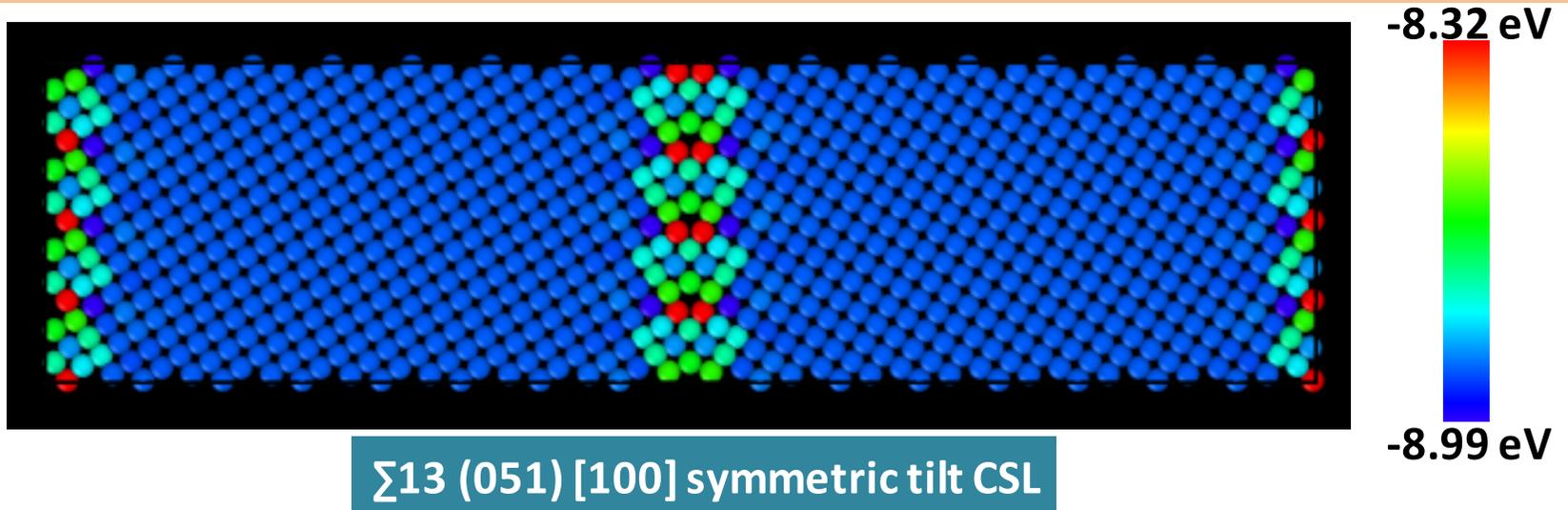
Vacancy Formation Energy

$$E_{vf} = E_{GB,v} - E_{GB} + E_{cohesive}$$

Interstitial Formation Energy

$$E_{SIA,f} = E_{GB,SIA} - E_{GB} - E_{cohesive}$$

Defect Formation Energy about the Grain Boundary plane



Future work

- Simulation of damage in polycrystalline W
- Stresses and movement of point defects
- Study of defect-H interaction

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1. Chandan Danani, IPR: Neutronics discussions
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