Statistical study of defects caused by primary knock-on atoms in fcc and bcc metals using molecular dynamics simulations

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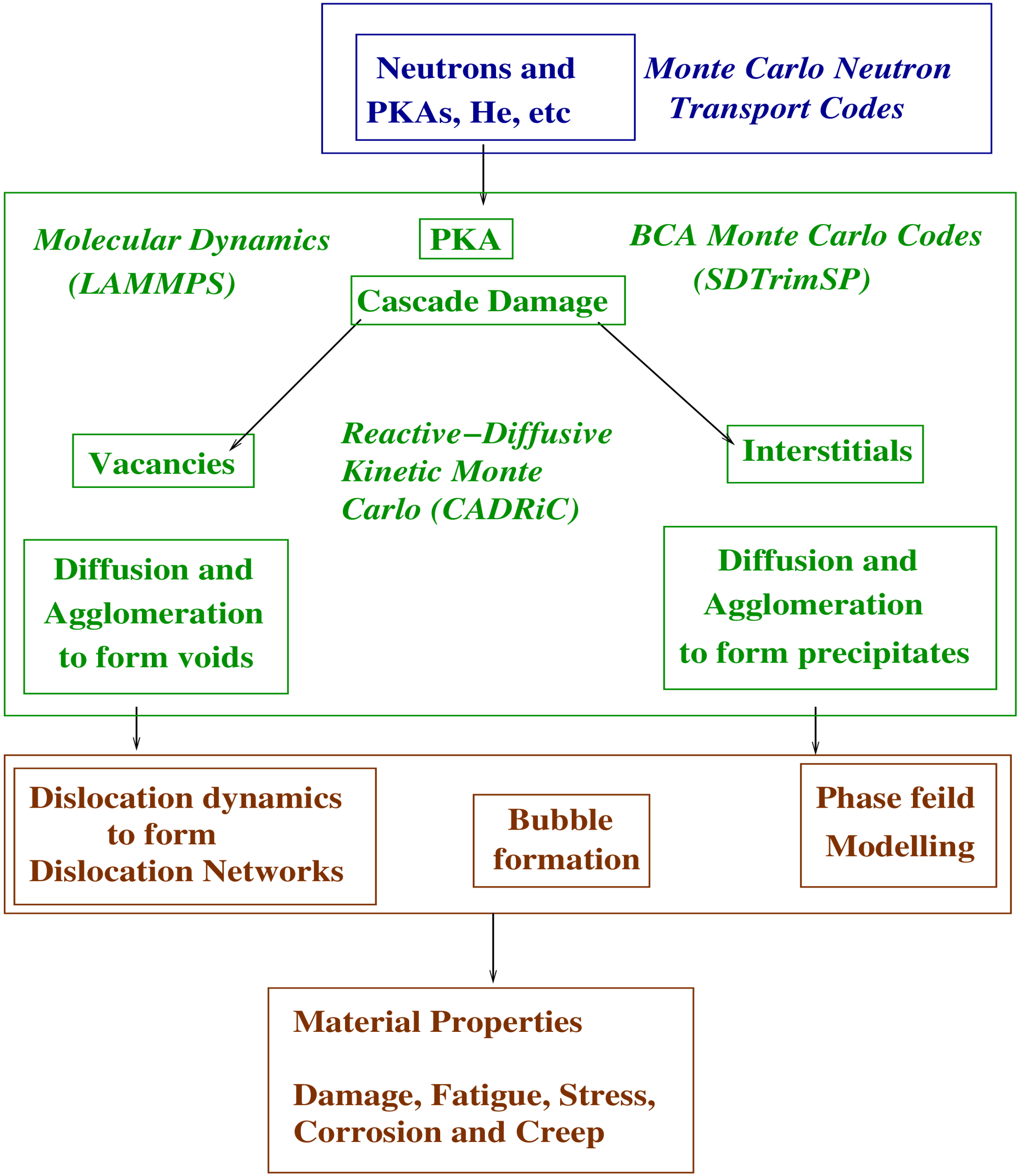
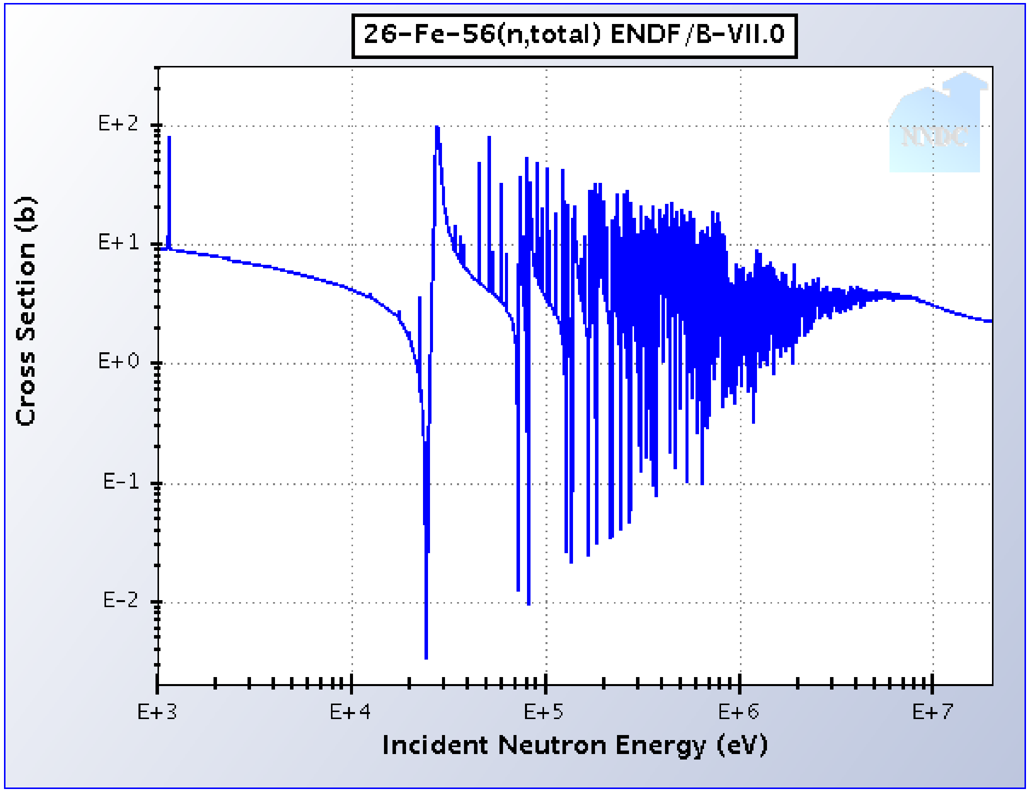
Motivation – Big picture – Multi-scale model



Focus of the talk

- MD of collision cascades
- MD of interstitial diffusion
- Scaling up to dynamic MC

Obtaining PKA Energy Distributions



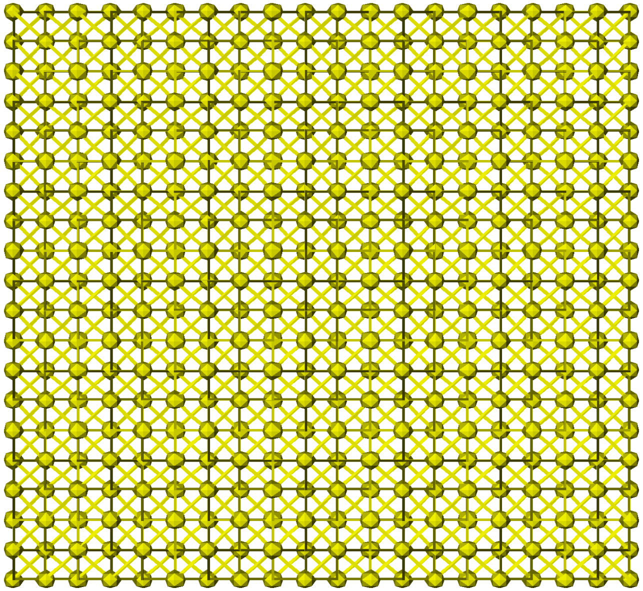
Cross section from http://www.nndc.bnl.gov/

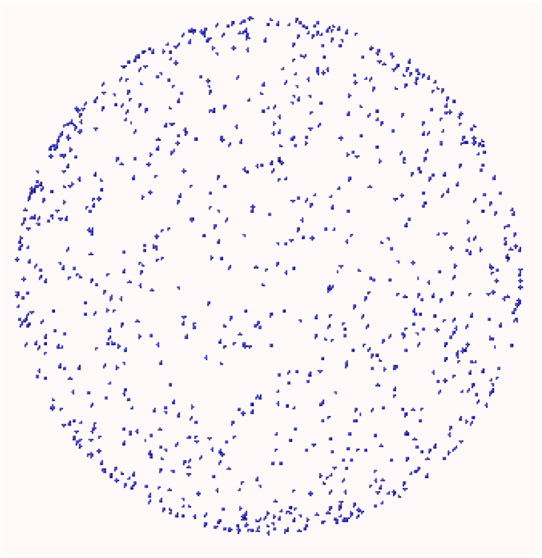
Table from:
R.E. Stoller and L.R. Greenwood,
Jnl. Nucl. Mater. 271&272 (1999) 57-62

- Cross-sections available.
- One has to implement not only elastic collisions, but also the relevant transmutation reactions.
- How do others do it? SPECTRE code, SPECOMP code

n energy (MeV)	Avg. PKA Energy (keV)
0.00335	0.116
0.0175	0.236
0.0358	1.24
0.0734	2.54
0.191	6.6
0.397	13.7
0.832	28.8
1.77	61.3
14.1	487.0

Molecular Dynamics Simulations using LAMMPS

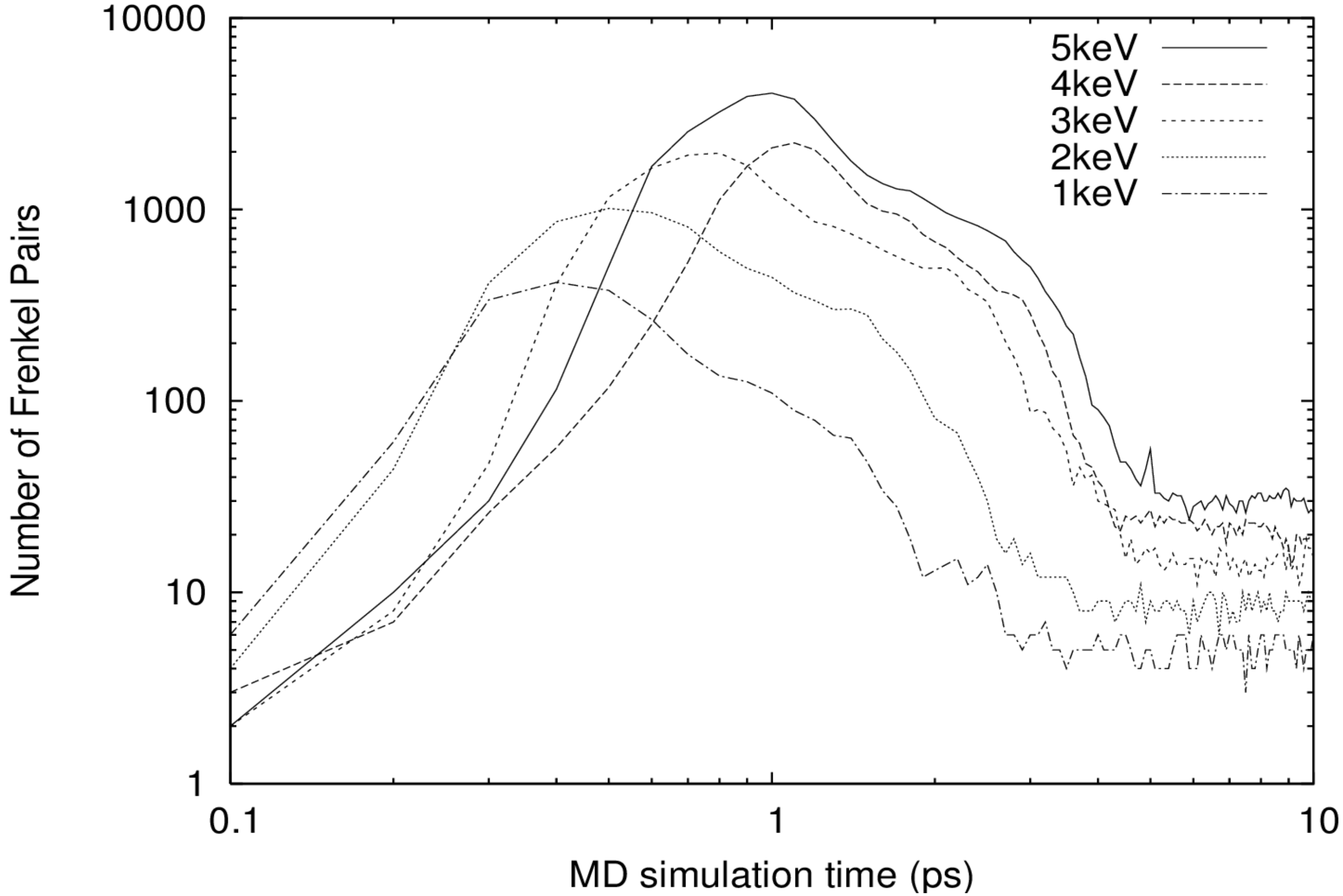




- Concentration dependent EAM Potential for FeCr (not stiffened)
- BCC crystal, NPT for 10 ps
- PBCs along X-Y-Z, 10 ps NPT at 300 K, 10 ps NVE collision cascade
- Variable time stepping, Boundaries fixed
- Electronic losses not included
- PKA launched in 1000 random directions at 0.1, 0.5, 1, 2, 3, 4, 5 keV

How many simulations are required for acceptable statistics?

Cascade evolution with time

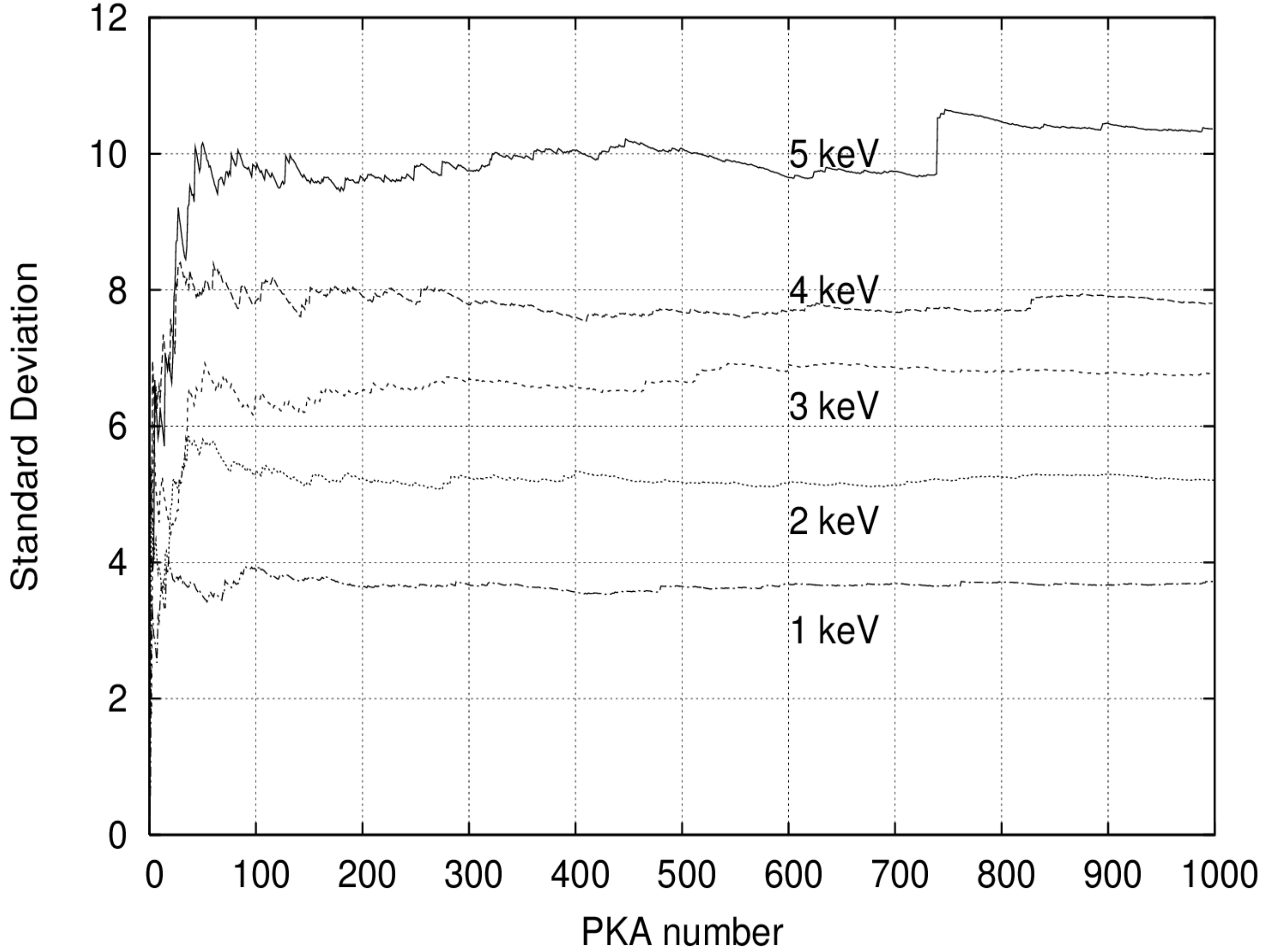


Cascade dynamics lasts a few pico-secs

Higher energy cascades take a longer time to play out

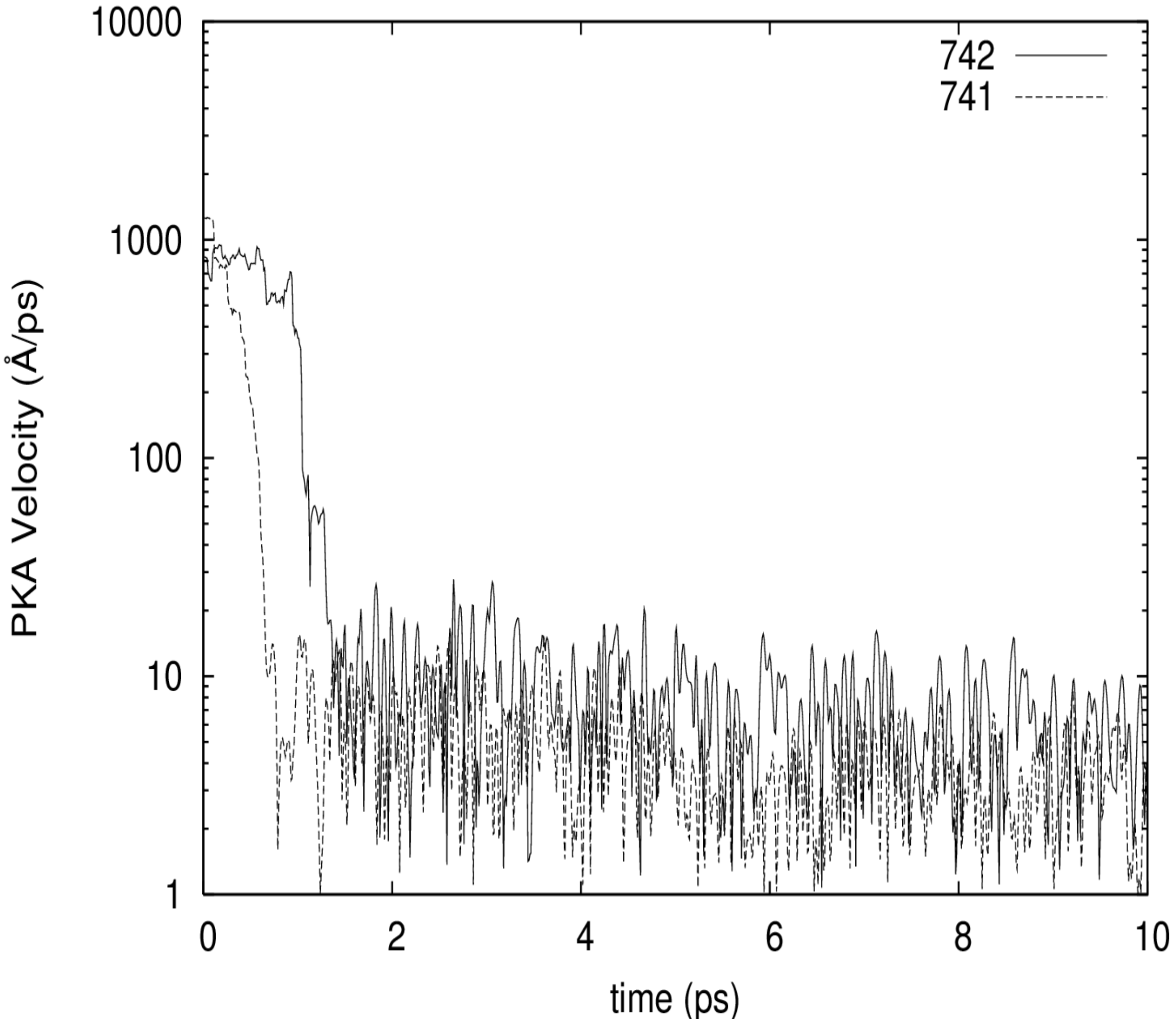
Most of the interstitials formed, recombine during the cascade

Number of Displaced atoms (directional statistics)



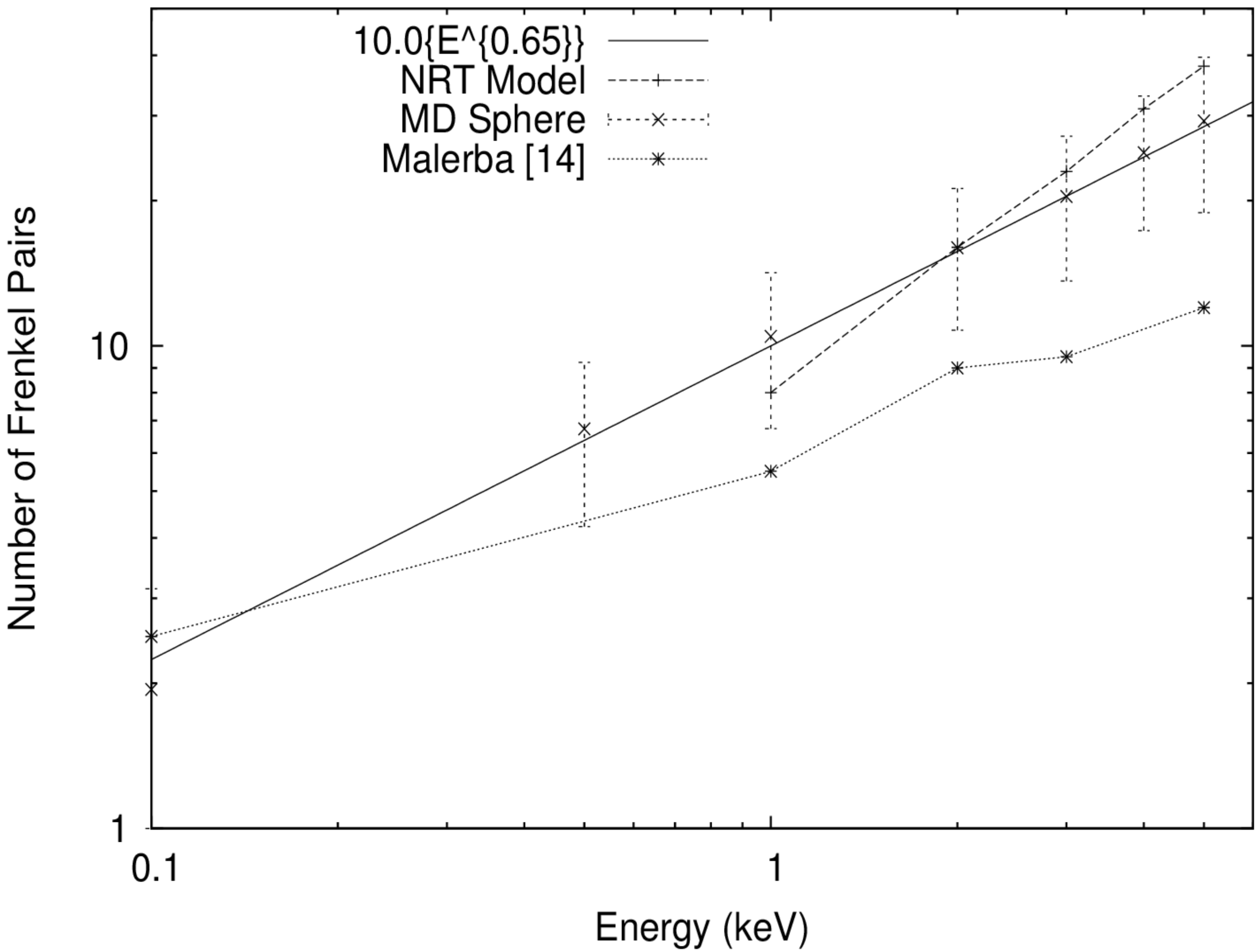
A few hundred random directions have to be explored for the standard deviation to stabilize

PKA energy attenuation



742nd PKA seems to have initially lost energy only in small angle collisions, thereby losing energy more slowly initially as compared to the 741st PKA

Comparison with the NRT model



Error bars in MD are the variance for 1000 PKA simulations

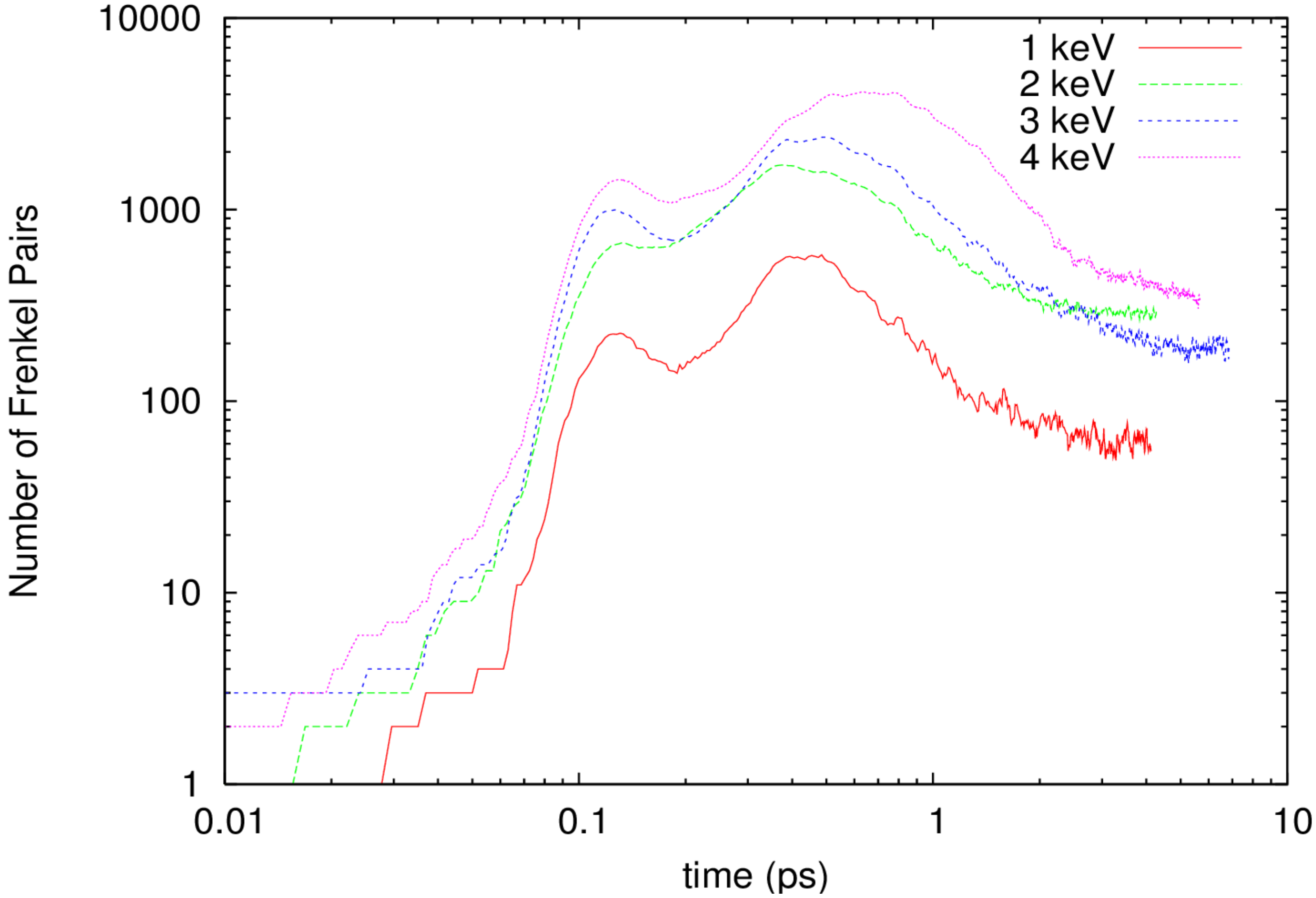
Number of Surviving Frenkel Pairs follows a power law

Tabled statistics for FeCr

Table I: Direction averaged values of N_{FP}, Sample size in terms of number of unit cells of size 2.8553 Å, the number of Frenkel Pairs, $MaxD$, the maximum displacement and $PKAD$, the displacement of the PKA. The value after the $\pm$ sign is the standard deviation of these quantities.

E_{PKA} (keV)	Sample Size	N_{FP}	$MaxD$ (Å)	$PKAD$ (Å)
0.1	20x20x20	2 ± 1	3.5 ± 1.1	3.1 ± 1.5
0.5	30x30x30	7 ± 3	8.4 ± 2.1	7.5 ± 2.7
1.0	30x30x30	11 ± 4	12.5 ± 4.1	10.9 ± 4.4
2.0	40x40x40	16 ± 5	20.5 ± 8.6	17.8 ± 9.2
3.0	40x40x40	20 ± 7	28.5 ± 13.6	24.2 ± 14.1
4.0	50x50x50	25 ± 8	35.4 ± 18.6	30.8 ± 19.5
5.0	50x50x50	30 ± 10	42.0 ± 24.1	35.8 ± 25.4

Cascade evolution in FCC Cu

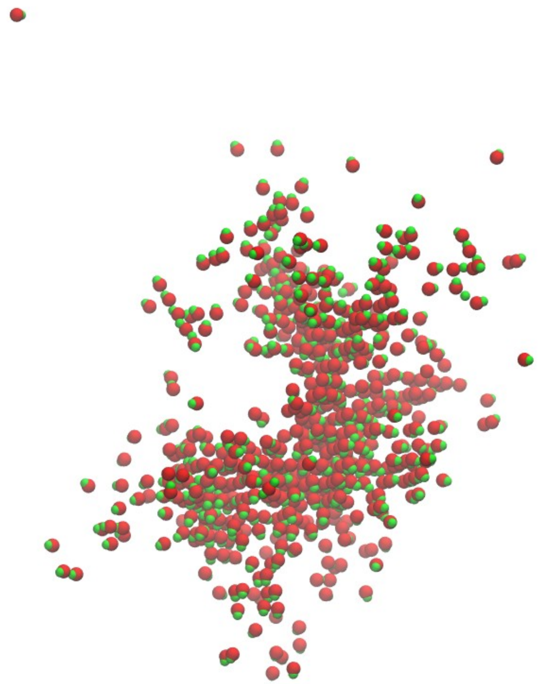


Double hump – Is this common for FCC crystals?

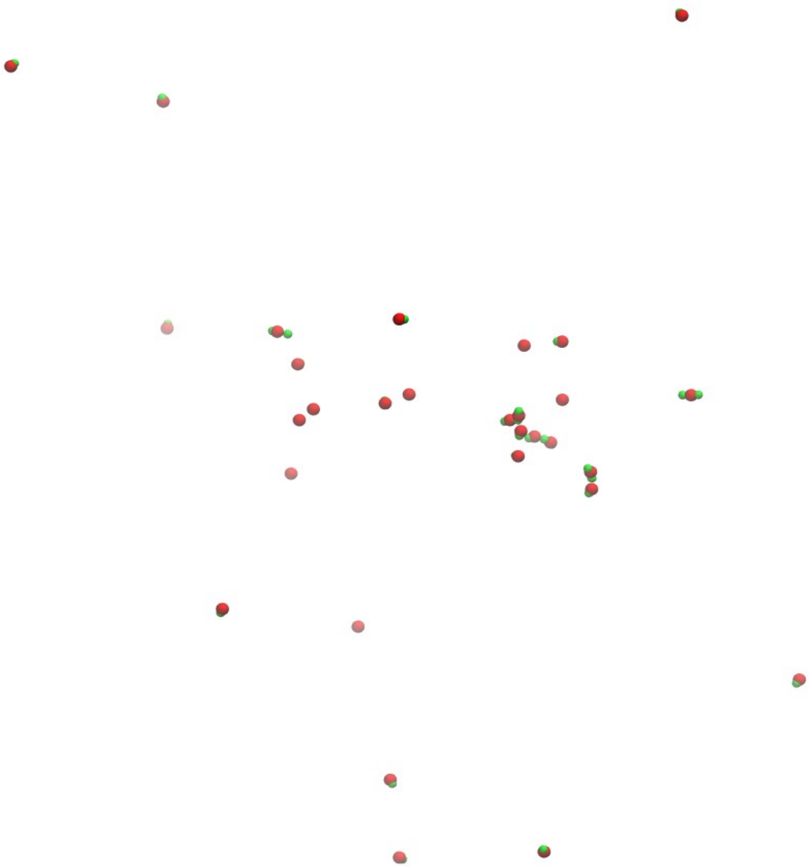
Non stiffened potentials – Kai has given me stiffened

Potentials for Cu, Fe and W – ToDo ..

Cascade characteristics in Cu



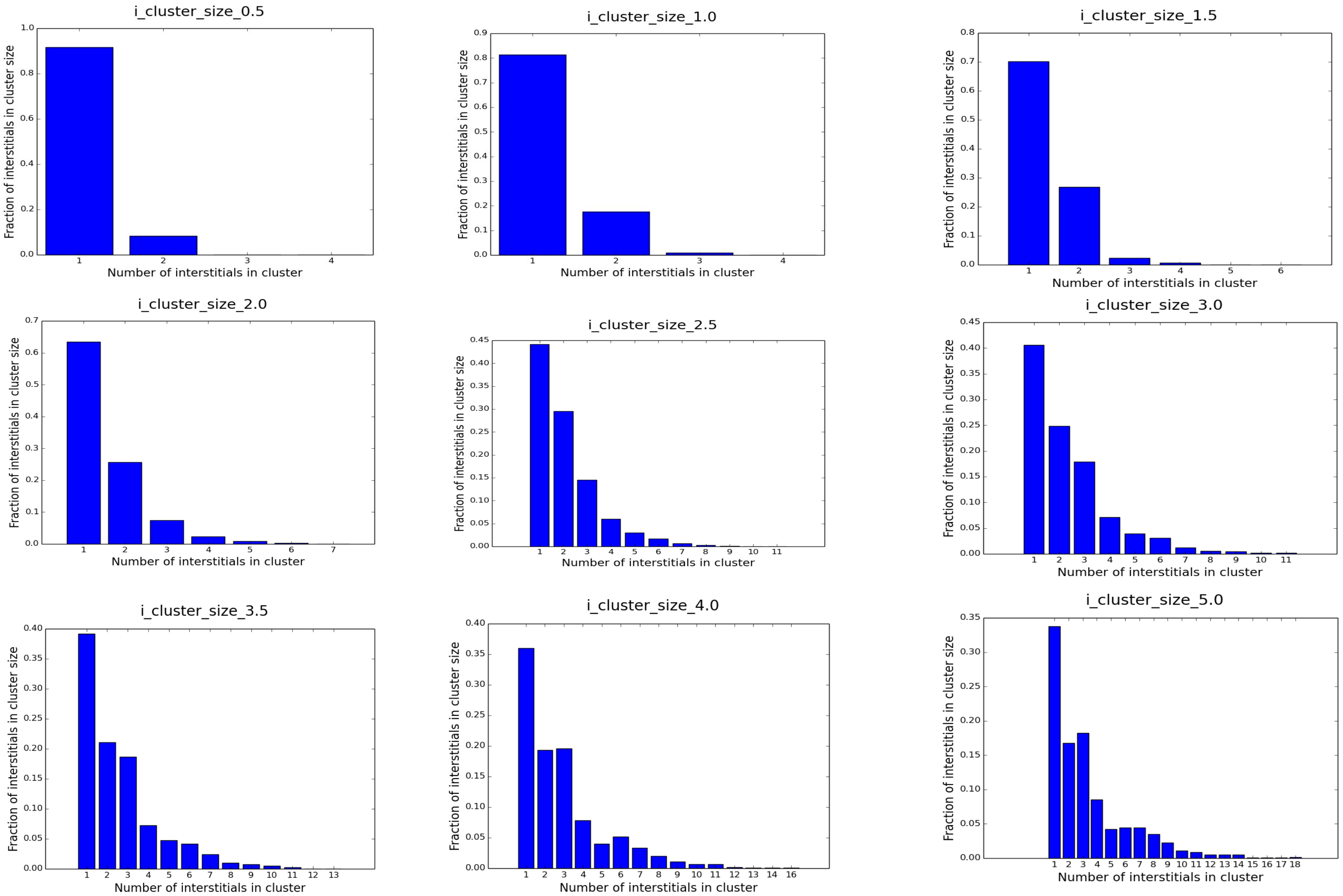
At Cascade Peak



After Stablizing

Stoller - At peak interstitials are in close proximity which then recombine in an athermal process until steady state value is reached

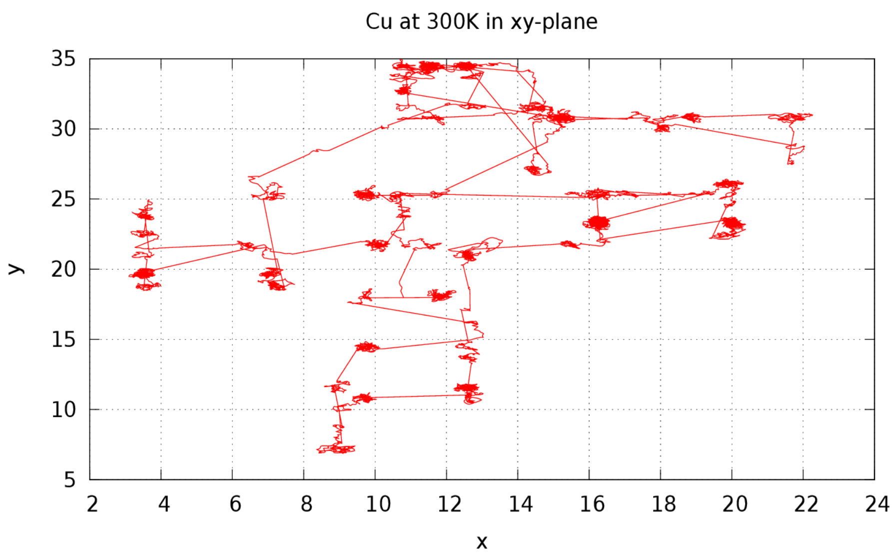
Clustering of interstitials in Cu cascade

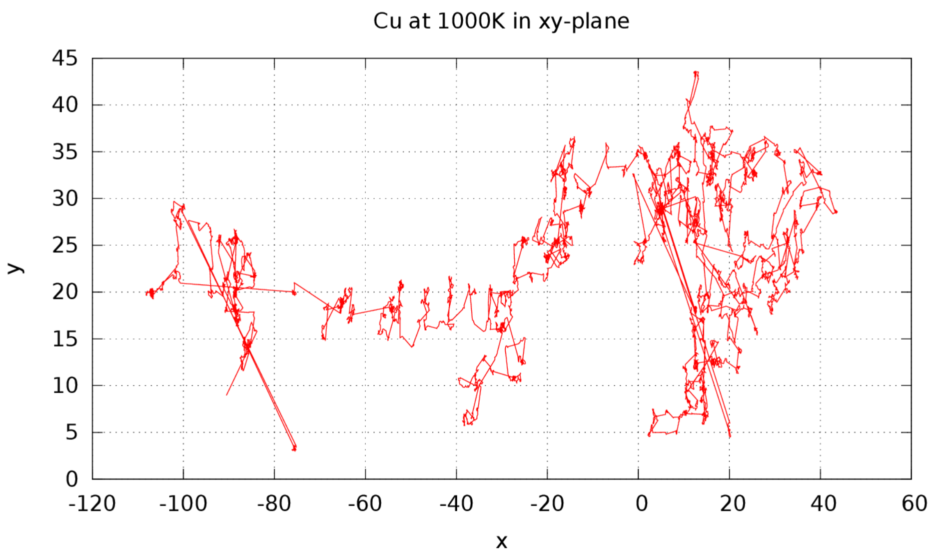


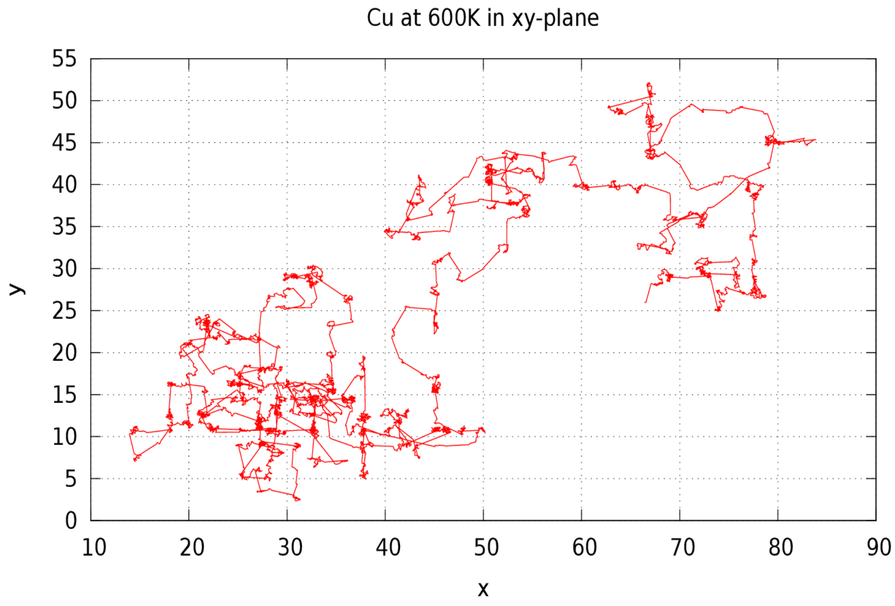
Cluster identification algorithms - DBSCAN

Interstitialcy Diffusion

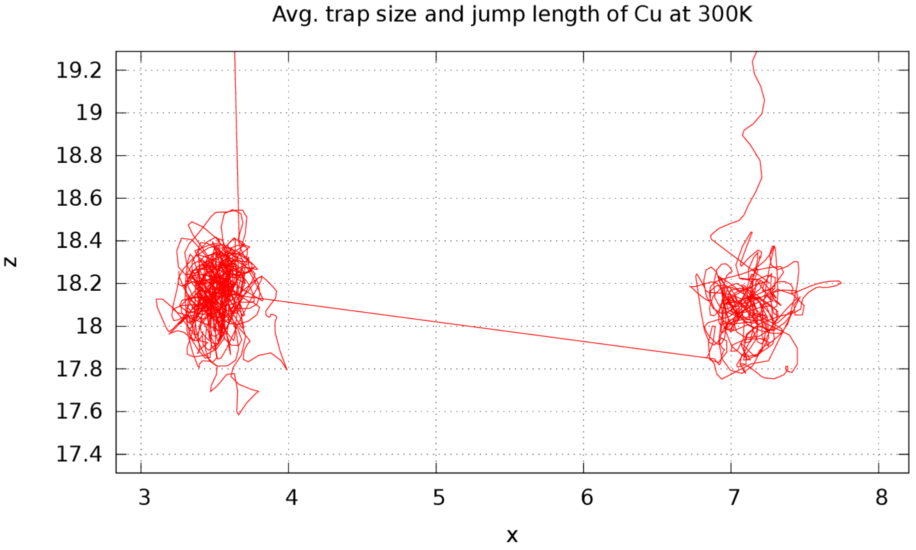
Interstitialcy Diffusion in Cu

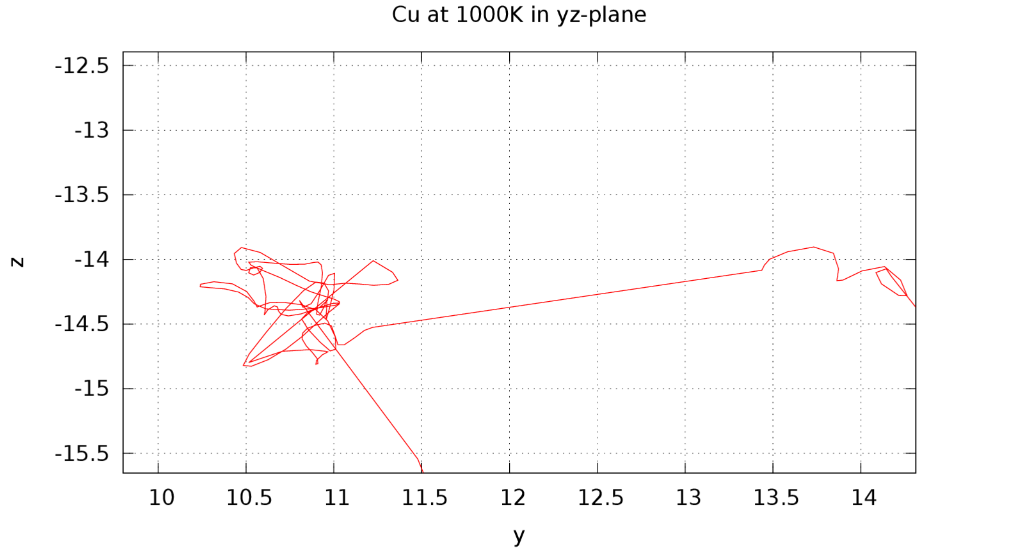


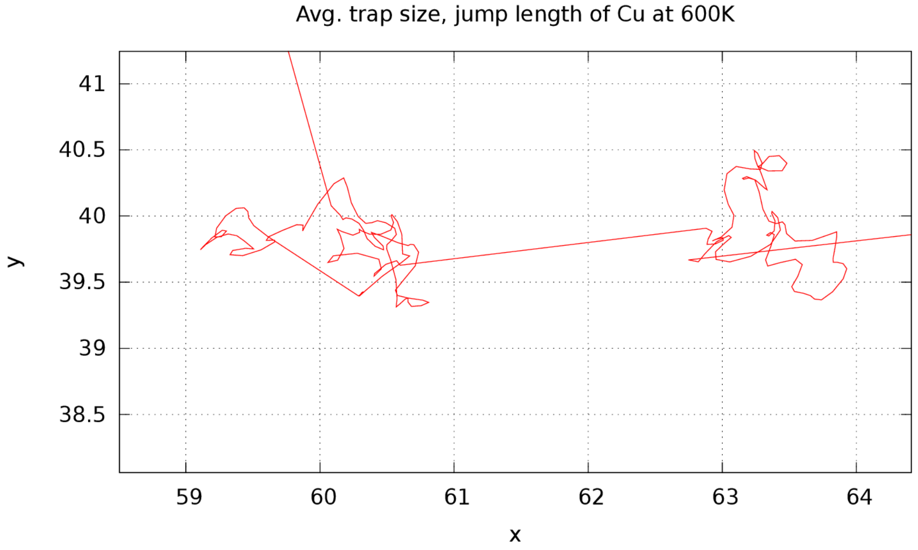




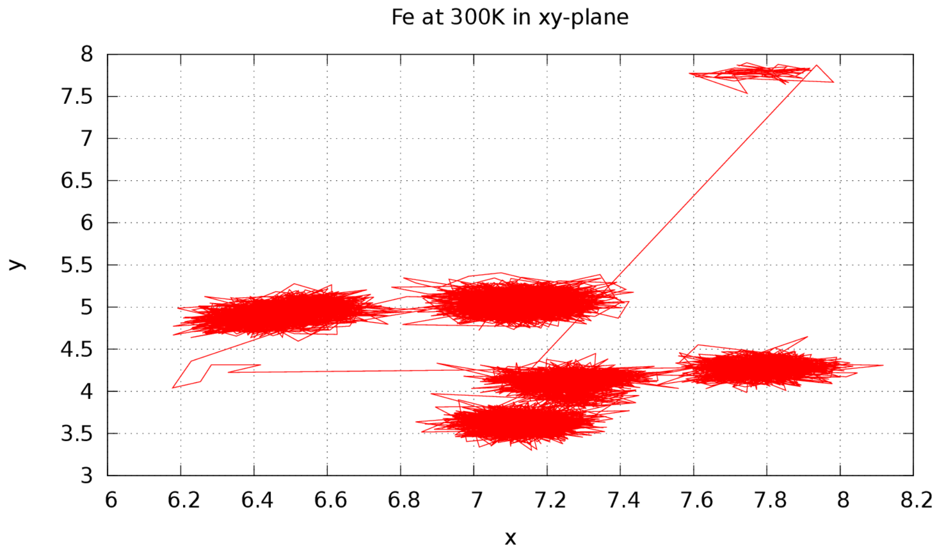
Interstitialcy Diffusion in Cu

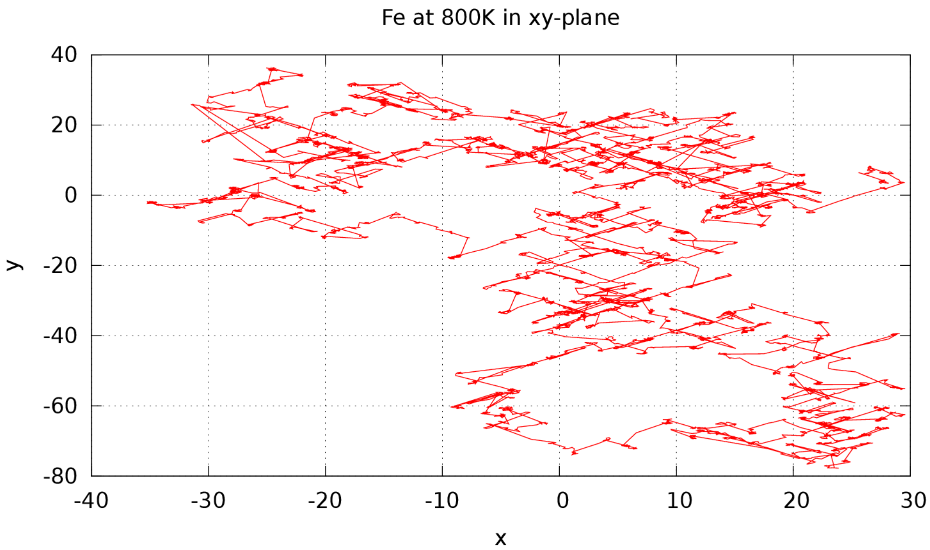


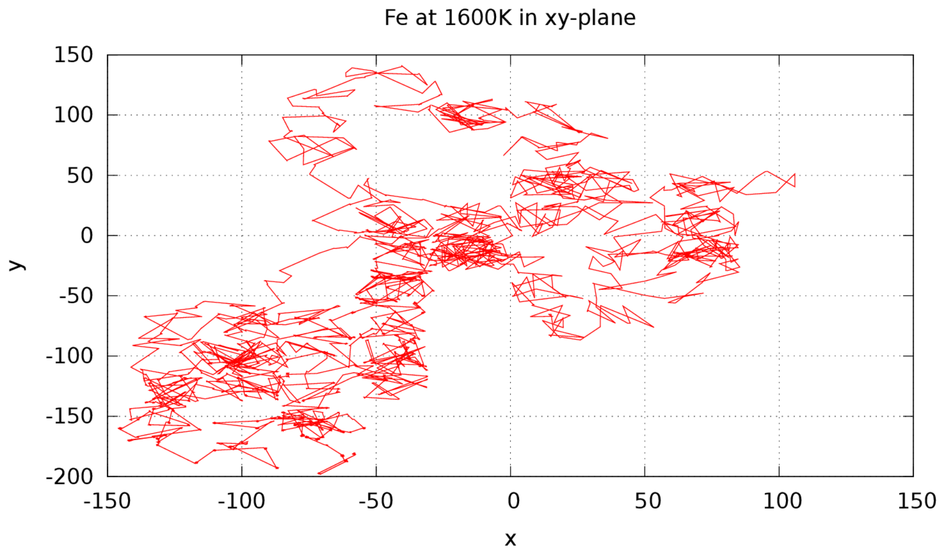




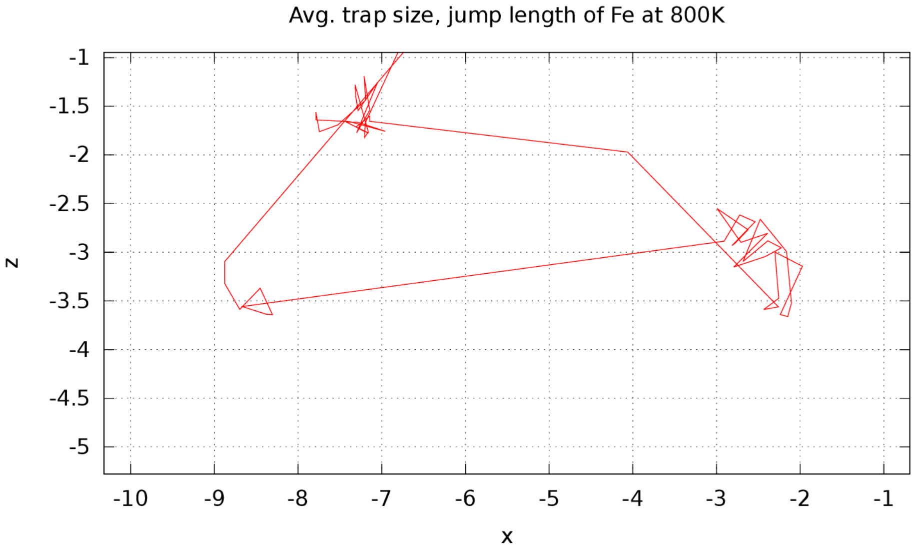
Interstitialcy Diffusion in Fe

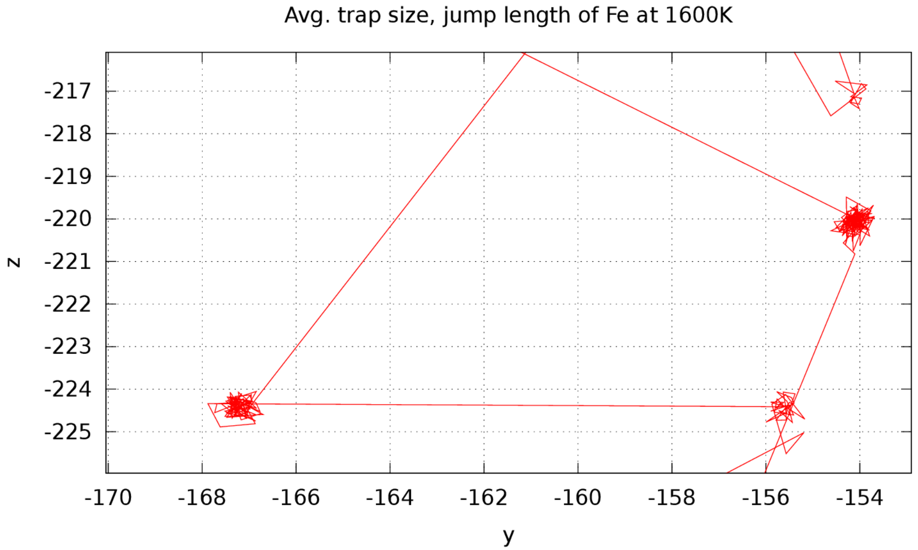




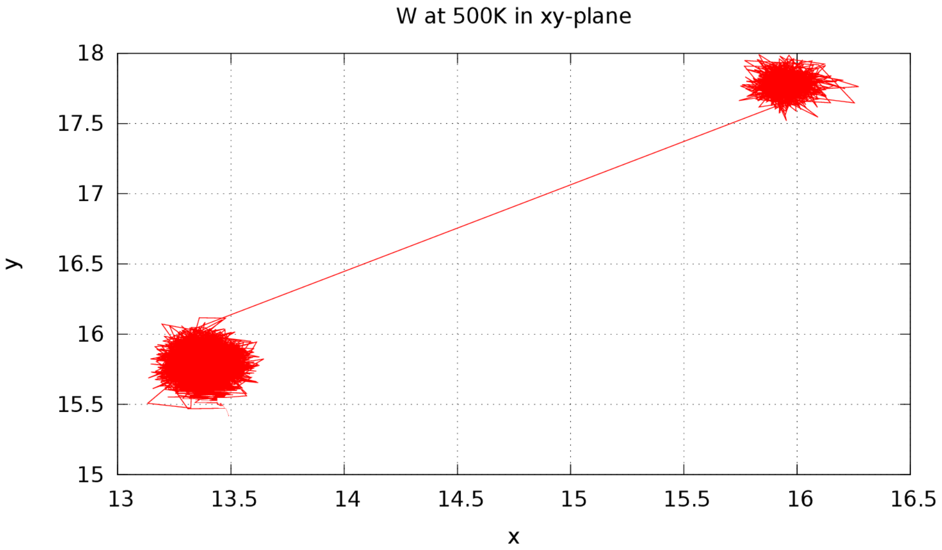


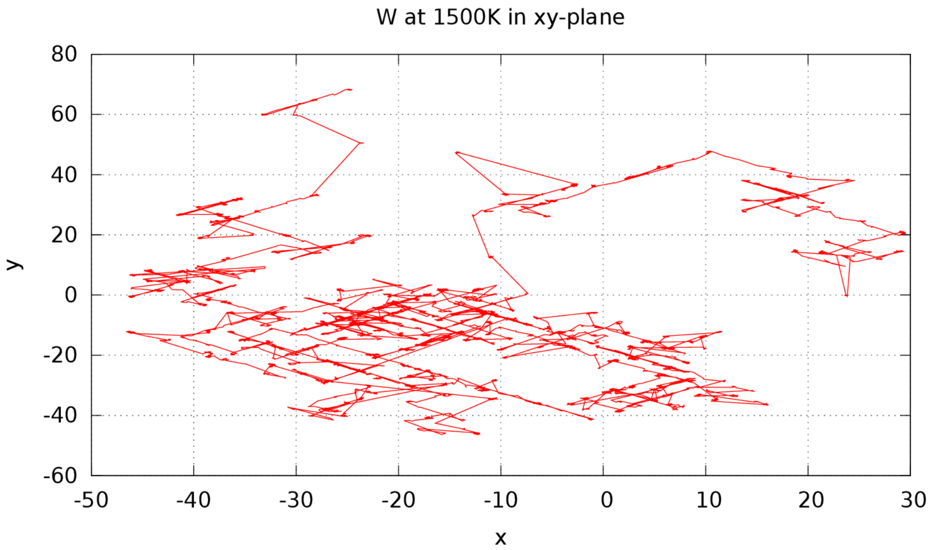
Interstitialcy Diffusion in Fe

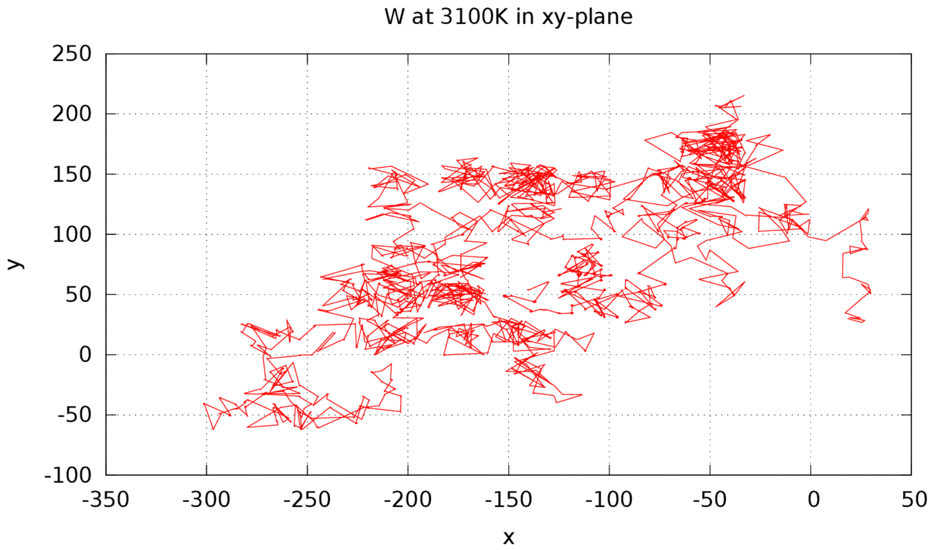




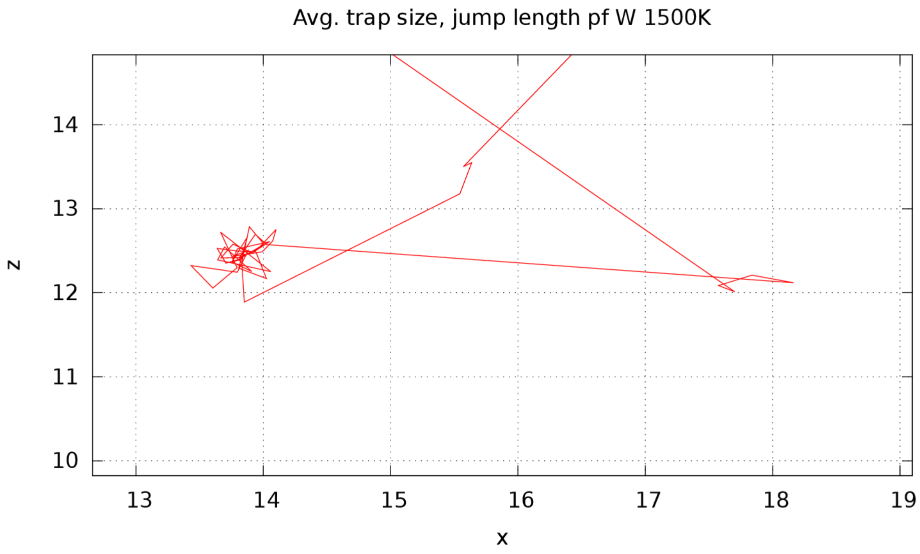
Interstitialcy Diffusion in W

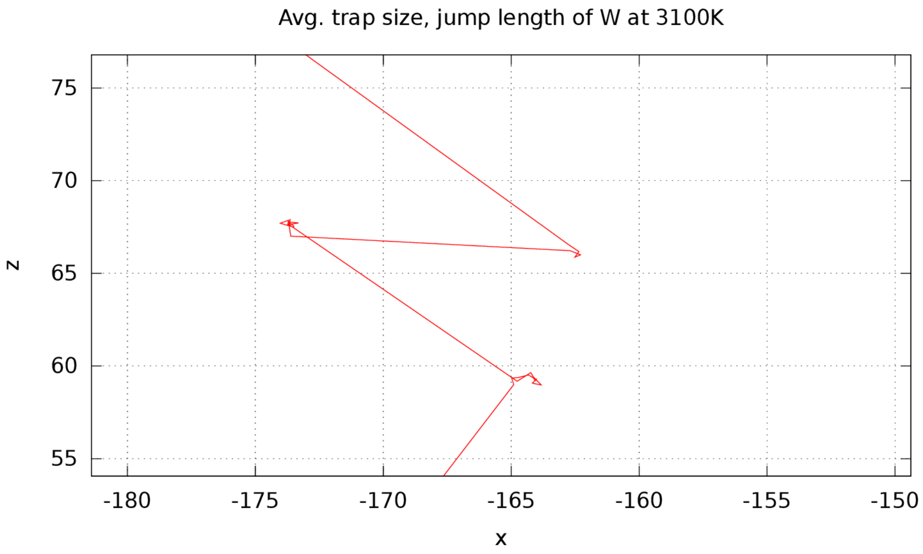




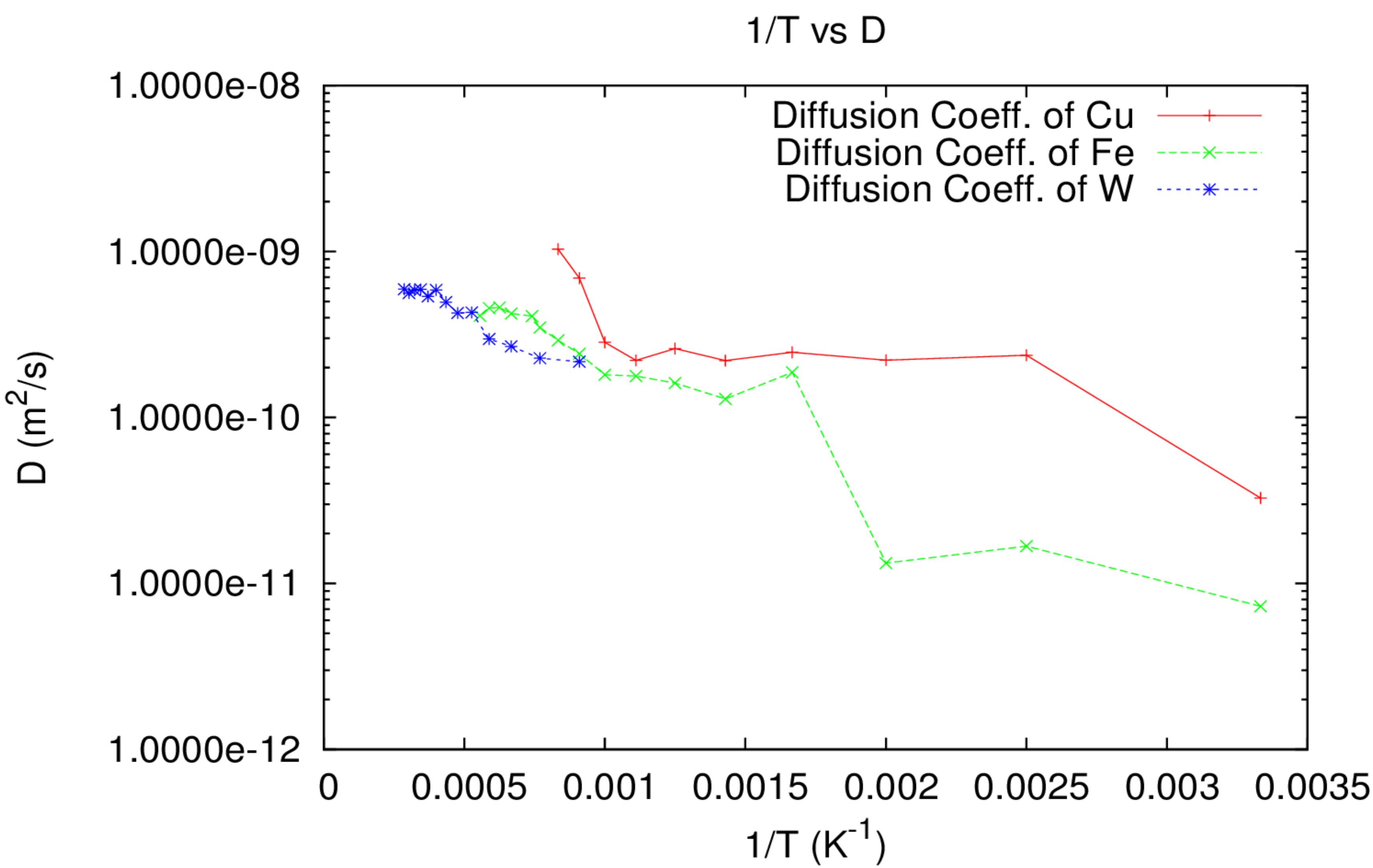


Interstitialcy Diffusion in W



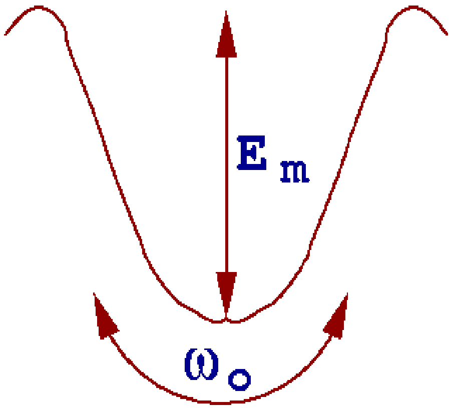


Interstitialcy Diffusion Coefficients



Note the gray color – Needs further analysis – see poster to discuss details of analysis

Scaling up KMC - MCD



$$\omega^{l,h} = \omega_o^{l,h}\, e^{-E_m^{l,h}/(k_B T)}$$

$$\Delta t = \frac{-\ln(U)}{N(\omega^l + \omega^h)}$$

Poisson process (assigns real time to the jumps)

Jumps are independent (no memory)

One particle per time-step – inputs E_m, jump lengths, jump directions

Monte Carlo Diffusion (MCD) used to simulate TGD

$$\Delta X = \sqrt{2D\Delta t}\,\varsigma + V_c \Delta t$$

All particles per time-step – inputs Diffusion coefficients

Neighbour lists – 3-d tree?, parallelization using domain decomposition

O-KMC for end of cascade clusters and

MCD for larger clusters of interstitials, vacancies and He bubbles?

Conclusions

- A few 100 random directions have to be explored to obtain saturation
- in the standard deviation in number of displaced atoms in bcc FeCr.

- In 35 % of the cases at high secondary recoils have a higher range than the PKA.

- Large displacements seen in 0.2 to 0.9 % of PKAs at energies > 2keV.

- In situ post-processing for N_{FP}, clustering developed.

- Interstitialcy diffusion has time scales of a few tens of pico-secs. This will be analyzed for inputs to a O-KMC code and MCD code.

- Comparison of MD results with TRIM-SP planned (MARLOWE available?)

- Diffusion in Grain boundaries also needs to be studied (See A. Abishek's poster on He diffusion in grain boundaries).