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Cascade Morphologies in BCC Metals

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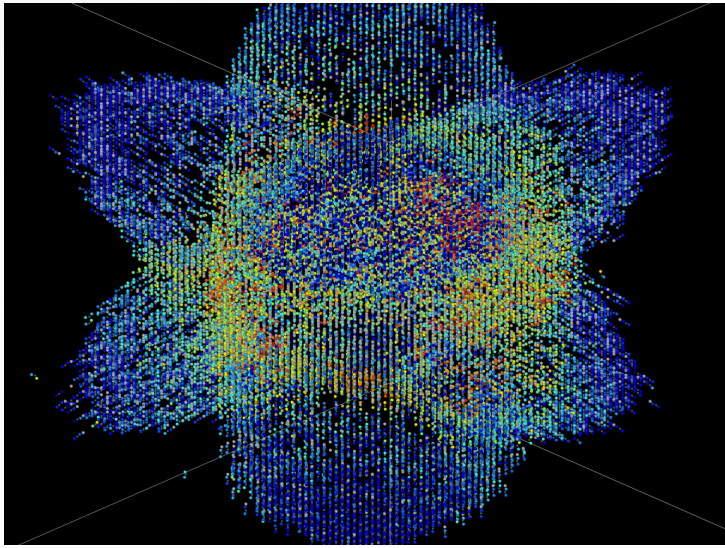

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Introduction

Motivation

- Compare different cascade morphologies in bcc metals.
- Study the effect of morphology on defect production.
- Study the effect on defect clustering/distribution.

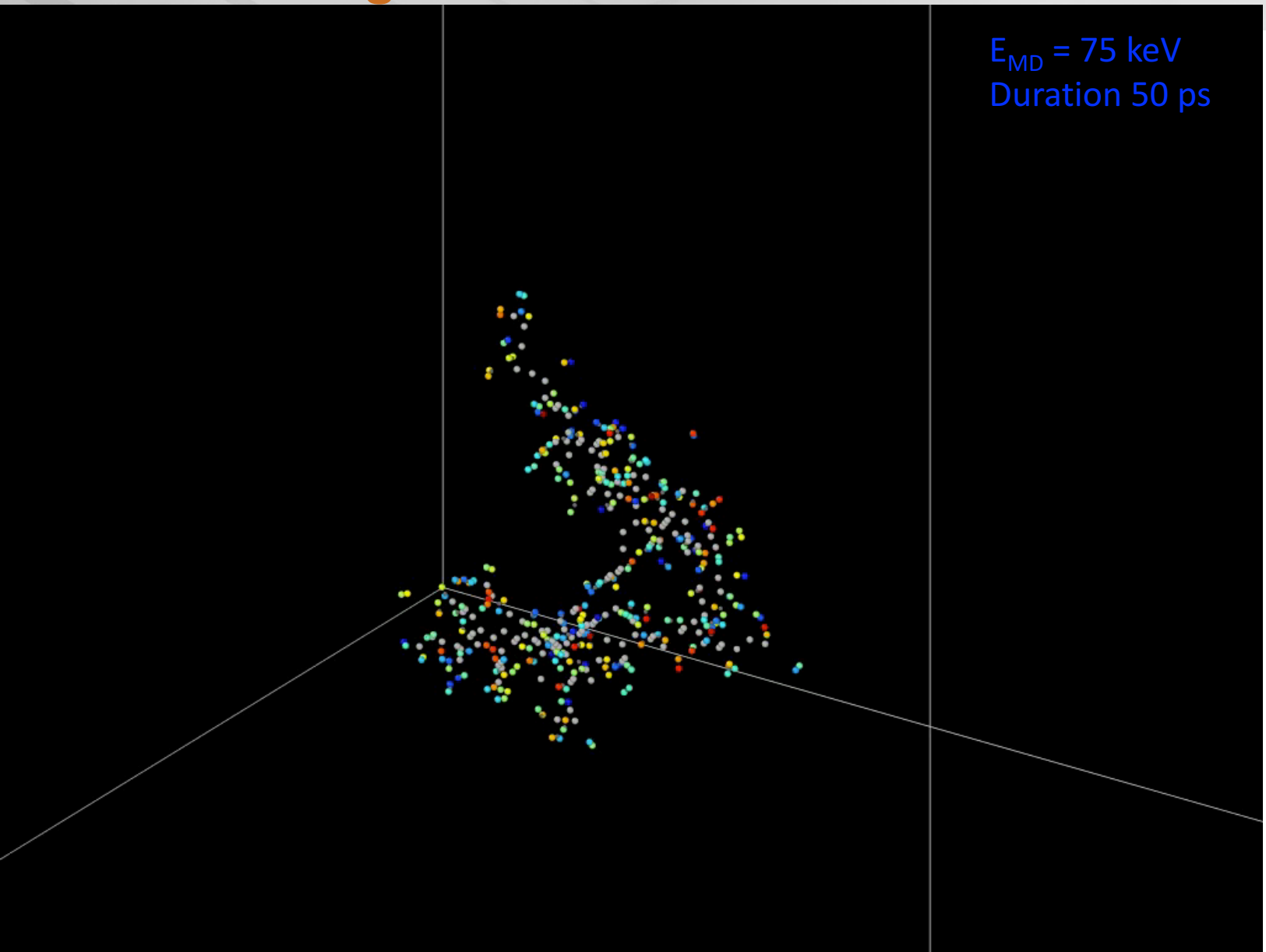
Interatomic potentials for MD

- Cr: EAM by Bonny *et al* [PhilMag **91**, 1724 (2011)], ZBL added by N. Juslin for this study.
- Fe: Finnis-Sinclair [PhilMag A **50**, 45 (1984)], modified by Calder *et al* [JNM **207**, 25 (1993)].
- Mo: Ackland-Thetford [Philmag A **56**, 15 (1987)], modified by Salonen *et al* [JPCM **15**, 5845 (2003)].
- W: Ackland-Thetford, modified by Juslin *et al* [JNM **432**, 61 (2013)], denoted as ATJ potential.
- W-björkas: Derlet-Dudarev [PRB **76**, 054107 (2007)], modified by Björkas *et al* [NIMB **267**, 3204 (2009], denoted as DDB potential.

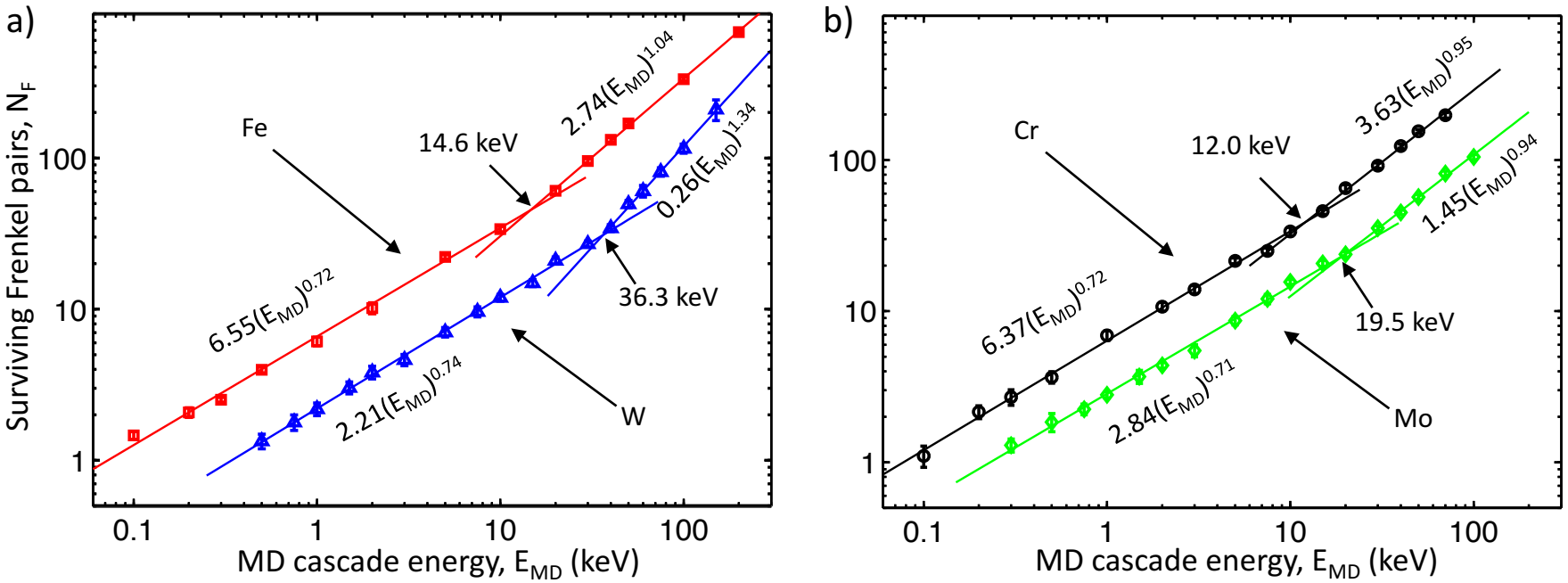
Simulations were performed with LAMMPS code at 100 K (Fe) and 300 K (Cr, Mo, W).
Electronic loss was excluded.
Defect was determined based on occupancy of Wigner-Seitz cell.

More information of the setup: JPCM **27**, 225402 (2015).

Movie of Large Cluster Formation in W



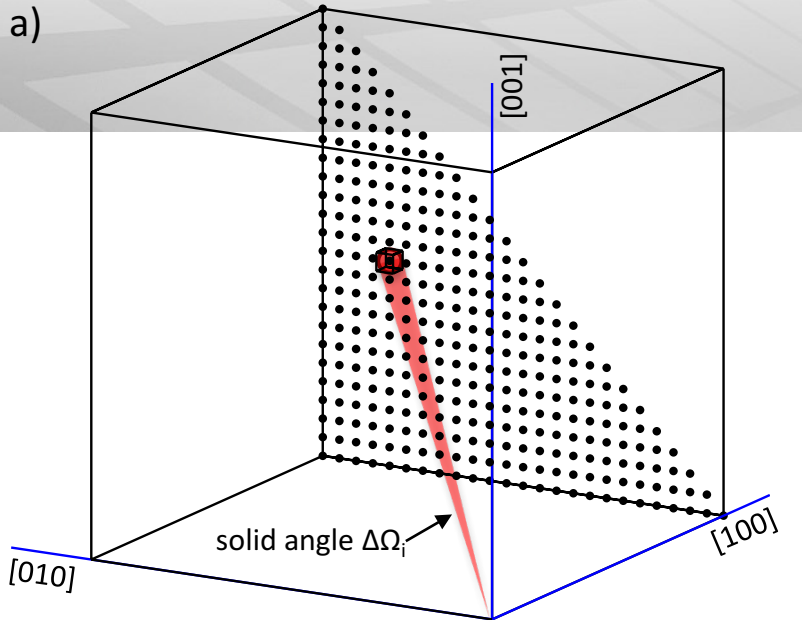
Observation of Different Cascade Regimes



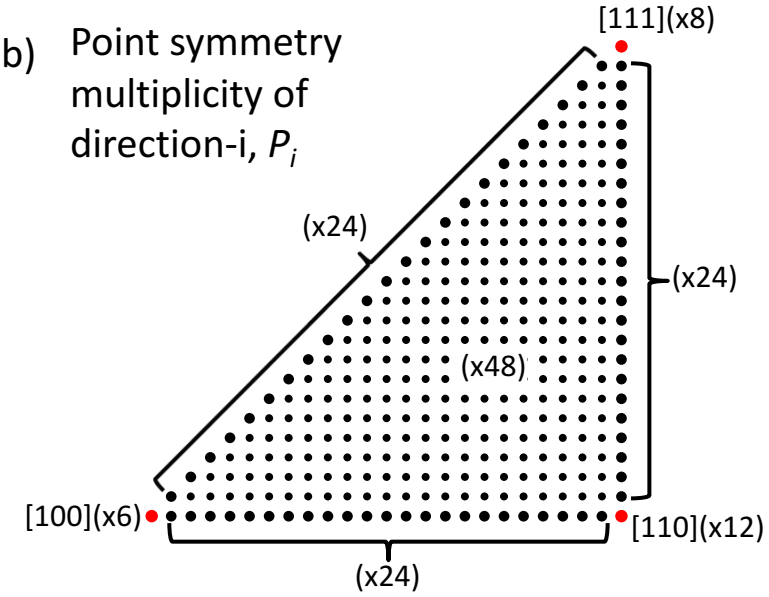
- A kink in the N_F curve is evident in W.
- We propose that the kink also exists in Cr, Fe, and Mo.
- Hence, we perform a bilinear fit and determine the inflection point (transition energy).
- The transition energy, μ, marks the onset of a different power-law regime.
- Depending on one's view, there could be a transition at the low-energy end: before and after "cascade-like" behavior is fully developed, as suggested in Fe [JNM **251**, 49 (1997)] and W [JNM **462**, 329 (2015)].

Displacement Threshold Energy, E_d

a)



b) Point symmetry multiplicity of direction-i, P_i



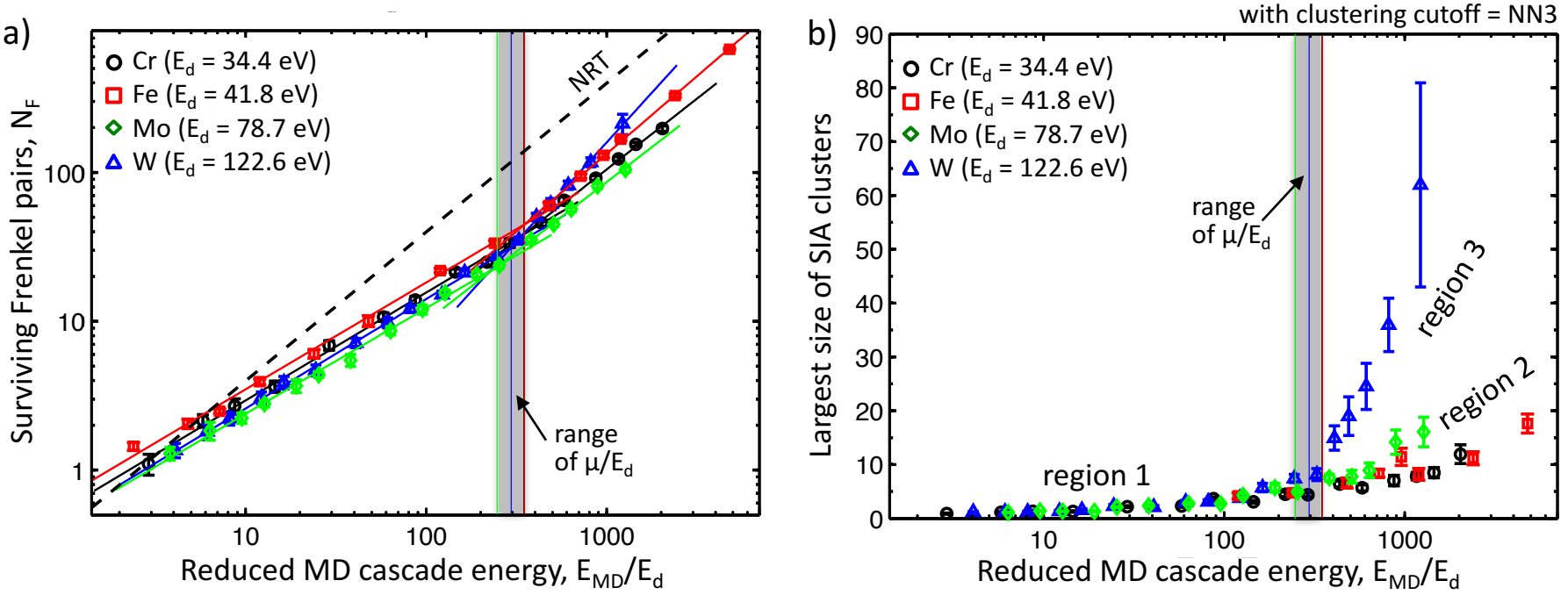
$$E_{\mathrm{d}} = \sum_i E_{d,i} P_i \Delta\Omega_i \Big/ \sum_i P_i \Delta\Omega_i ,$$

$$\Delta\Omega_i(h,k,l) = 2\pi \left(1 - \frac{\sqrt{h^2+k^2+l^2}}{\sqrt{h^2+k^2+l^2+D^2/4}}\right),$$

Interatomic potential	E_{d} (eV)
Cr	34.4 ± 1.5
Fe	41.8 ± 1.6
Mo	78.7 ± 2.9
W	122.6 ± 4.4

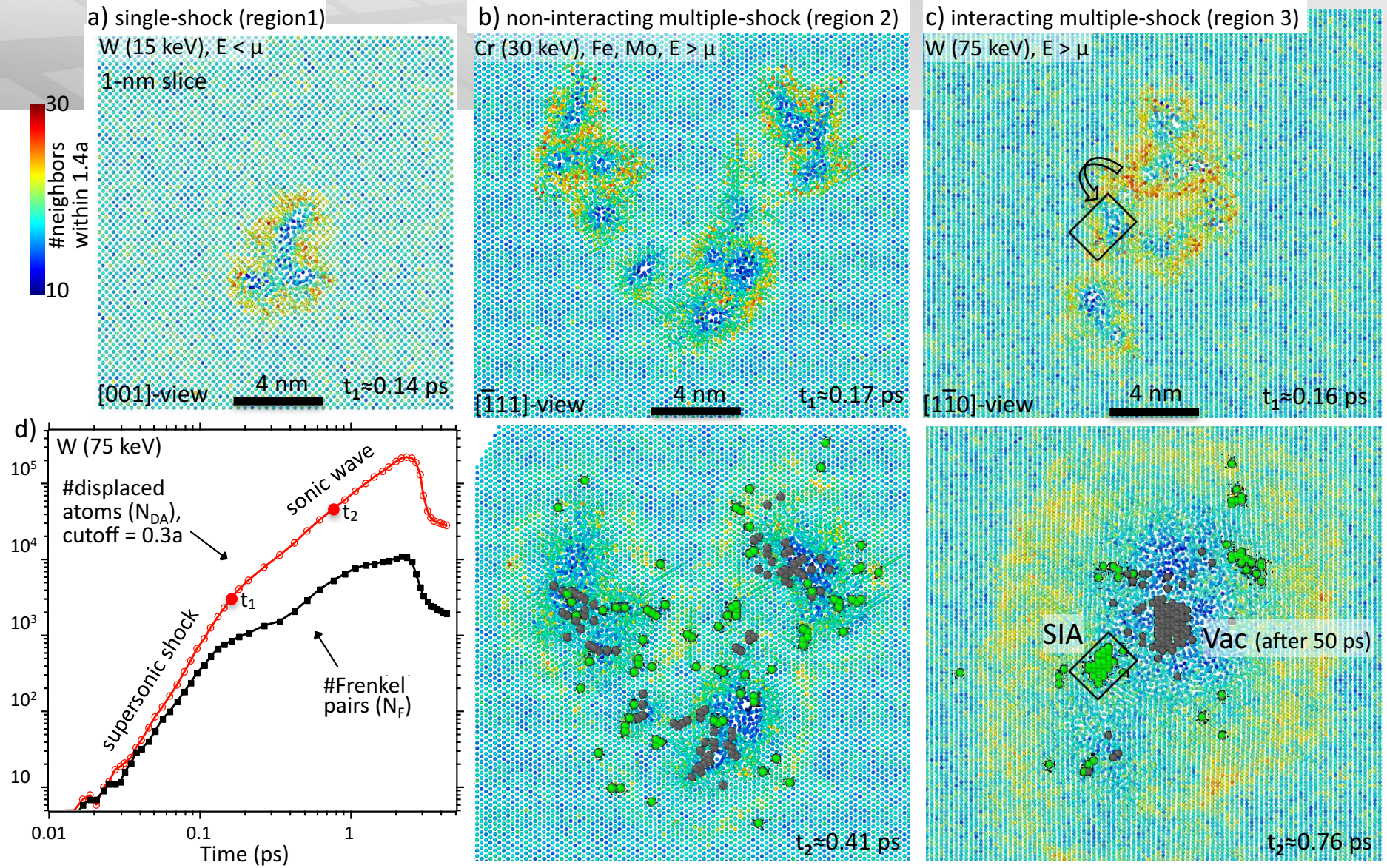
Box size = 20x18x16 supercell.

Normalization of Cascade Energy Scale



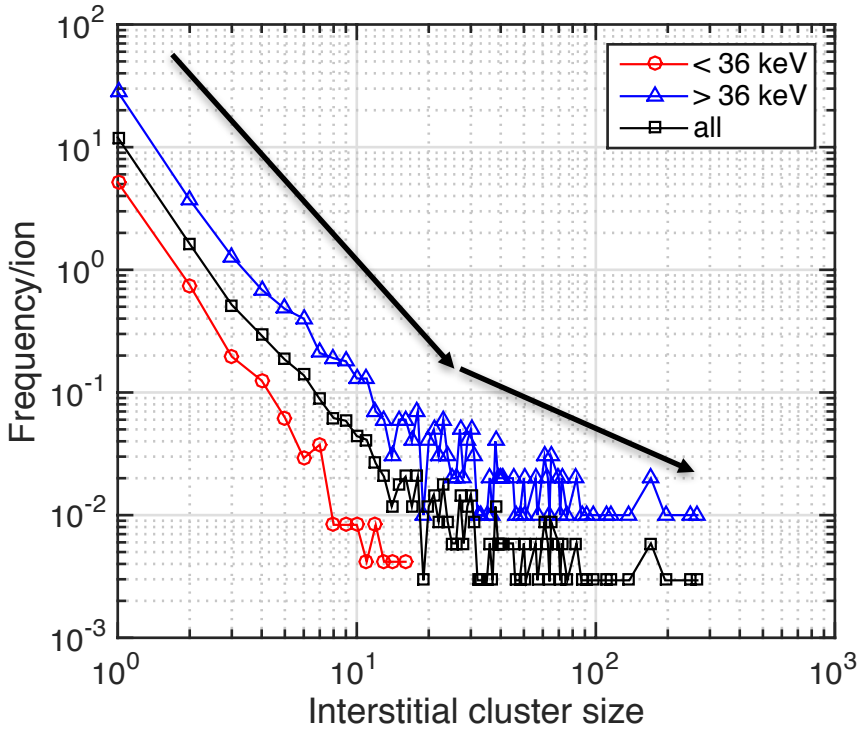
- To find a possible scaling of μ, we normalize the cascade energy with the displacement threshold energy, E_d.
- Indeed, the μ of Cr, Fe, Mo, and W fall in a narrow range of the normalized energy scale, around $\mu/E_d \approx 300$.
- μ also marks the onset of the formation of large SIA clusters in W and to a lesser extent in Mo, Fe, and Cr.

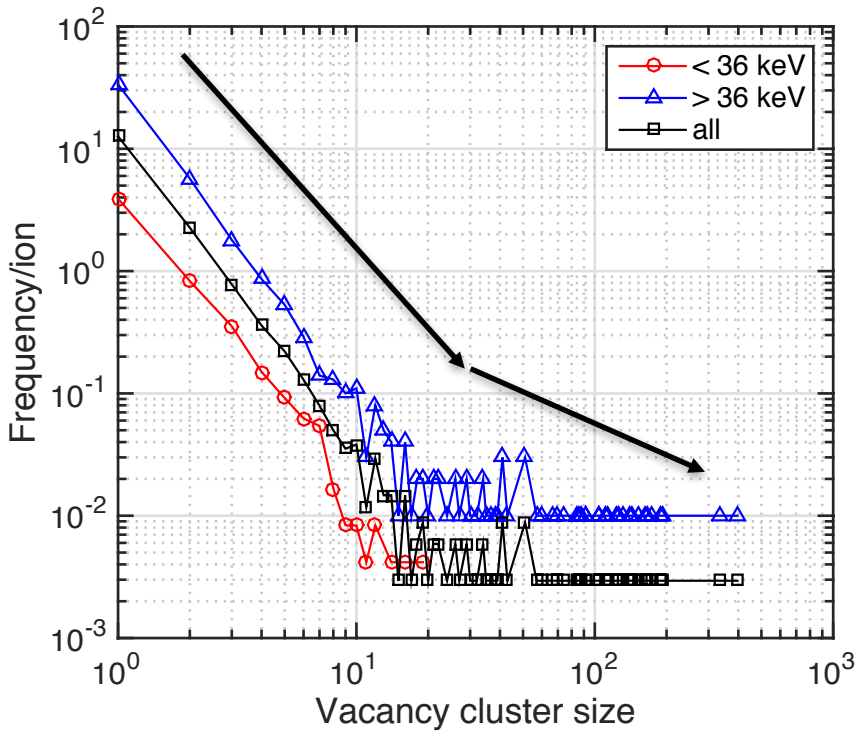
Cascade Morphology Comparison



Interacting multiple supersonic shocks facilitate the formation of the large SIA clusters and vac clusters, was first suggested by Calder *et al* in Fe with 2 Bi PKAs [PhilMag **90**, 863 (2010)].

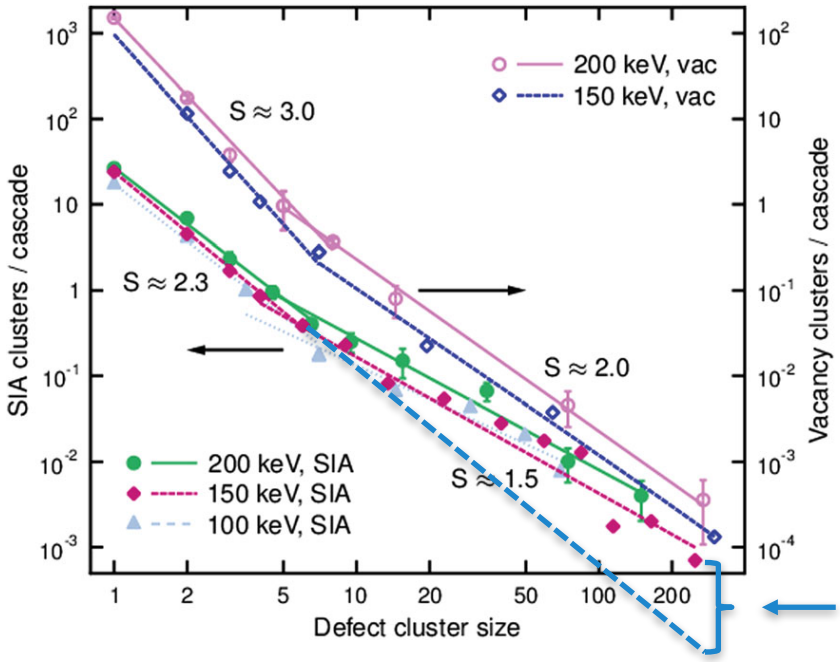
Effect of Cascade Morphology on Size Distribution of Defect Clusters in W





Slope change → associated with different cluster formation mechanism of the underlying cascade morphology.

Effect of Cascade Morphology on Size Distribution of Defect Clusters in W



Large clusters form more frequently in an interacting multiple-shock cascade than expected from a single-shock cascade.

Figure 2. Size–frequency distributions of defects in W derived from MD simulations of cascades initiated by PKAs with various energies. Results are averaged over 20, 36 and 10 cascades for 100, 150 and 200 keV PKAs, respectively. Note the different slopes of scaling laws for SIAs and vacancies. For clarity the vacancy plot is shifted upwards with respect to the SIA plot. The scale of the axes is the same for both cases.

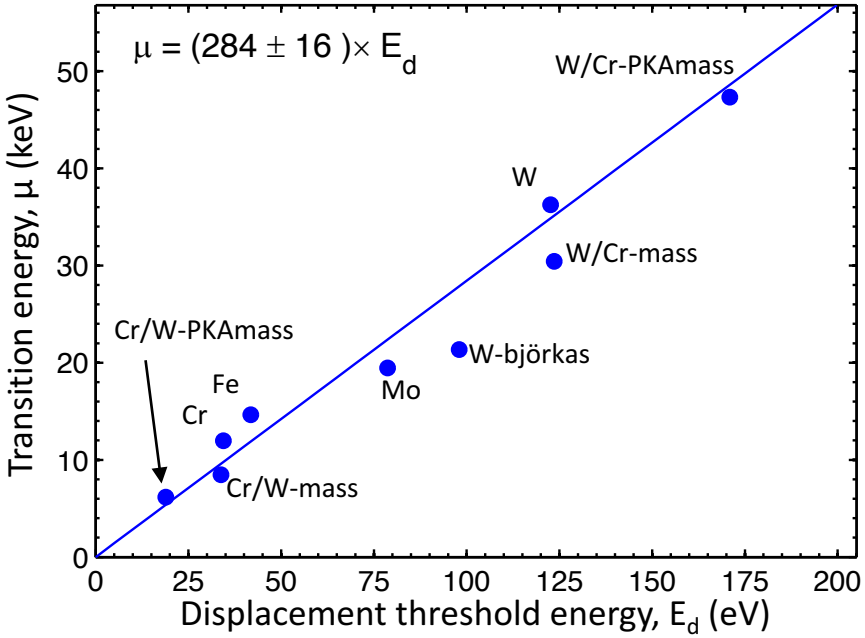
A. E. Sand *et al*, MatResLett **5**, 357 (2017).

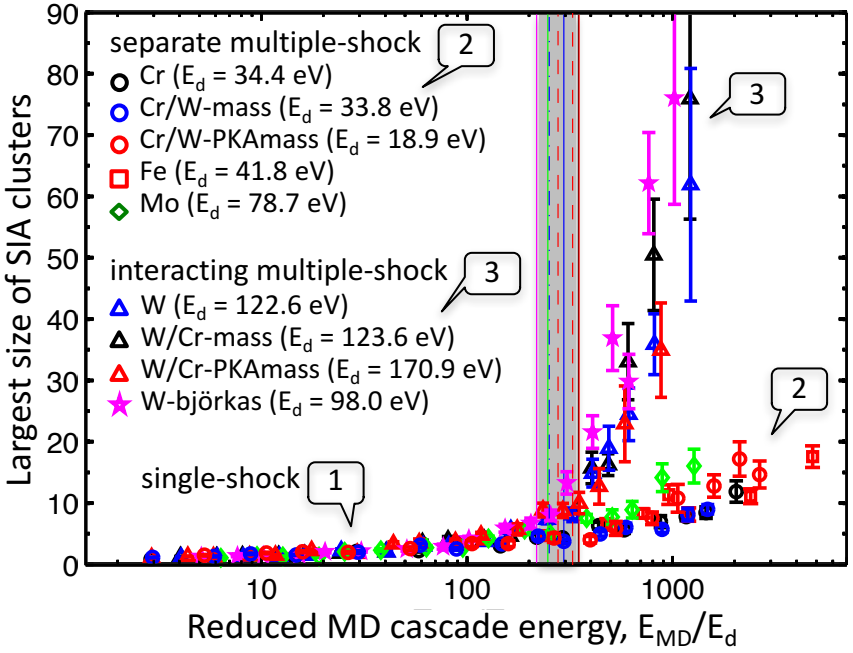
Additional BCC Test Systems

Interatomic potential	E_d (eV)	Note	
Cr	34.4 ± 1.5	As is.	
Fe	41.8 ± 1.6	As is.	
Mo	78.7 ± 2.9	As is.	
W	122.6 ± 4.4	As is.	
Cr	33.8 ± 1.4	With W mass.	(Cr/W-mass)
Cr	18.9 ± 1.1	With W PKAmass.	(Cr/W-PKAmass)
W	123.6 ± 4.4	With Cr mass.	(W/Cr-mass)
W	170.9 ± 6.7	With Cr PKAmass.	(W/Cr-PKAmass)
W-björkas	98.0 ± 3.7	As is.	

- PKAmass ↑ E_d ↓, and vice versa, related to momentum transfer.
- All-atom mass has negligible effect on E_d, due to similar collision kinematics.

Transition Energy Model





- μ is found to be reasonably proportional to E_d:
  - ✓ The transition energy can be estimated based on only one parameter, i.e. E_d.
  - ✓ The effect of different mass, PKA mass, and the force field on μ is embedded in their effect on E_d.

W. Setyawan *et al*, JPCM **27**, 225402 (2015)

Linear vs Bilinear Fit of N_F Data

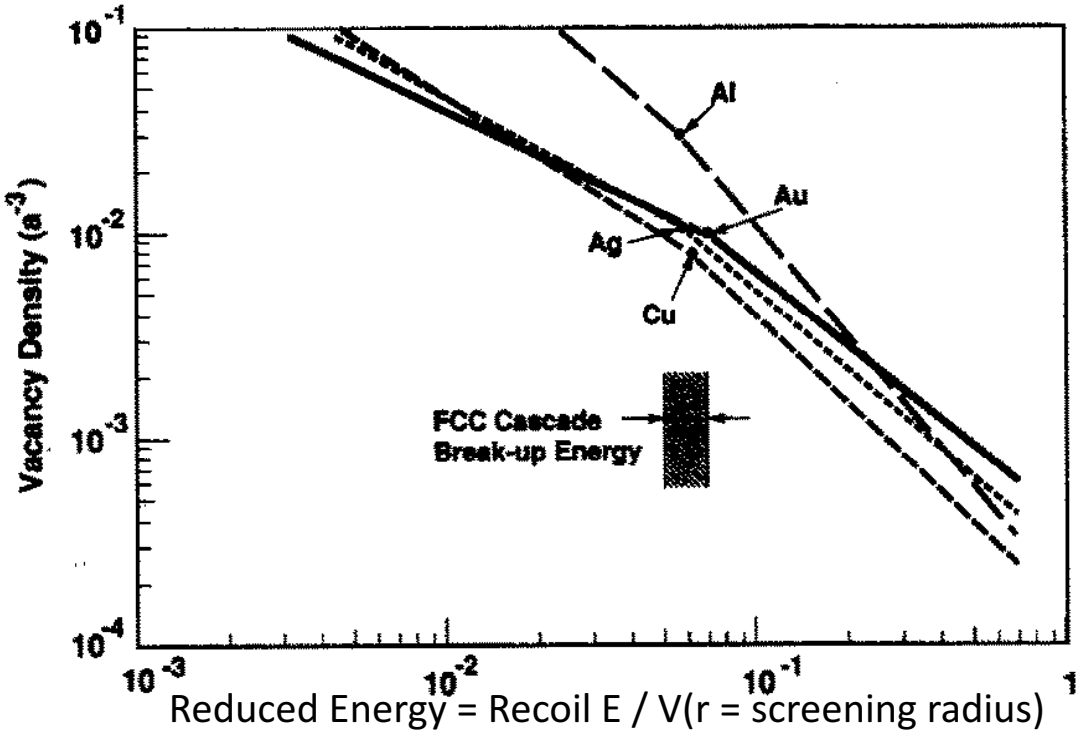
System	Two-line fit $\delta_{\text{rms}}(\%)$	One-line fit $\delta_{\text{rms}}(\%)$
Cr	5.1	10.2
Fe	5.9	18.8
Mo	5.0	9.3
W	3.3	19.9
Cr/W-mass	5.8	12.4
Cr/W-PKAmass	5.3	18.4
W/Cr-mass	5.6	24.2
W/Cr-PKAmass	5.5	11.8
W-björkas	6.3	34.0

$$\delta_{\text{rms}} = 100\sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\frac{y_i - y_{i,\text{fit}}}{y_{i,\text{fit}}}\right)^2}$$

- The two-line (bilinear) fit performs significantly better than the one-line (linear) fit.

Early Studies of Sub-Cascade with Binary Collision Approximation (BCA)

Heinisch et al, JNM **179**, 893 (1991)



Element	Reduced energy factor [a] (eV^{-1})	Cascade break-up recoil energy (keV)	Reduced break-up damage energy
Al	2.34×10^{-5}	2.5	0.052
Cu	3.05×10^{-6}	20	0.049
Ag	1.28×10^{-6}	50	0.055
Au	4.18×10^{-7}	200	0.071
Fe	4.00×10^{-6}	50	0.15
Mo	1.80×10^{-6}	130	0.19
W	5.10×10^{-7}	300	0.13

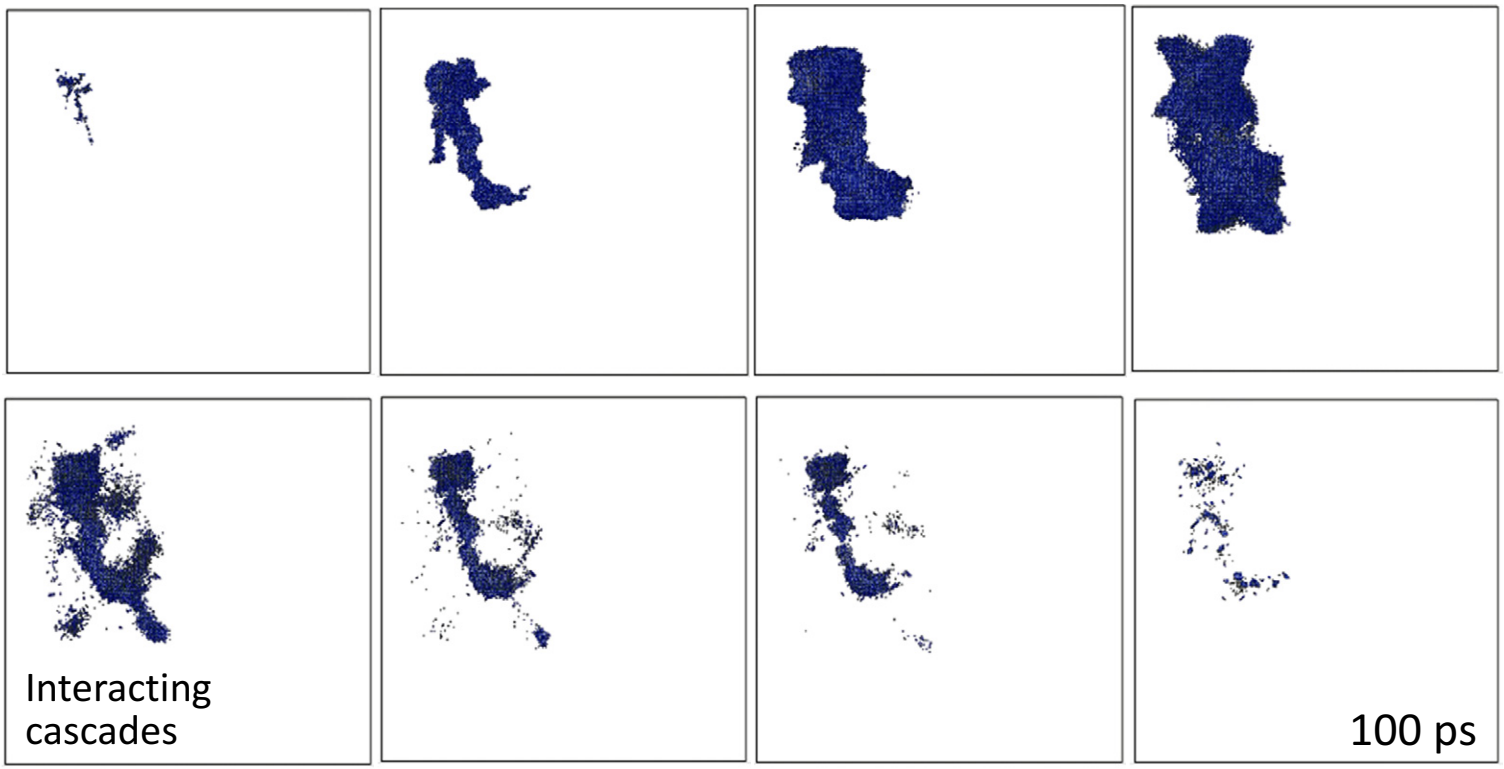
- BCA shows that cascade transition occurs both in bcc and fcc metals and over a narrow range of reduced cascade energy.
- Only non-interacting cascades (sub-cascades) were predicted by using BCA (many body collisions are ignored). MD shows that W exhibits interacting cascade (no sub-cascades).
- In W, will the next transition occur? i.e. interacting cascade → non-interacting cascade.

300-keV Cascade in Tungsten

E. Zarkadoula *et al*, JPCM **27**, 135401 (2015).

2T-model = electronic stopping (friction model) + electron-phonon coupling

E_{PKA} = 300 keV with DDB potential.



Non-interacting cascades are still not observed at 300 keV.

Electronic Stopping Effect in Tungsten

A. Sand *et al*, EPL **103**, 46003 (2013).
A. Sand *et al*, JNM **455**, 207 (2014).
Electronic stopping (ES) was modeled as a friction term when atom's kinetic energy > T_c.
E_{PKA} = 150 keV, simulation at 0 K.

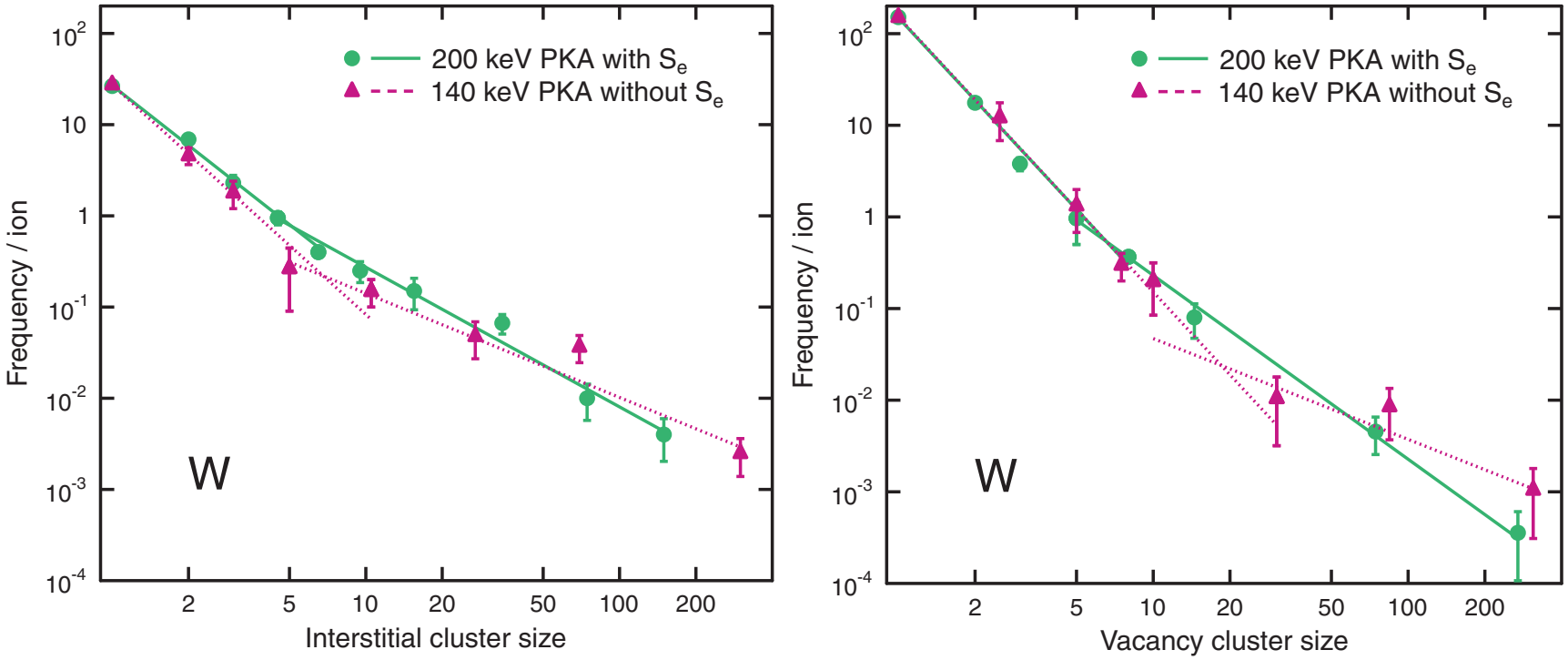
Friction Model				Our Fit (without ES)	
T_c (eV)	E_{ES} (keV)	N_F	N_{sim}	E_{dam} (keV)	N_F
5	48	183 ± 28	9	102	192
10	43	179 ± 21	10	107	206
20	39	183 ± 18	5	111	216
100	35	257 ± 50	5	115	228
10	40	124 ± 16	10	110	137

Derlet-Dudarev-Björkas (DDB)
[PRB **76**, 054107 (2007); NIMB **267**, 3204 (2009)]

Ackland-Thetford-Juslin (ATJ)
[PhilMag A **56**, 15 (1987); JNM **432**, 61 (2013)]

- Compared to the friction model, ignoring ES overestimates N_F even though still reasonably within the standard errors.

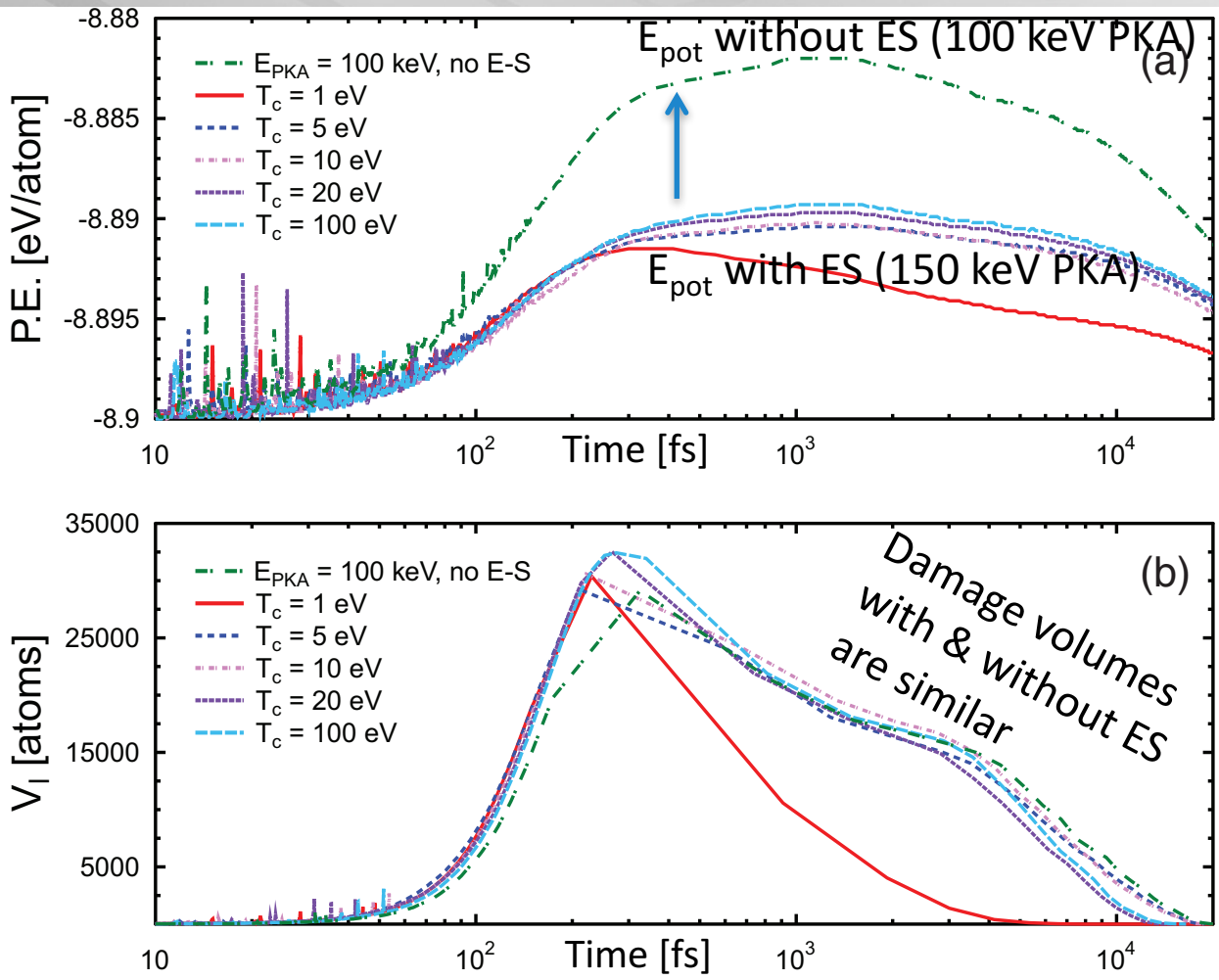
Electronic Loss Effect on Size Distribution of Defect Clusters in W

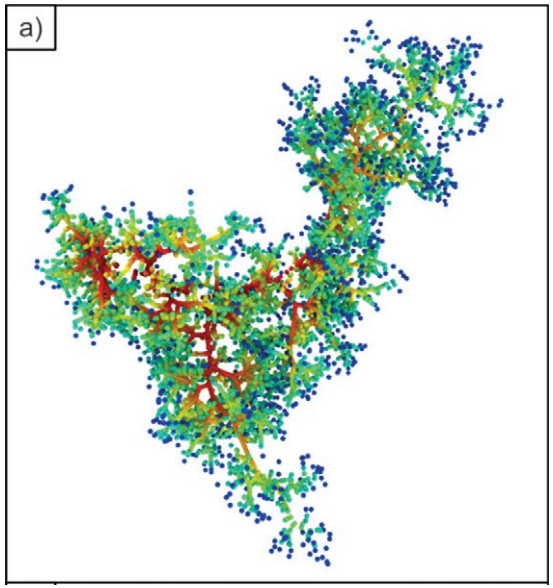


Large cluster probability is smaller with electronic loss.

A. E. Sand *et al*, EPL **115**, 36001 (2016).

A. Sand *et al*, EPL **103**, 46003 (2013).
A. Sand *et al*, JNM **455**, 207 (2014).





Path of energetic atoms from 0 fs (red) to 200 fs (blue) showing interconnected regions, consistent with our results.

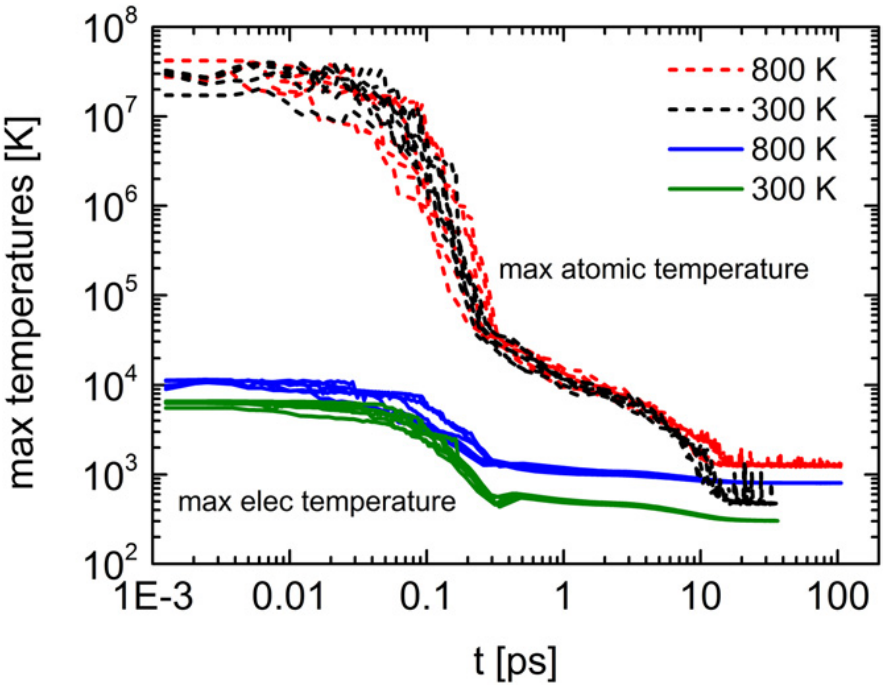
Ignoring ES increases potential energy → energy density → larger defect clusters.
Nevertheless, friction model also predicts interacting multiple-shock morphology.

Electron-Phonon Coupling Effect in Tungsten

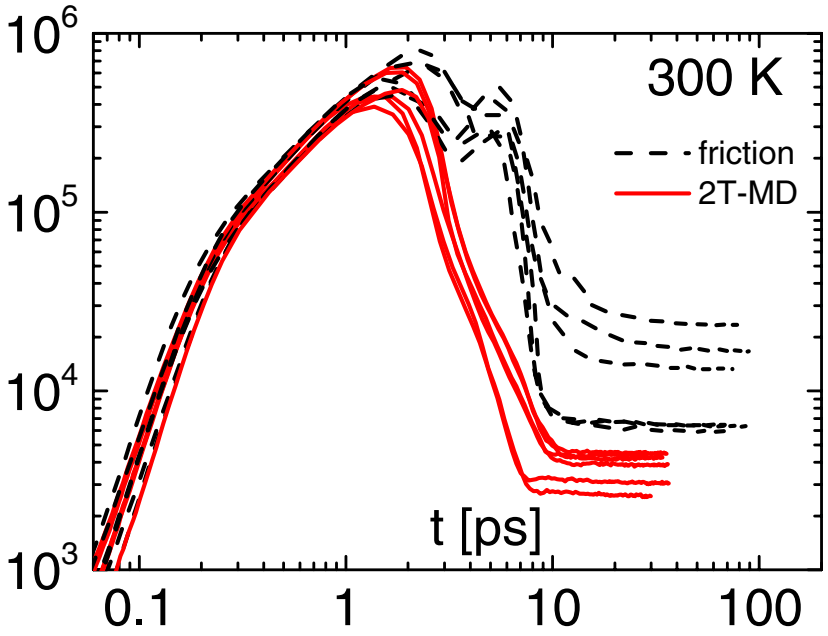
E. Zarkadoula *et al*, JPCM **27**, 135401 (2015).

2T-model = electronic stopping (friction model) + electron-phonon coupling

E_{PKA} = 300 keV with DDB potential.



N_{def}



Through out simulation, $T_{atom} > T_{electron}$ → electrons act as additional heat sinks.

N_{def} with 2T model < with friction model (note that the amount of net damage energy is not the same, hence the net effect of the 2T model is difficult to infer).

Summary

- Three cascade morphologies are observed:
  - Single-shock cascade (before sub-cascade).
  - Separate (non-interacting) multiple-shock (sub-cascade in Cr, Fe, Mo).
  - Interacting multiple-shock (connected sub-cascade in W) → formation of large clusters.
- A transition energy separates different energy regimes of cascade morphology:
  - different power-law in defect production and cluster size distributions.
  - Hence data should be fit with a bilinear curve.
- In simple bcc metals, the transition energy occurs at damage energy approximately $300E_d$.