Present state-of-the-art dpa models

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Acknowledgement

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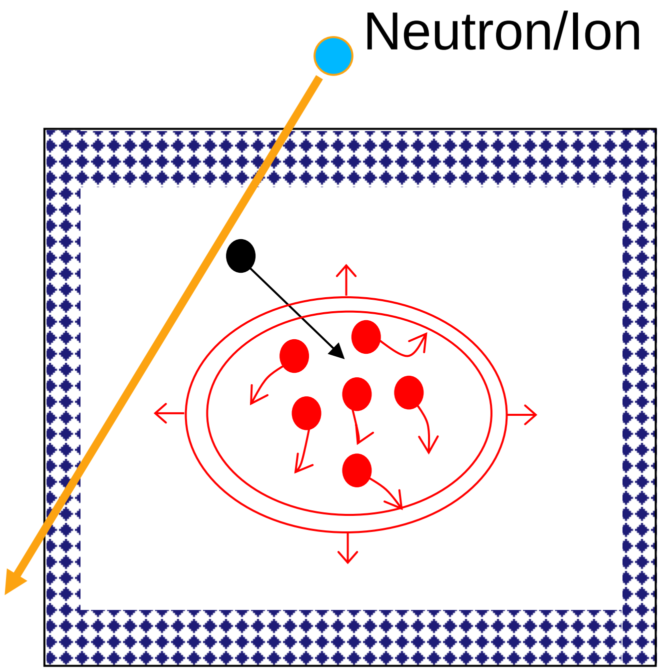
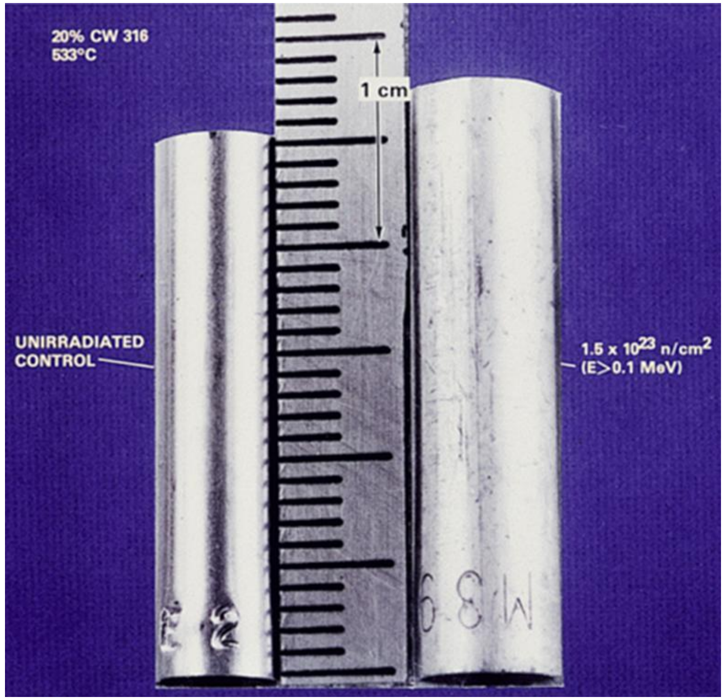
INTRODUCTION / MOTIVATION

- Neutrons/Ion will damage the reactor
- The primary damage is formed as the incoming particle hits a lattice atom and gives it recoil energy
- This can/will then cause macroscopic changes to the material

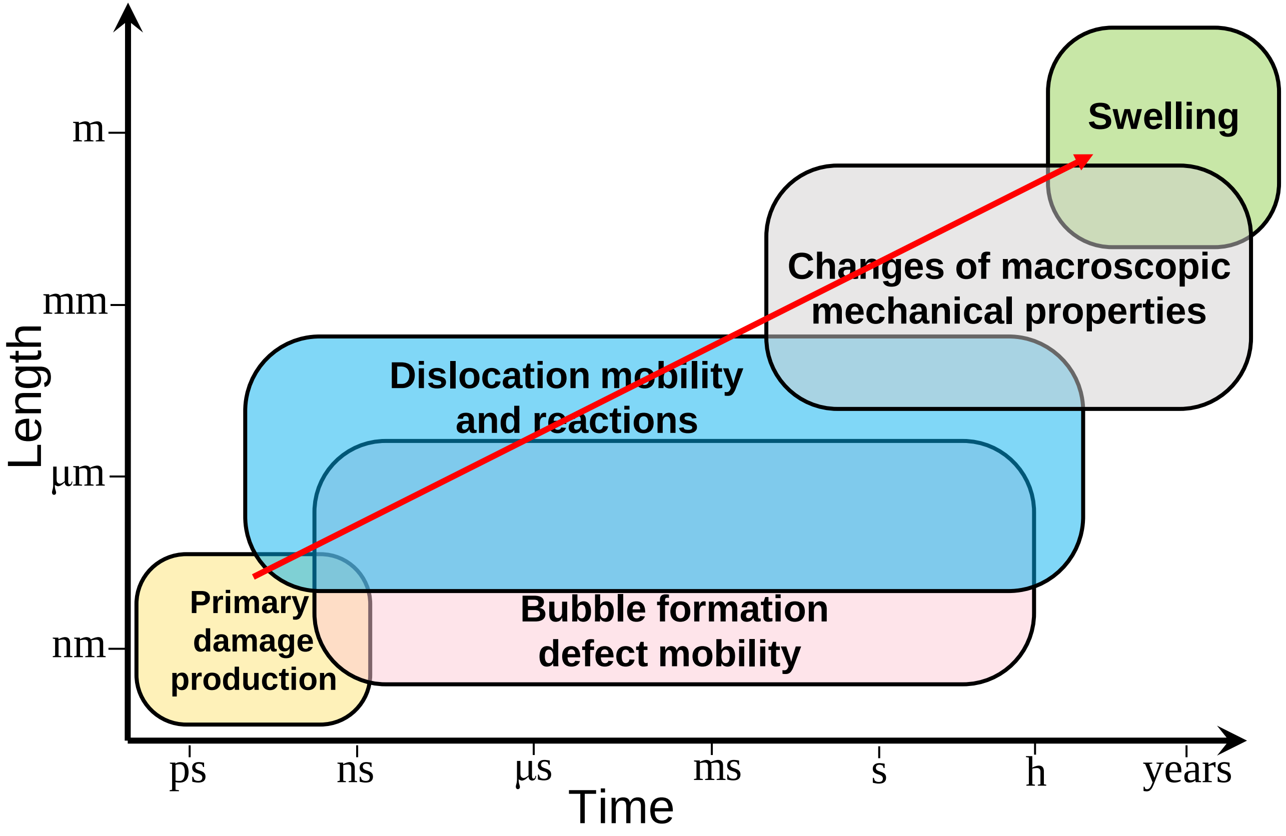




Straalsund J L, et al. J. Nucl. Mater. 108/109 299-305 (1982)

INTRODUCTION / MOTIVATION

- The primary damage will then evolve and ultimately cause macroscopic changes
- But it is clear that to understand the macroscopic behavior we need to understand the primary damage
- Also, the ”dose” we use to quantify the damage at large scale is related directly to the primary damage

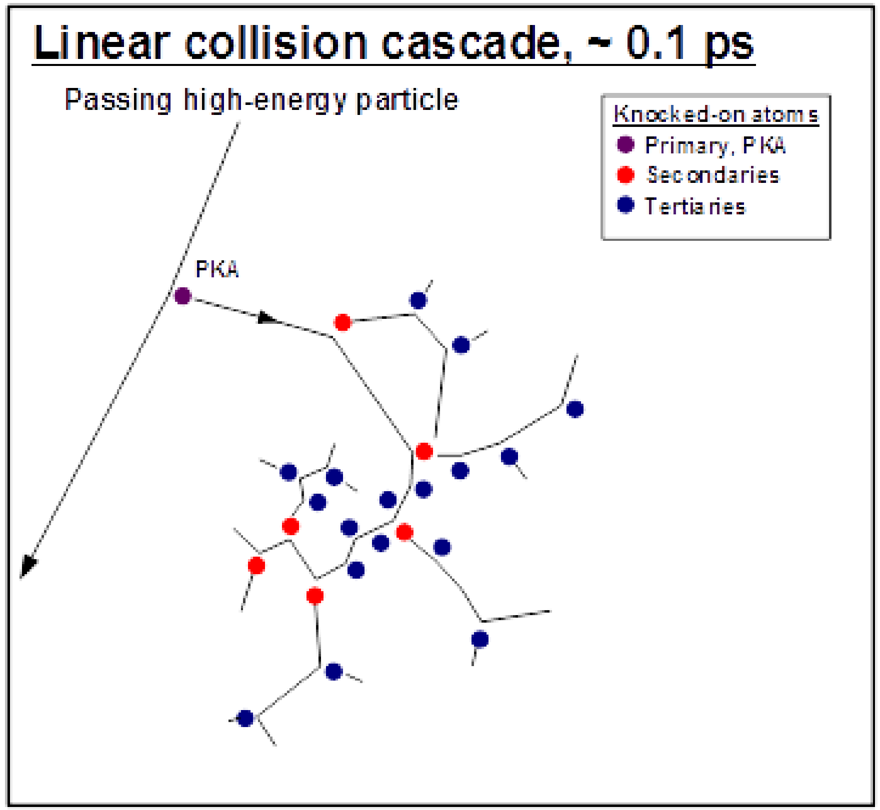


DISPLACEMENTS PER ATOM / DPA
NRT-dpa

- If radiation damage would be only formed in a sequence of binary collisions, it should scale linearly with damage energy T_d
- This leads to the NRT-dpa equation for the number of defects N_d

$$N_\mathrm{d}(T_\mathrm{d}) = \begin{bmatrix} 0 & , & T_\mathrm{d} < E_\mathrm{d} \\ 1 & , & E_\mathrm{d} < T_\mathrm{d} < \dfrac{2E_\mathrm{d}}{0.8} \\ \dfrac{0.8T_\mathrm{d}}{2E_\mathrm{d}} & , & \dfrac{2E_\mathrm{d}}{0.8} < T_\mathrm{d} < \infty \end{bmatrix}$$

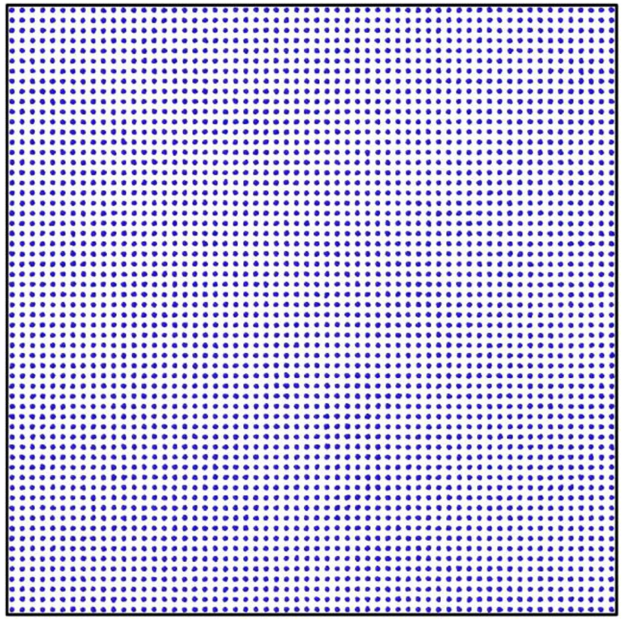
M. J. Norgett et al. Nuc. Eng. Des. 33 (1975) 50-54

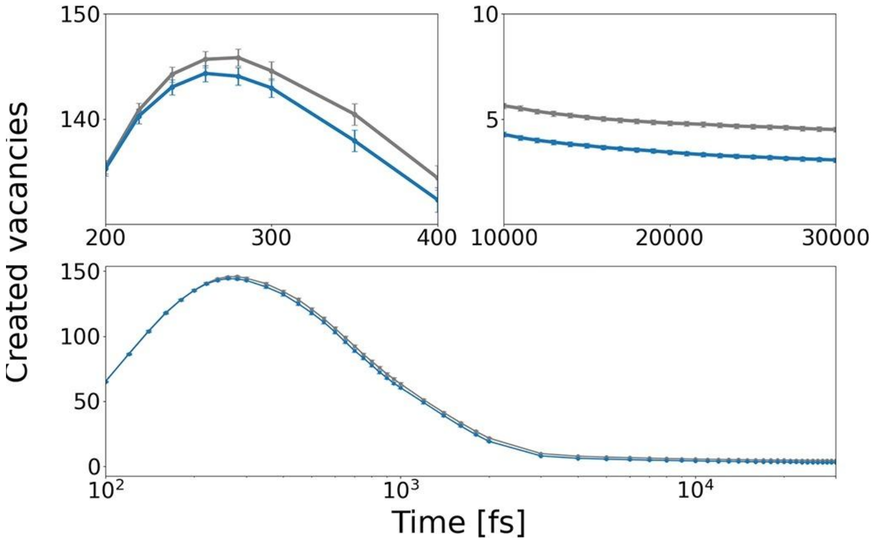


K. Nordlund et al. J. Nucl. Mater. 512 (2018) 450-479

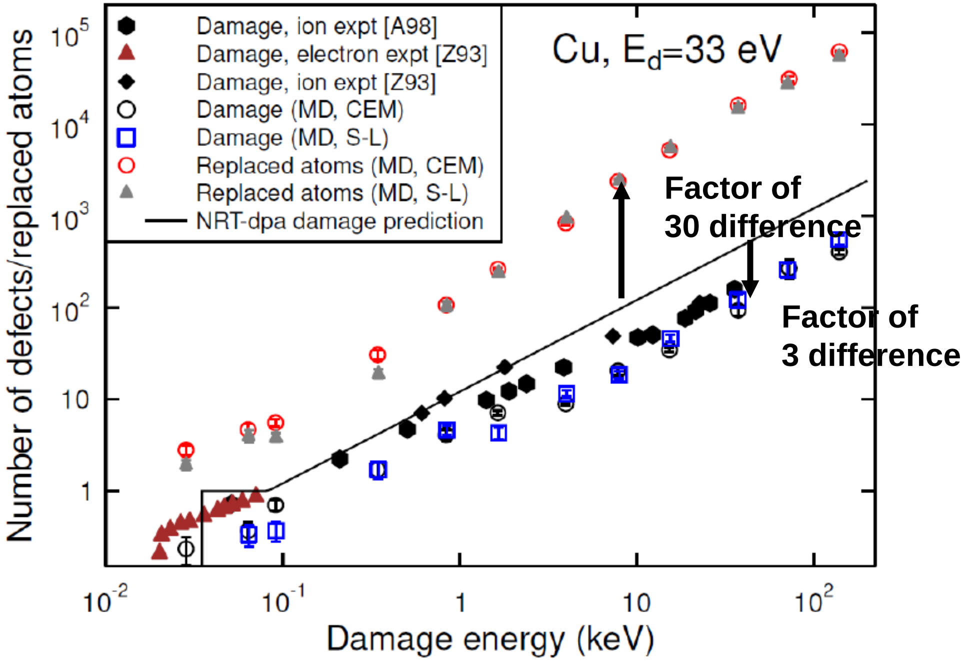
DISPLACEMENTS PER ATOM / DPA
Problems with NRT-dpa

- The PKA event is not a binary collision sequence, but a many-body problem





V. Lindblad et al. J. Nucl. Mater. 603 (2025) 155422



K. Nordlund et al. J. Nucl. Mater. 512 (2018) 450-479

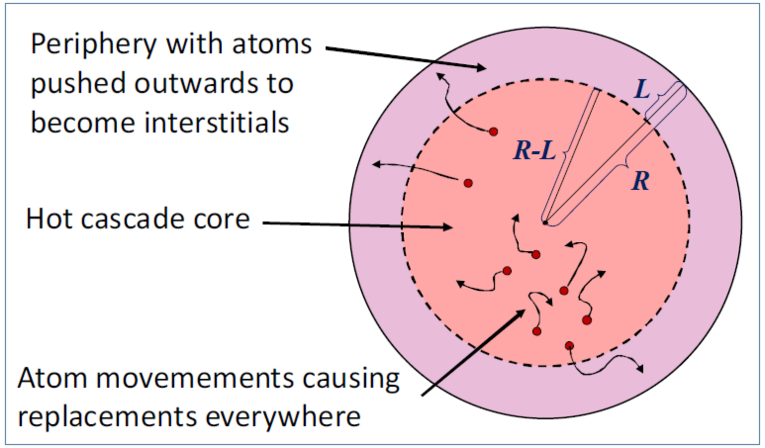
DISPLACEMENTS PER ATOM / DPA
Why a improved analytical model is needed

- The MD simulations are easily doable thanks to modern computers, and can in principle replace NRT-dpa
- However, for parameterizing higher-scale models (neutronics damage models, FEM, …) it is not really feasible to do MD simulations for every recoil
- If a simple analytical model can be fit to the data, huge advances are gained:
  - Analytical equation: **nanosecond on one core**
  - MD simulation: **one week on thousand cores**

DISPLACEMENTS PER ATOM / DPA
arc-dpa

- Considering the heat spike as two spherical zones with perfect recombination inside ***R*,** and a shell ***R-L*** with surviving interstitials, the surviving defect fraction:

$$\xi_{\mathrm{survive}} = \frac{V_{\mathrm{outer}} - V_{\mathrm{inner}}}{V_{\mathrm{outer}}} = \frac{\frac{4\pi R^3}{3} - \frac{4\pi (R-L)^3}{3}}{\frac{4\pi R^3}{3}} = 3\frac{L}{R} - 3\frac{L^2}{R^2} + \frac{L^3}{R^3} \approx 3\frac{L}{R}$$



- The cascade radius is $R \propto T_{\mathrm{d}}^{x}$ where x < 1
- Then $N'_{\mathrm{d}}(T_{\mathrm{d}}) \frac{0.8T_{\mathrm{d}}}{2E_{\mathrm{d}}} \xi_{\mathrm{survive}} = \frac{0.8T_{\mathrm{d}}}{2E_{\mathrm{d}}} 3\frac{L}{R} \propto \frac{0.8T_{\mathrm{d}}}{2E_{\mathrm{d}}} 3\frac{L}{T_{\mathrm{d}}^{x}} \propto T_{\mathrm{d}}^{1-x}$
- At high energies cascades split into sub-cascades

-> linear, and demanding consistency with the

NRT-dpa at the threshold, one arrives at the final form

$$\xi_{\mathrm{arcdpa}}(T_{\mathrm{d}}) = \frac{1 - c_{\mathrm{arcdpa}}}{(2E_{\mathrm{d}}/0.8)^{b_{\mathrm{arcdpa}}}} T_{\mathrm{d}}^{b_{\mathrm{arcdpa}}} + c_{\mathrm{arcdpa}}$$

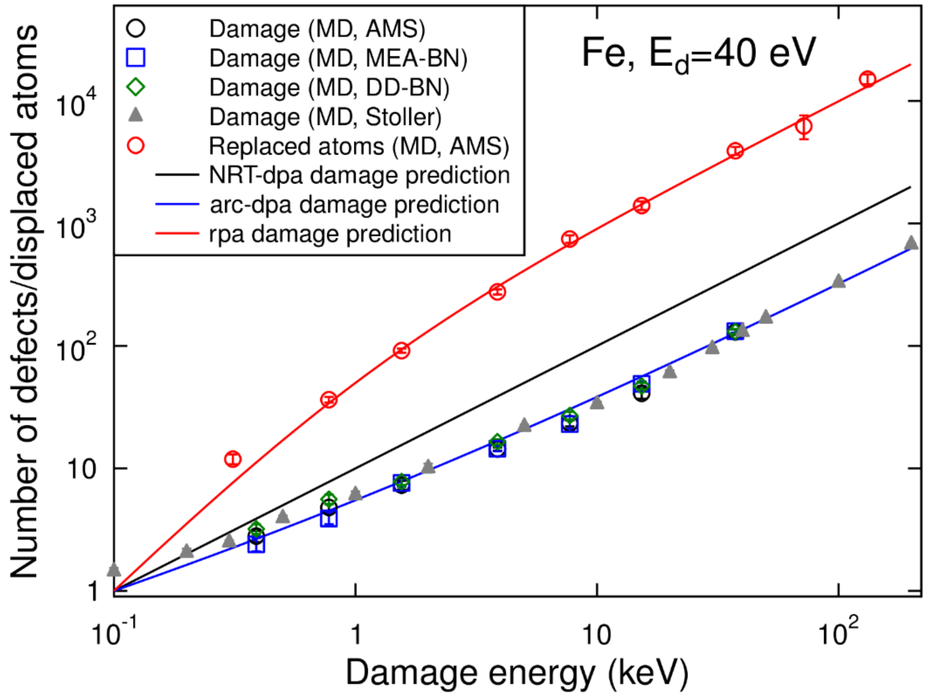
K. Nordlund et al. Nat. Commun. 9 (2018) 1084

DISPLACEMENTS PER ATOM / DPA
rpa

- Consider now the atomic mixing (replacements)
- It is actually a very good approximation that all atoms within the core are replaced. Hence simply $N \propto R^3$.
- Combining this with the previously noted $R \propto T_d^x$, and demanding linearity:

$$\xi_{\mathrm{rpa}}(T_{\mathrm{d}}) = \left(\frac{b_{\mathrm{rpa}}^{c_{\mathrm{rpa}}}}{(2E_{\mathrm{d}}/0.8)^{c_{\mathrm{rpa}}}} + 1\right)\frac{T_{\mathrm{d}}^{c_{\mathrm{rpa}}}}{b_{\mathrm{rpa}}^{c_{\mathrm{rpa}}} + T_{\mathrm{d}}^{c_{\mathrm{rpa}}}}$$

- We need four parameters in addition to the threshold displacement energy per material



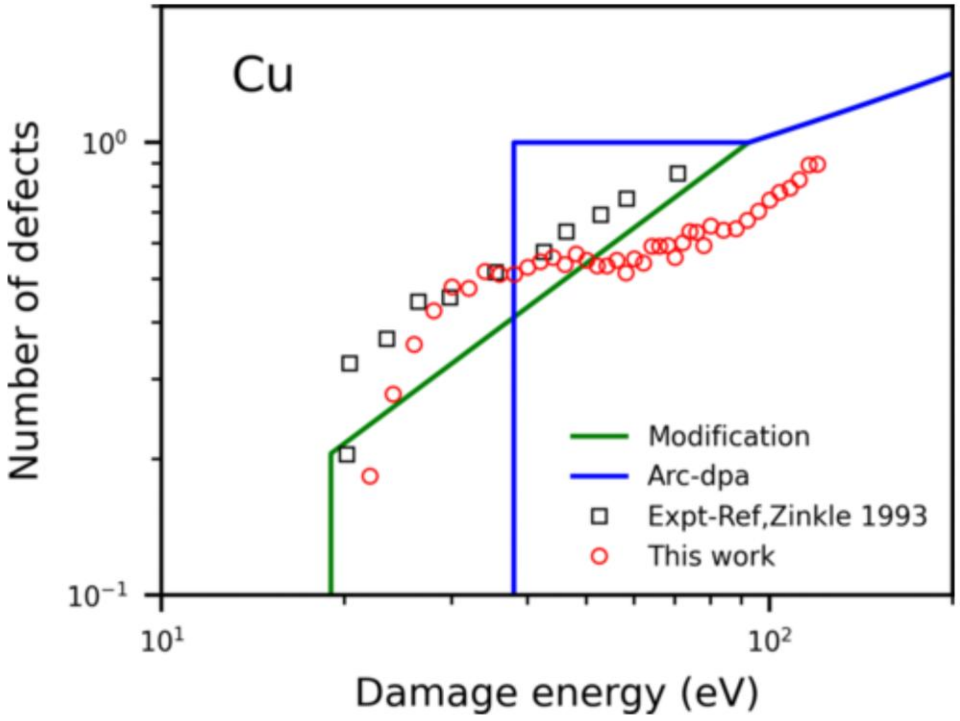
K. Nordlund et al. Nat. Commun. 9 (2018) 1084

DISPLACEMENTS PER ATOM / DPA
Limitation of arc-dpa -> full energy range dpa

- The hard cut-off at the E_d
  - E_d an average energy needed, not the minimum
  - In an alloy, this is also PKA specific
  - Linear correction to the minimum added

$$N_d(E) = \begin{bmatrix} 0 & E < E_d \\ 1 & E_d < E < 2E_d/0.8 \\ \frac{0.8E}{2E_d}\xi(E) & 2E_d/0.8 < E < \infty \end{bmatrix}$$

$$N_d(T_d) = \begin{cases} 0, & T_d < E_d^{\min} \\ \frac{0.8T_d}{2E_d^{\text{avr}}}, & E_d^{\min} < T_d < \frac{2E_d^{\text{avr}}}{0.8}, \\ \frac{0.8T_d}{2E_d^{\text{avr}}}\xi(T_d), & \frac{2E_d^{\text{avr}}}{0.8} < T_d \end{cases}$$



Q. Yang and P. Olsson, Phys. Rev. Mater. 5 (2021) 073602

DISPLACEMENTS PER ATOM / DPA
Limitation of arc-dpa -> crc-dpa

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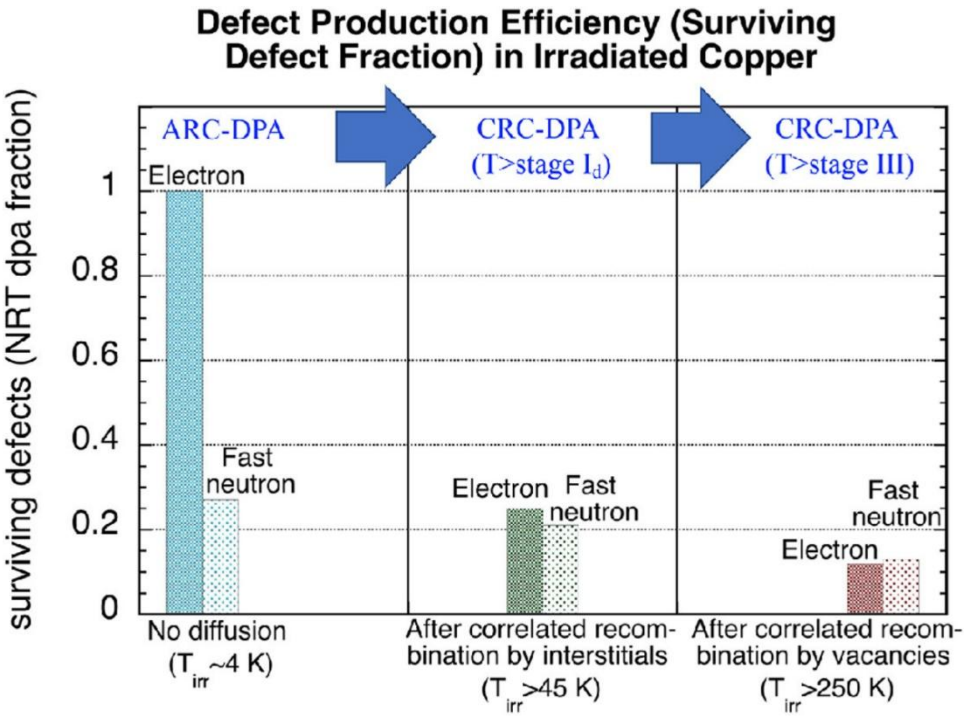
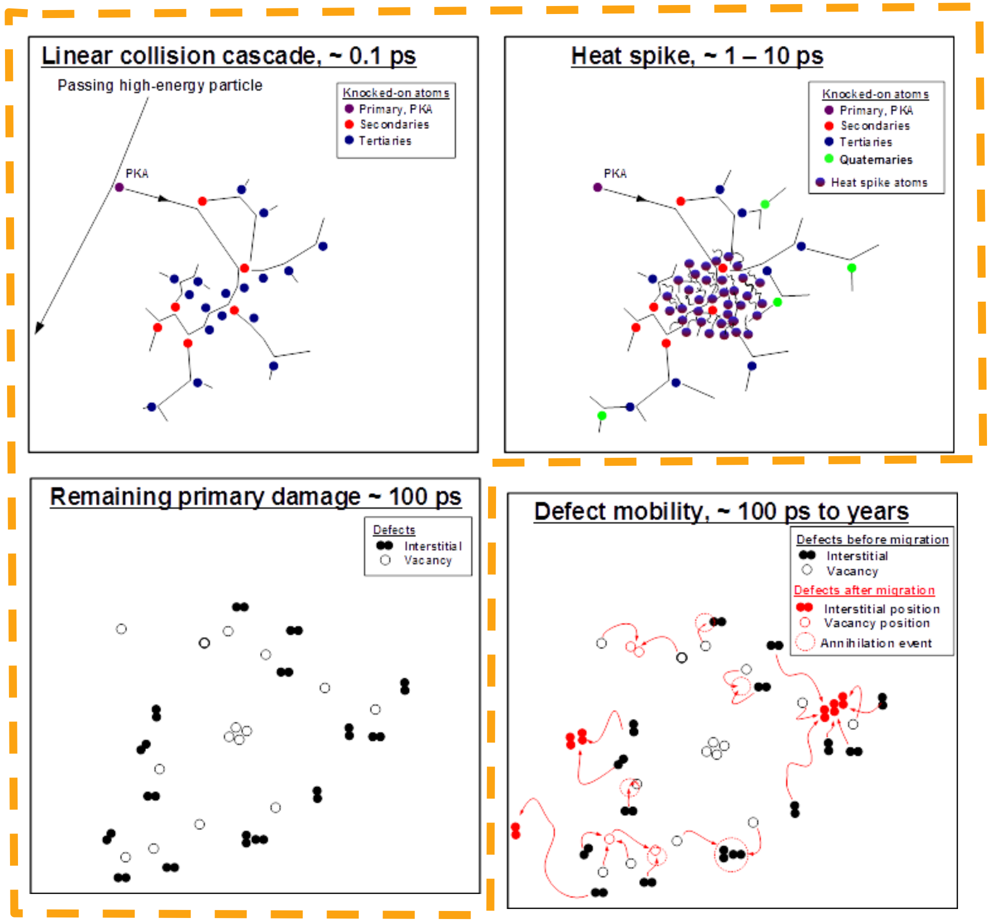
- Defect mobility: taking into account correlated movement of interstitials and vacancies, separately.





S. J. Zinkle and R. E. Stoller, J. Nucl. Mater. 577 (2023) 154292

DISPLACEMENTS PER ATOM / DPA
Current status

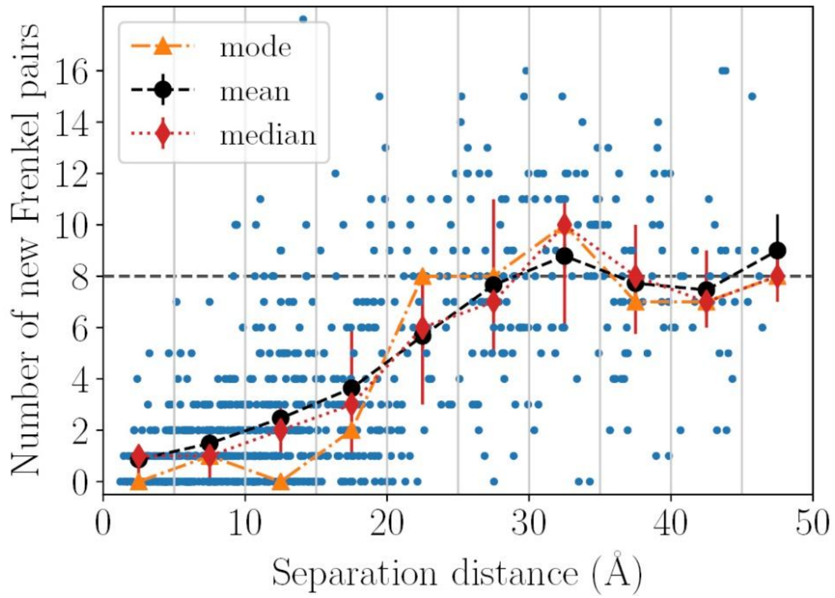
- With current models we can take into account the:
  - Defects produced from binary collisions (NRT-dpa) [1]
  - Account for the heat-spike [2,3]
    - Corrects real damage (arc-dpa)
    - and replacements (rpa)
  - Correction to low energy regime, full energy range dpa [4]
  - Account for thermal correlated movement, crc-dpa [5]
- What is still missing:
  - Defect production a range, not exact value/morphology
  - High energies, stable defect clusters can form

[1] M. J. Norgett et al. Nuc. Eng. Des. 33 (1975) 50-54
[2] K. Nordlund et al. Nat. Commun. 9 (2018) 1084
[3] K. Nordlund et al. J. Nucl. Mater. 512 (2018) 450-479
[4] Q. Yang and P. Olsson, Phys. Rev. Mater. 5 (2021) 073602
[5] S. J. Zinkle and R. E. Stoller, J. Nucl. Mater. 577 (2023) 154292

LIMITATIONS
Cascade overlap

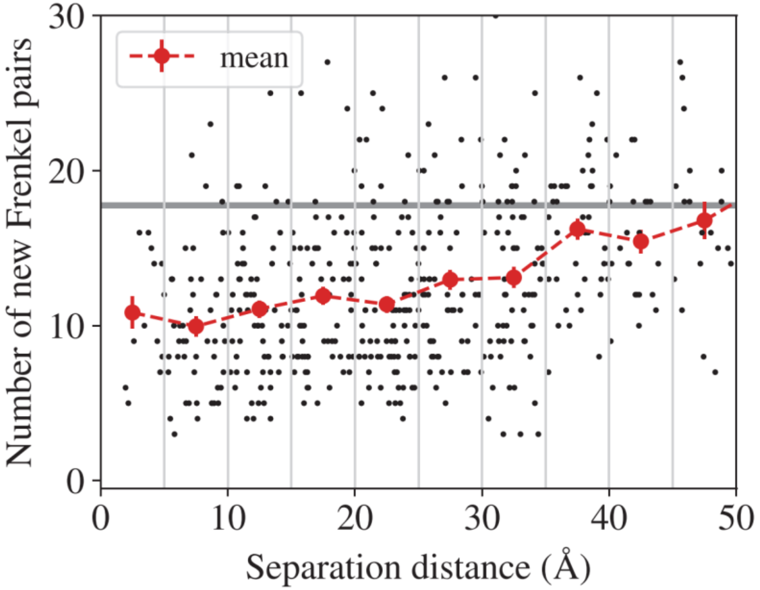
- The dpa models can account for single PKAs in pristine material, however…
  - The dose is micro- to milli-dpa, maybe not relevant

Interstitials



J. Byggmästar et al. J. Phys. Condens. Matter 31 (2019) 245402

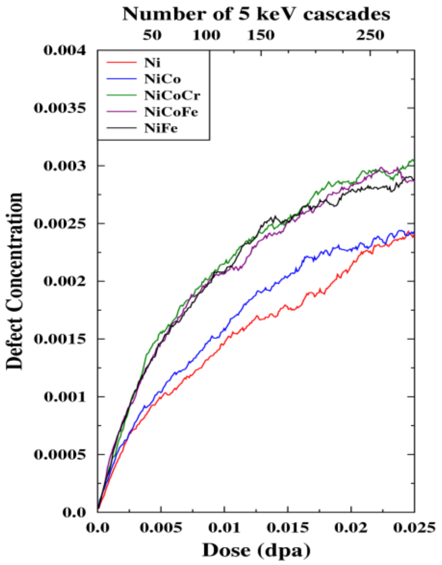
Vacancies

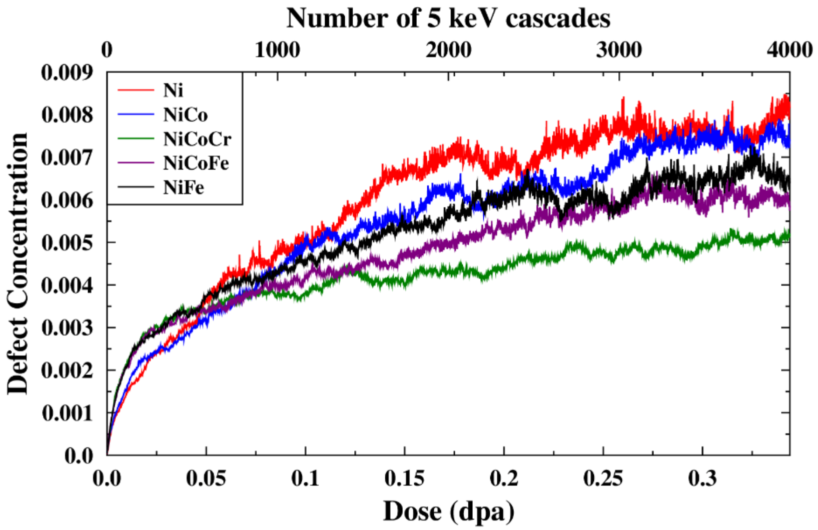


F. Granberg et al. Eur. Phys. J. B. 92 (2019) 146

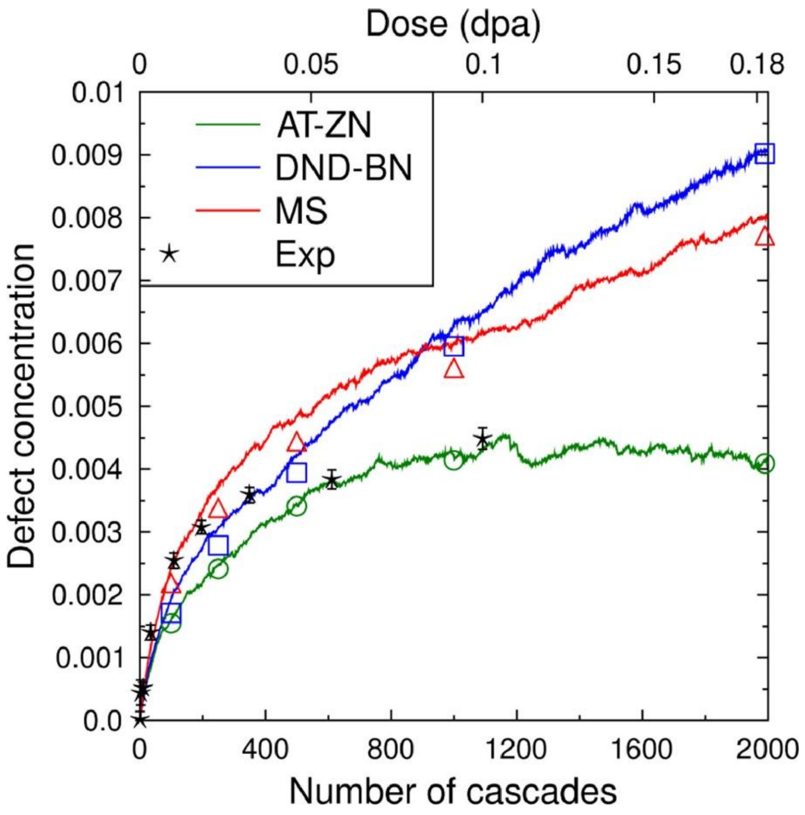
LIMITATIONS
Cascade overlap/High-dose simulations

- The dpa estimate only applies when there is practically no cascade overlap





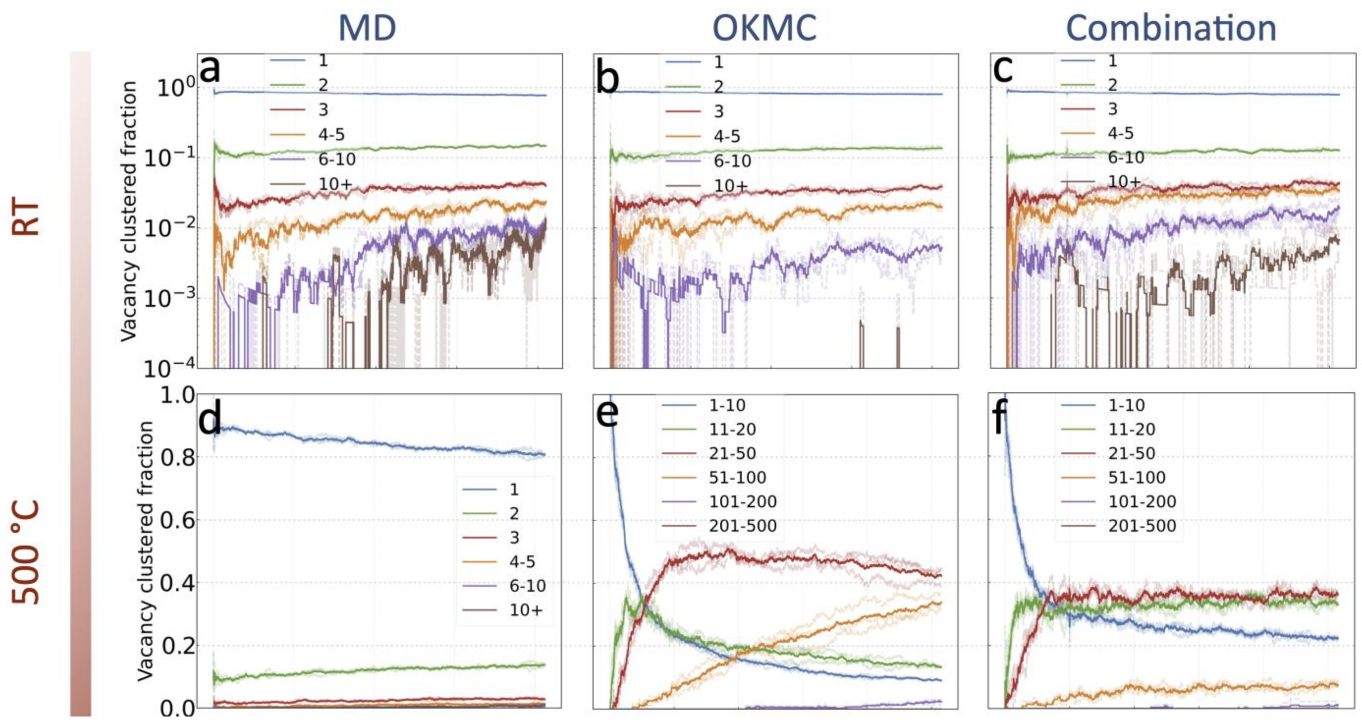
E. Levo et al. J. Nucl. Mater. 490 (2017) 323-332



F. Granberg et al. J. Nucl. Mater. 556 (2021) 153158

EXAMPLE: Multiscale modelling Need for ”cascade overlap”

- Utilize DFT-based ML potentials to carry out MD cascades and utilize OKMC to evolve the time to experimental ones.
- Initial studies, on W, show that utilizing only OKMC with a MD database is not giving the same evolution as the full combination



J. Wu et al. https://arxiv.org/abs/2409.15856

CONCLUSIONS

- The NRT-dpa value is still the most used measure for dose, used for comparison
- Better models do exist to predict the real damage or displacements
  - Considering heat-spike/recombination and long-term diffusion
- In single elements replacements are quite useless, however, in complex materials the replacements can be the real defects
- Current limit is high energies (material specific), where complex defects can form
- Still, the limit is when the PKA is not anymore in a pristine material
  - This happens quickly as the dose increases
  - Practically only solution is full simulations instead of analytical models

  ➔ We still need full-scale high-energy and high-dose simulations!

THANK YOU FOR YOUR ATTENTION