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# A spatially resolved stochastic cluster dynamics approach for simulating radiation damage accumulation in α-Fe


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## Abstract


In this work, a novel spatially resolved stochastic cluster dynamics (SRSCD) model is developed for simulating radiation damage accumulation irradiated metals in a three-dimensionally resolved fashion. Particular interest is placed the following challenges: (1) introduction of displacement cascades in a numerically efficient manner while accounting for spatially correlated reactions between defects, (2) accounting for interactions between defects already present in the material and cascades during the thermal spike phase, and (3) choosing appropriate cascade energies that reflect damage accumulation due to high-energy neutrons. Further, a numerical strategy relying on a synchronous parallel kinetic Monte Carlo algorithm is presented to extend the capabilities of the method. SRSCD is applied to the test case of neutron irradiation of α-Fe and results are compared to experimental results over the range of doses studied here. The computational efficiency and accuracy of this technique is discussed in light of several examples.


## SRSCD Description

$$\left(\frac{dC}{dt}\right)\left(\frac{V}{\Omega}\right)=\frac{dN}{dt}$$

$$A=\sum_{\mu}A_{\mu}$$

$$\tau=\frac{1}{A}\ln\left(\frac{1}{r_1}\right),\quad \sum_{\nu=1}^{\mu-1}A_{\nu}<r_2A\le\sum_{\nu=1}^{\mu}A_{\nu}$$

- Convert concentration rate equations from rate theory into number rate equations in a simulated volume
- Compile reaction rates $A_\mu$ for allowed reactions
- Choose reaction $\mu$ and timestep $\tau$ using kinetic Monte Carlo (KMC) algorithm

## Synchronous Parallel Kinetic Monte Carlo

$$A_{max}=\max_{d}\{A^d\}$$

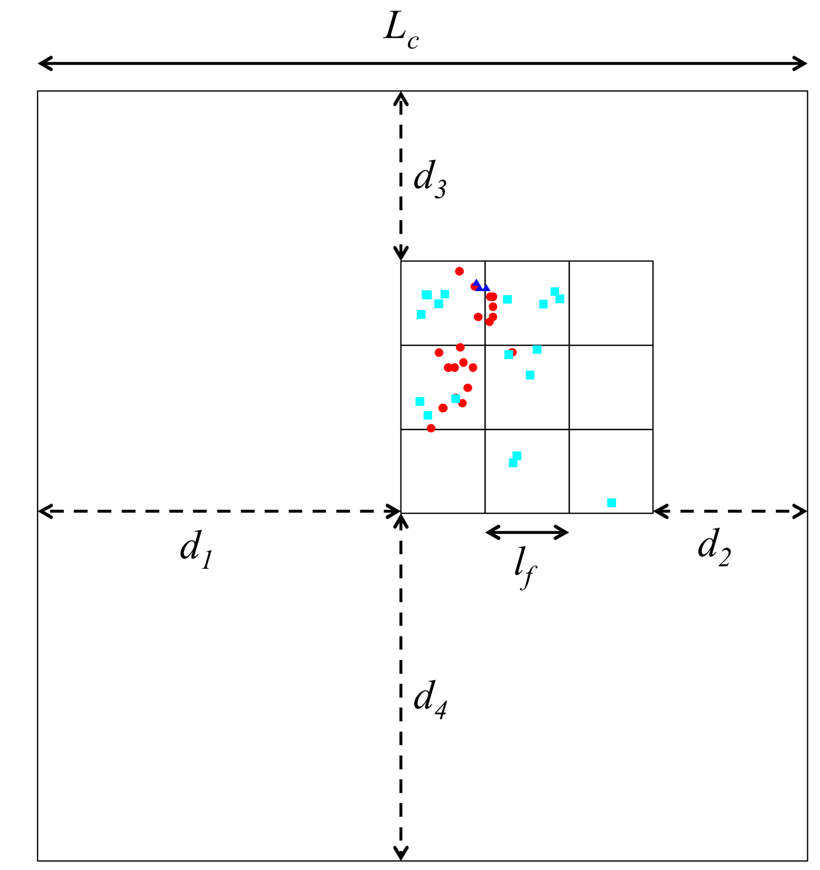
$$A_0^d=A_{max}-A^d$$

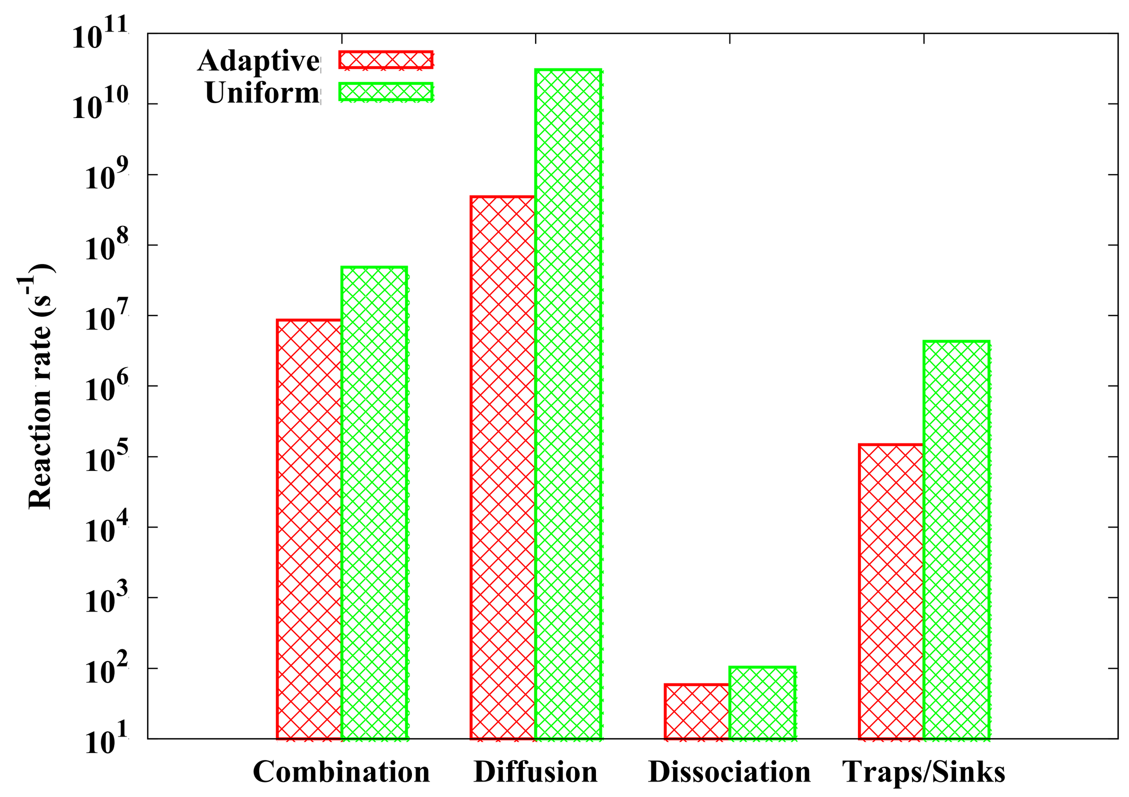
$$\tau=\frac{1}{A_{max}}\log\left(\frac{1}{r_1}\right)$$

$$\sum_{\nu=0}^{\mu-1}A_{\nu}^d<r_2^dA_{max}\le\sum_{\nu=0}^{\mu}A_{\nu}^d$$

- Find total reaction rate $A^d$ in each sub-domain $d$
- Find max total reaction rate across all sub-domains
- Create *null event* in each sub-domain so that $A^d$ is the same in each sub-domain
- Choose a global timestep and a local reaction in each sub-domain (including null events)

## Adaptive Meshing

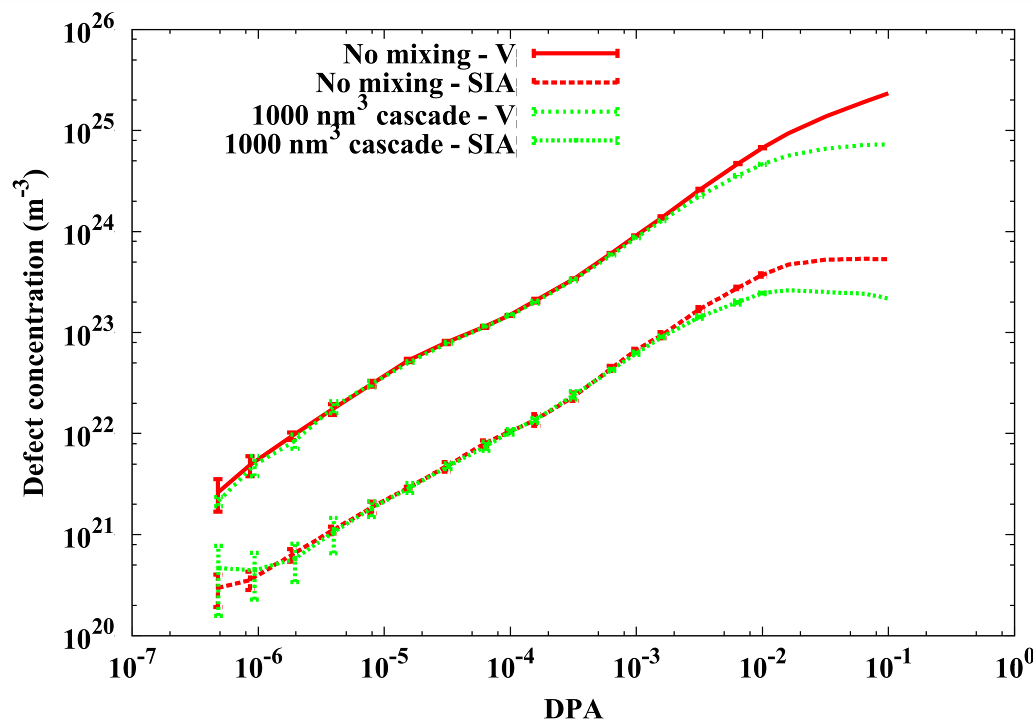


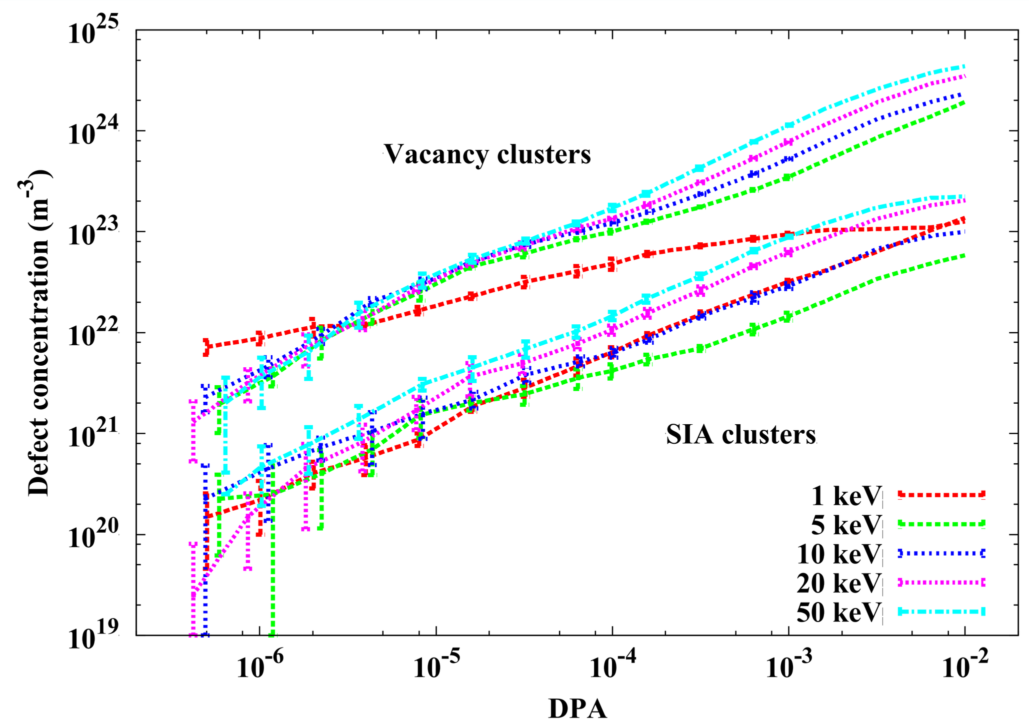




- When cascade event is chosen, create fine mesh within coarse mesh element
- When cascade is annealed, remove fine mesh and place defects within coarse mesh

- Comparison between total reaction rates using adaptive meshing scheme and uniform 5 nm mesh
- Adaptive meshing gives significant reduction in reaction rates and therefore computation time

## Effect of Cascade-Defect Interactions and Cascade Energy

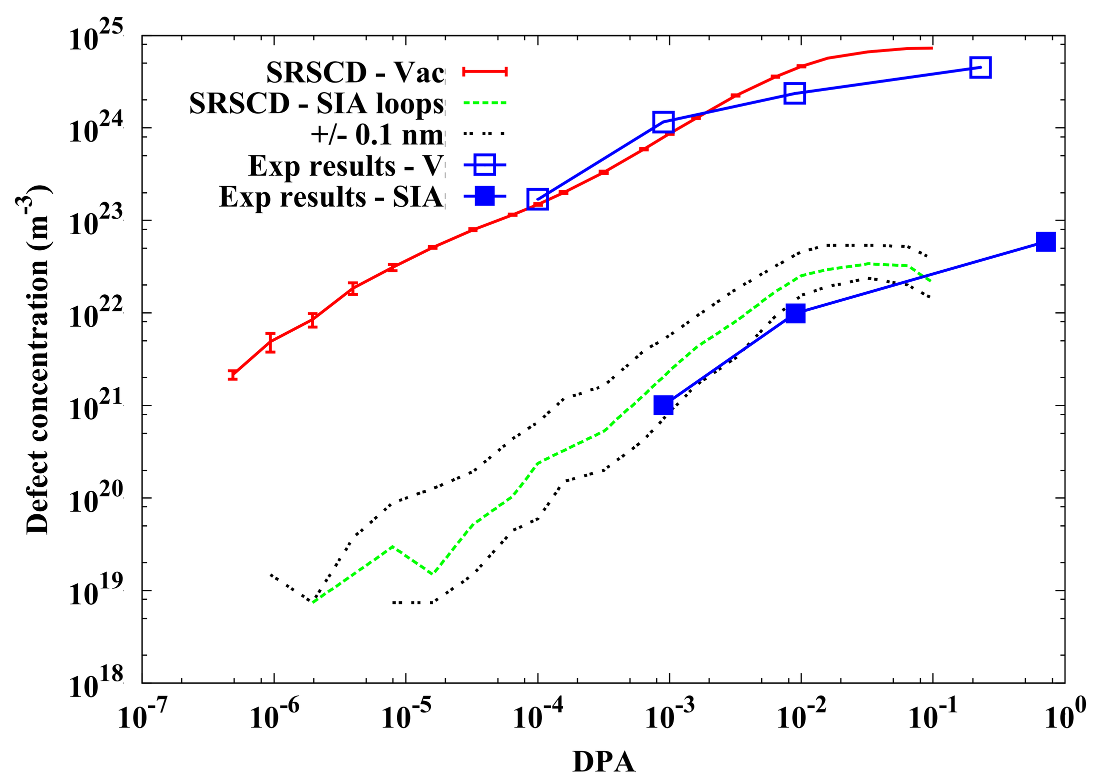



- Allowing cascades to mix with defects already present
- Effect significant by $10^{-2}$ dpa, stronger for larger cascades

- Higher energy cascades have large number of defects and clusters
- Similar behavior for cascades > 5 keV

## Application: Neutron Damage in Room Temperature Irradiated α-Fe

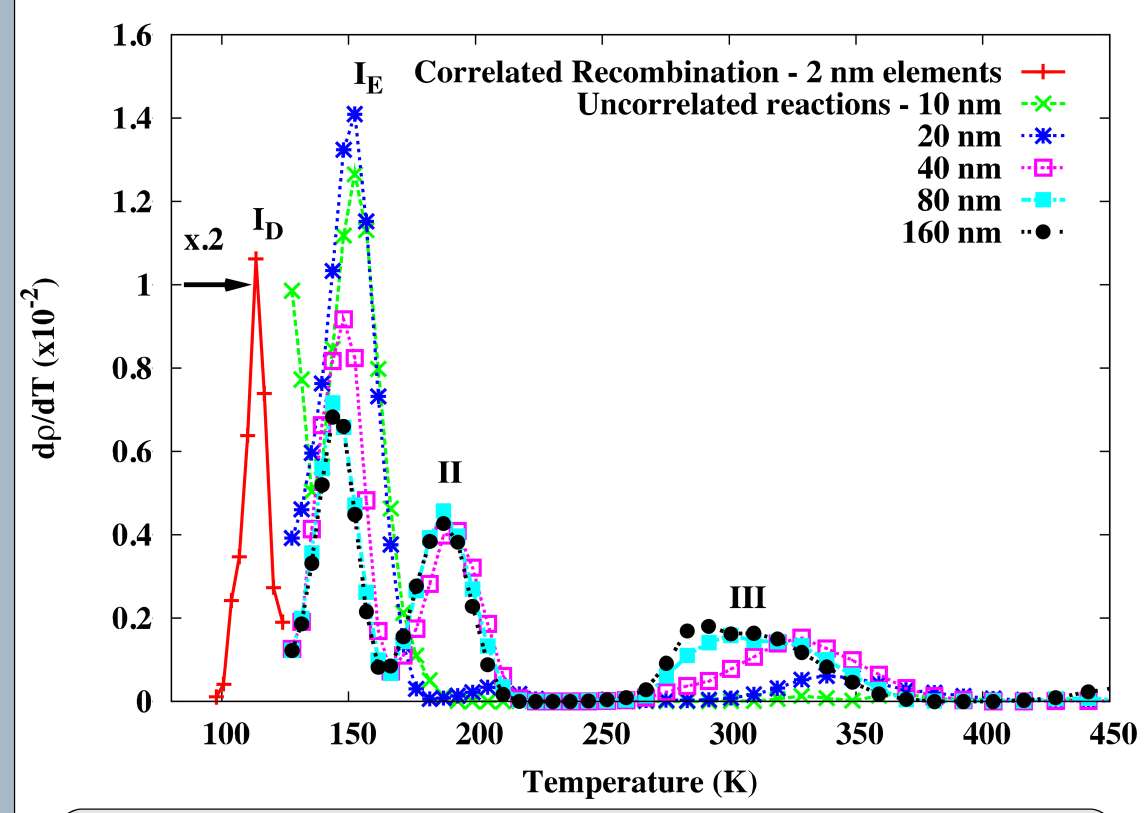



- Using adaptive meshing scheme, cascade-defect interactions, and 20 keV cascades, simulated damage in bulk α-Fe to $10^{-1}$ dpa

- Results show qualitative agreement with experimental results from neutron irradiation (blue, Eldrup et al. (2002))

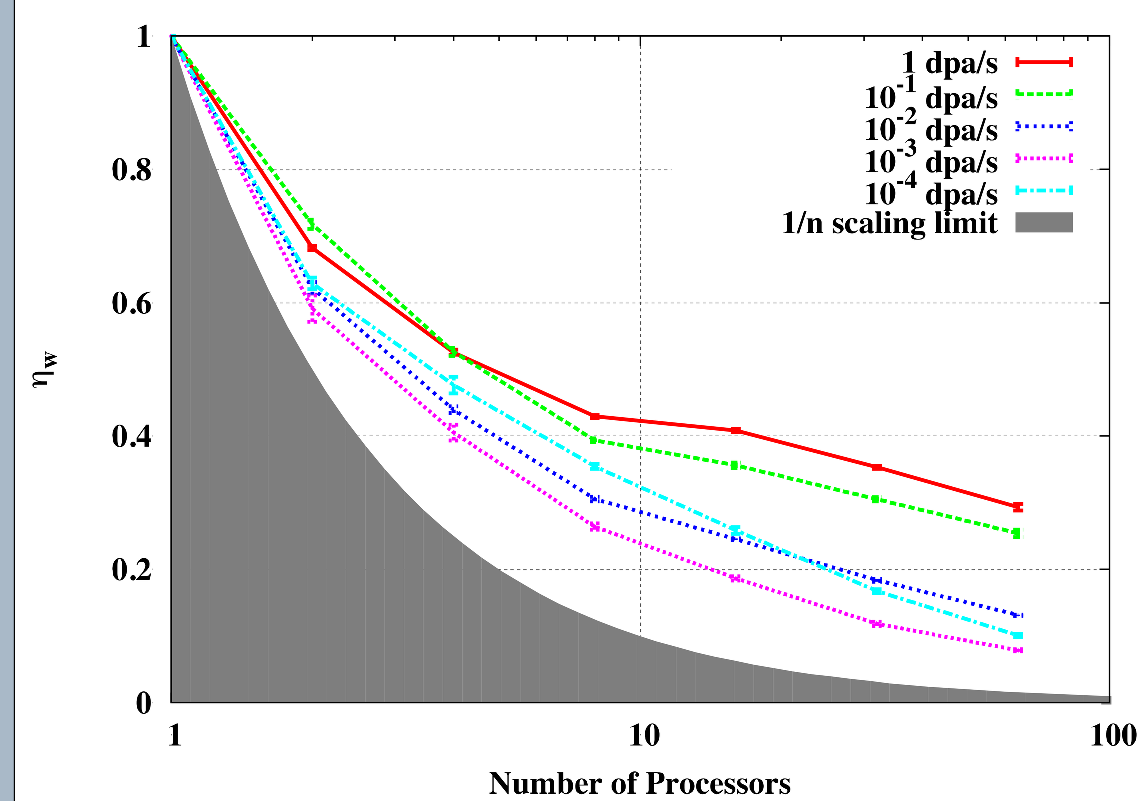
- Differences likely due to details in cascade-defect interaction process not addressed here

## Effect of Spatially Correlated Reactions: Resistivity Recovery in Frenkel Pair Irradiated α-Fe




- Electron irradiation of α-Fe at low temperatures followed by annealing gives peaks in resistivity recovery when different mechanisms are activated (Takaki et al. (1983), Fu et al. (2004)).
- Standard cluster dynamics does combines peaks $I_D$ and $I_E$ (Dalla Torre et al. (2006)): correlated and uncorrelated recombination of Frenkel pairs
- SRSCD reproduces correlated recombination peak due to spatial resolution

## Weak Scaling of SRSCD in Parallel KMC Configuration




- Measure of parallel performance of SRSCD
- $\eta_w$ defined as time to run a simulation with 1 domain size $d$ in serial divided by time to run a simulation with $n$ domains size $d$ in parallel using $n$ processors
  - **Perfect scaling**: $\eta_w=1$ (no slowdown due to increasing computational domain)
  - **Worst case**: $\eta_w=1/n$ (no benefit from parallel algorithm)
- **Results**: scaling dependent on dose rate due to non-homogeneous distribution of reaction rates in domains (null events)