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Spatially resolved simulation of damage accumulation in nanocrystalline metals

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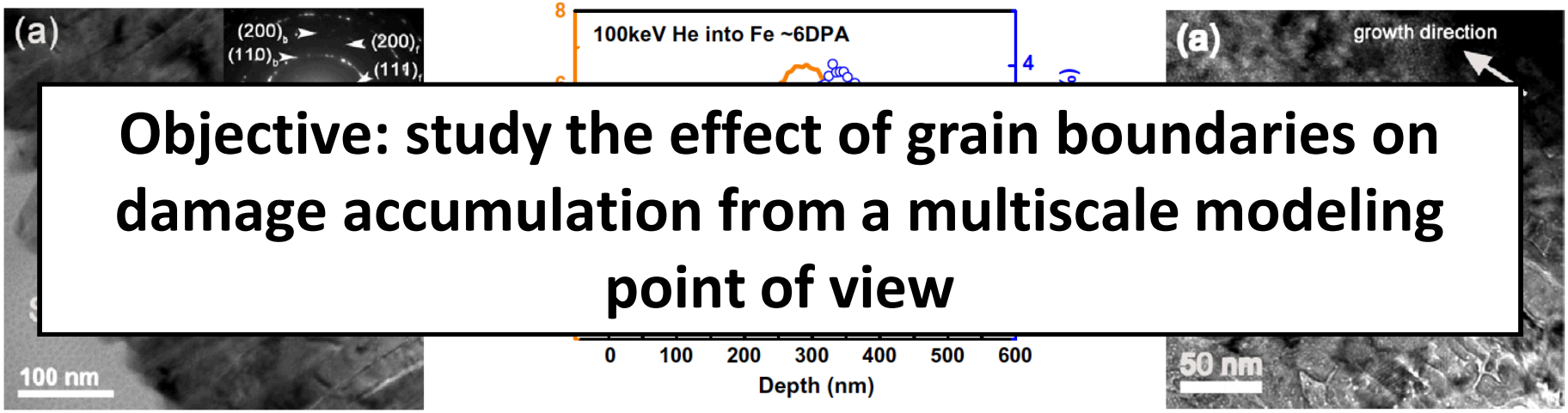
Outline

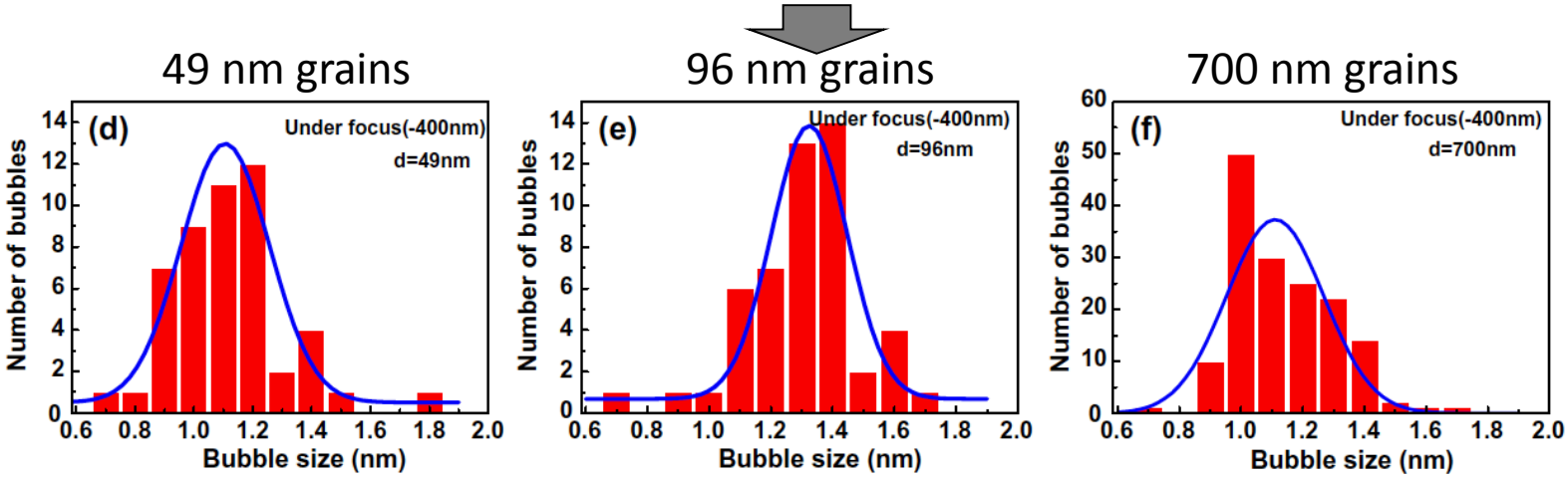
1. Motivation: radiation damage in nanostructured metals
2. Spatially Resolved Stochastic Cluster Dynamics (SRSCD): an efficient computational tool for simulating damage accumulation
3. Damage accumulation in polycrystalline Fe: effect of grain size
4. Impact of grain boundary defect behaviors on defect accumulation and sink efficiency: multivariate statistical analysis
   - Two-variable studies
   - Principal Component Analysis

Radiation damage in nanostructured metals



Objective: study the effect of grain boundaries on damage accumulation from a multiscale modeling point of view

Helium ion irradiation of nanocrystalline Fe thin films - He bubble growth Yu et al. (2012)

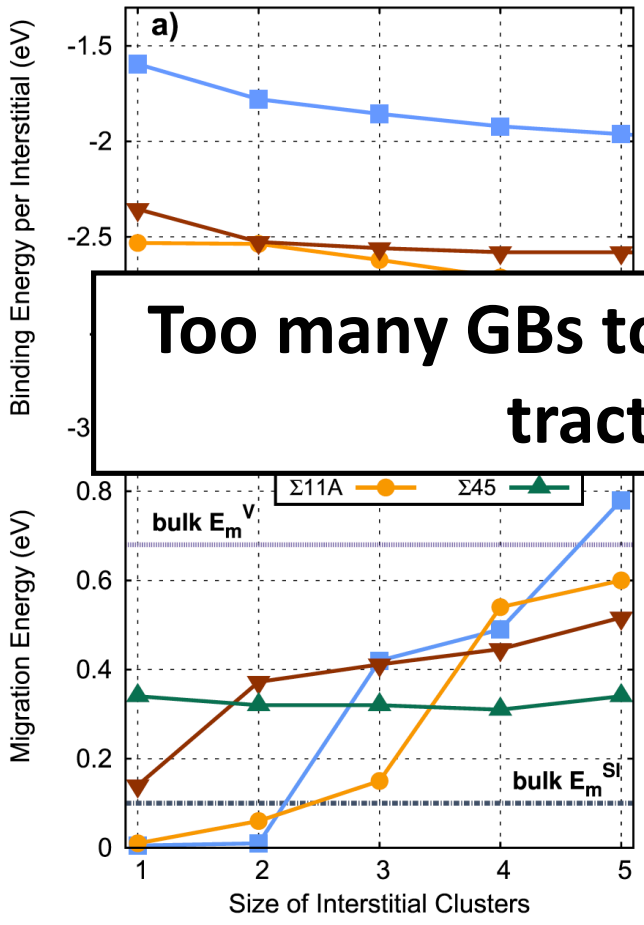


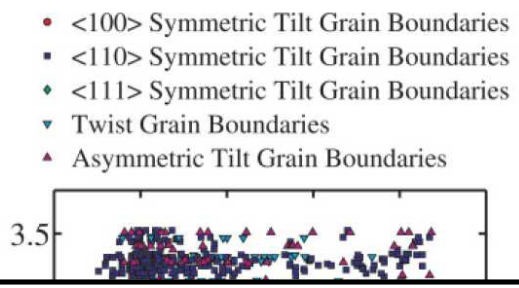
Defect behaviors at grain boundaries

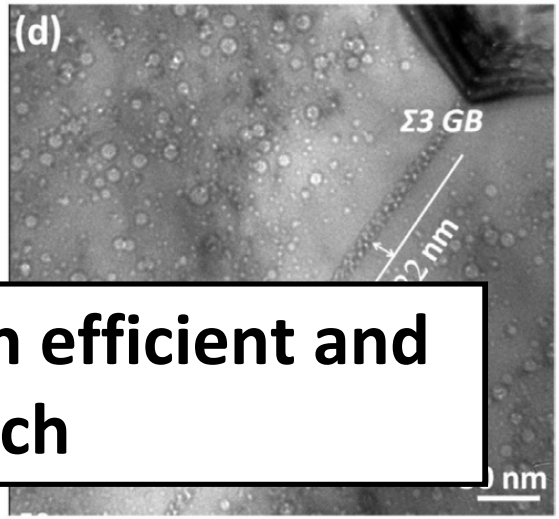
Diffusion and clustering inside GBs

Emission from GBs

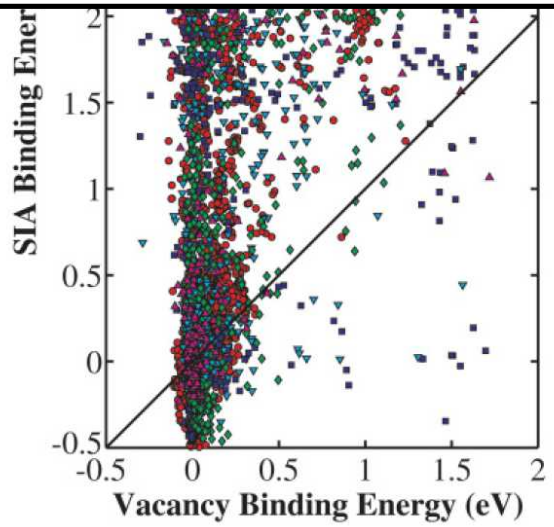
Denuded zone formation

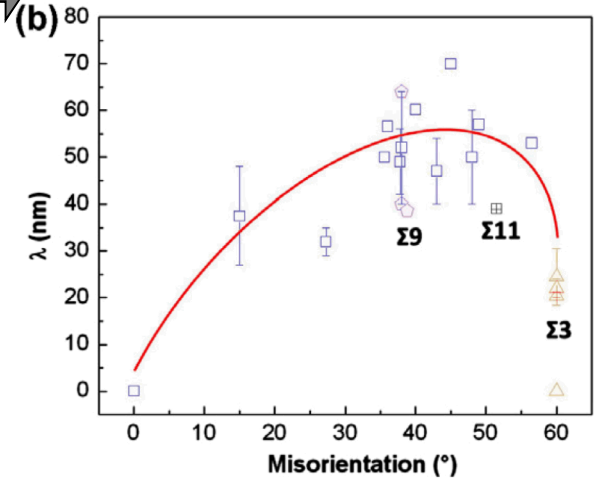






Too many GBs to include all types in an efficient and tractable modeling approach





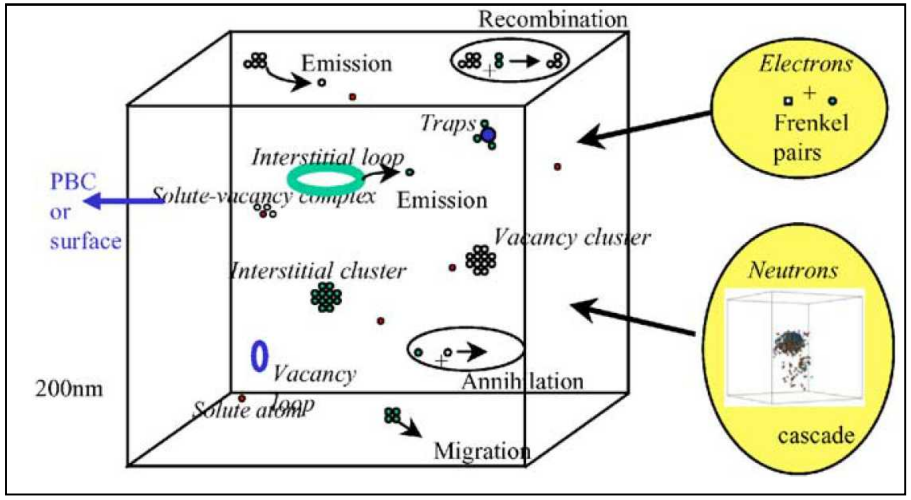
Uberuaga et al. (2015)

Tschopp et al. (2012)

Han et al. (2012)

Common Methods for Simulating Radiation Damage Accumulation

Object Kinetic Monte Carlo (OKMC)



Domain et al. (2004)

- Defects placed inside simulation volume
- Allowed reactions defined by user
- KMC algorithm used to choose reactions and advance time

Cluster Dynamics (CD)

$$\frac{dC_v(t)}{dt} = G_{NRT}(1-\varepsilon_r)(1-\varepsilon_{vcl}) - \left[\mu_R D_i C_i(t) C_v(t) + Z_v^d \rho D_v (C_v(t) - C_{v0}) + \sum_{x=2}^{x=\infty} P_{icl}(x) f_{icl}(x,t)\right] - [P_{vcl}(1) f_{vcl}(1,t) - (Q_{vcl}^v(2) + Q_{vcl}^i(x)) f_{vcl}(2,t)] - \sum_{x=1}^{x=\infty} (P_{vcl}(x) f_{vcl}(x,t) - Q_{vcl}^v(x+1) f_{vcl}(x+1,t)),$$

Stoller at al. (2008)

- Rate equations for concentrations of defect types
- Defects assumed homogeneously distributed in space
- Limited complexity of model
- Can simulate large doses / times

Traditional OKMC and CD methods do not explicitly include grain boundaries

Spatially Resolved Stochastic Cluster Dynamics (SRSCD)

Solving rate equations in a kinetic Monte Carlo setting (Marian and Bulatov, 2011):

1. Choose volume element size and convert all rate equations to number equations by multiplying by V/Ω:

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

1. Treat integer numbers of defects and compile the rates a_μ for all allowed reactions μ
2. Find the total reaction rate a inside the volume element
   Example: reaction rate for vacancy clustering

$$V_n + V_m \rightarrow V_{n+m}$$

3. $\omega(n^{\frac{1}{3}} + m^{\frac{1}{3}})(D_{Vn} + D_{Vm})N_{Vn}(t)N_{Vm}(t)\frac{\Omega}{V}$ se reaction:

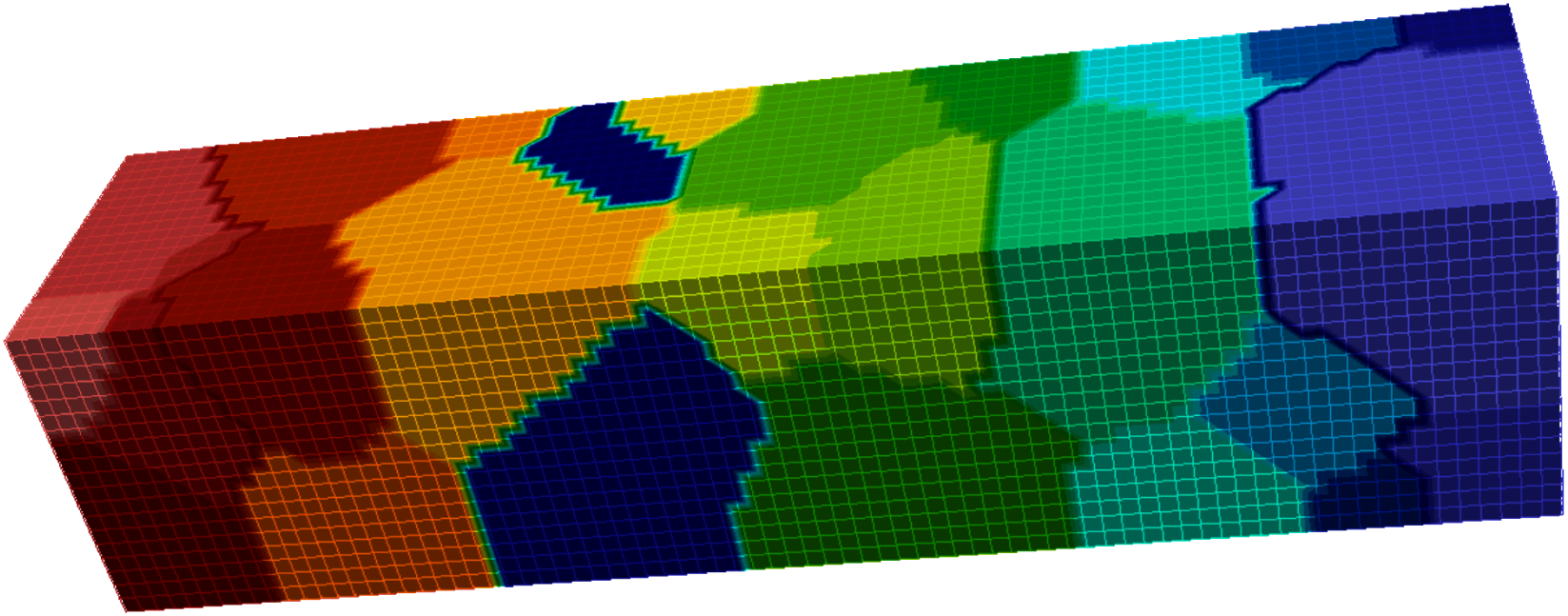
$$\tau = \frac{1}{a}\ln\left(\frac{1}{r_1}\right) \qquad \sum_{v=1}^{i} a_v < r_2 a < \sum_{v=1}^{i} a_v$$

4. Spatial resolution determined by volume element size

- **Benefits**: computationally efficient while including complex defects and reactions

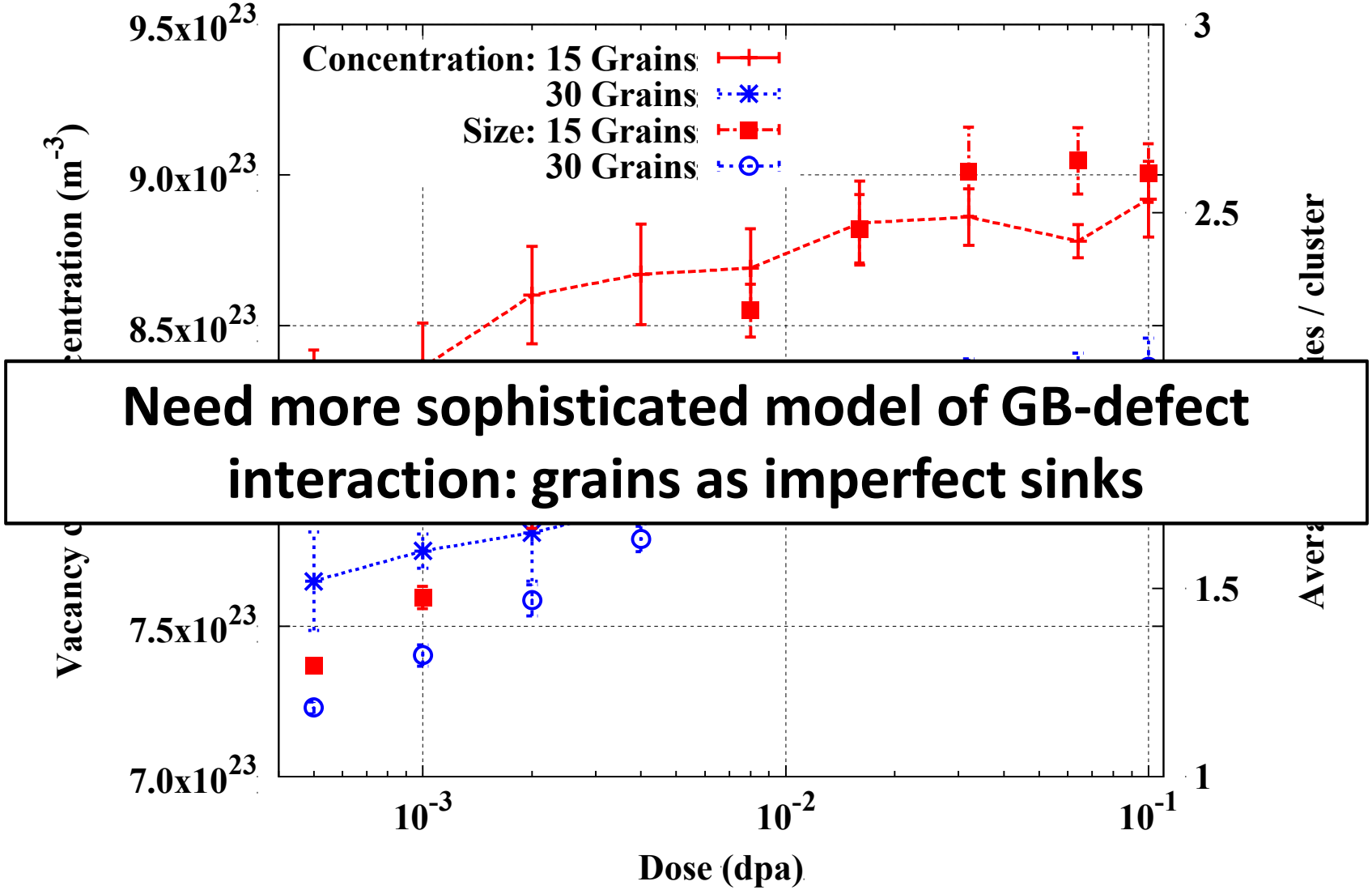
First approximation: treating grain boundaries as perfect sinks

- Uniform, room temperature Frenkel pair implantation in Fe at 7×10^{-7} dpa s^{-1} to a total dose of 10^{-1} dpa
- Two structures: 15 grains and 30 grains
- Total simulation volume: 400 nm x 100 nm x 100 nm, 5 nm elements
- Assume all grain boundaries are perfect sinks



Polycrystalline microstructure. Colors represent grain ID number.

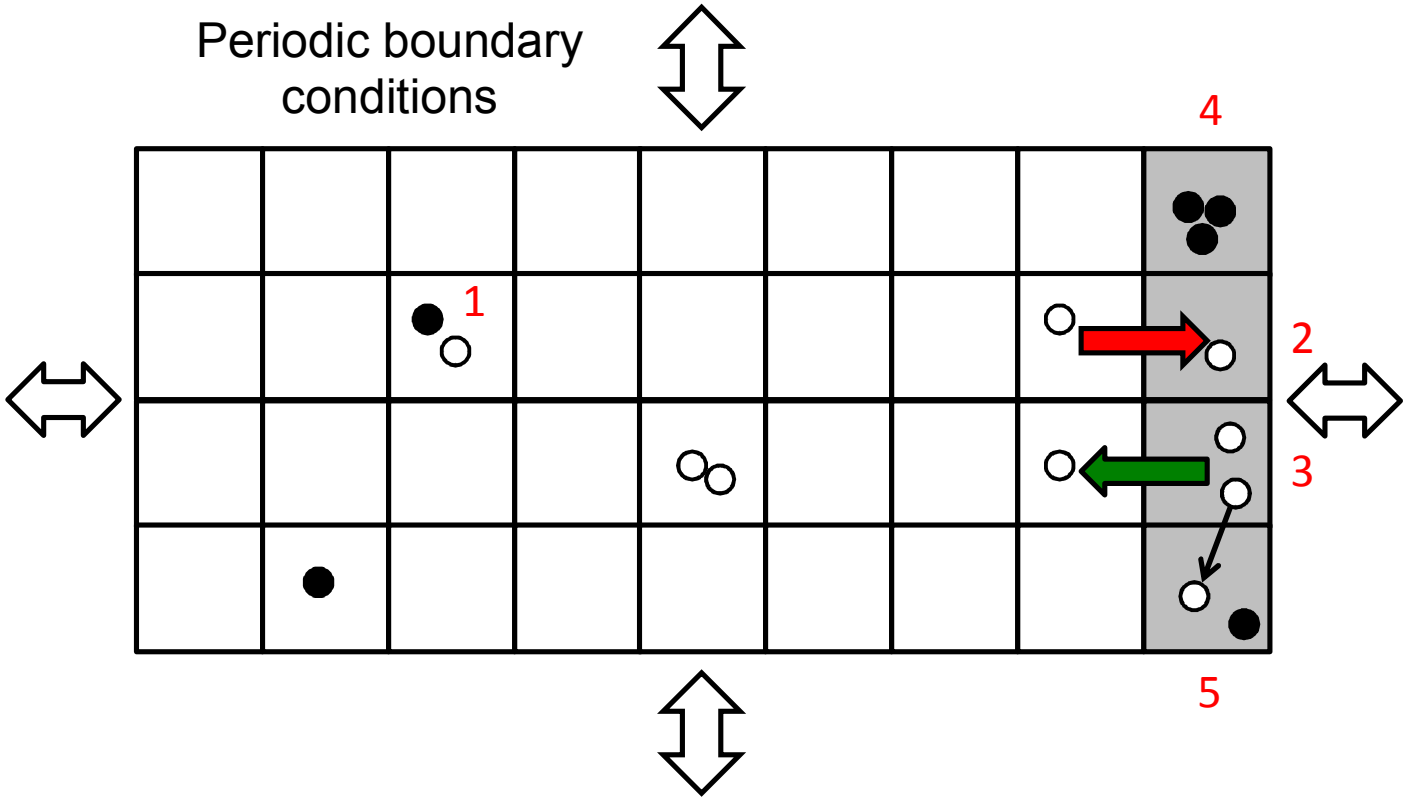
Effect of Grain Size on Damage Accumulation



Need more sophisticated model of GB-defect interaction: grains as imperfect sinks

- Reproduced experimental trend of Yu et al. (2012)

Strategy for investigating defect behaviors in grain boundaries



Allowed reactions:

1. Frenkel pair formation in bulk
2. Defect trapping at GB
3. Defect emission from GB
4. Defect cluster formation in GB
5. Defect diffusion within GB (2D surface)

2-D schematic of simulation layout for investigating effect of grain boundary defect parameters on sink efficiency

- Diffusion rates and cluster binding energies on GB treated as an unknown
- Binding energy for emission from GB treated as an unknown

Multivariate analysis: quantities varied

Quantity	E_m(V)	E_m(SIA)	E_m(V Clusters)	E_m(SIA Clusters)
Domain (eV)	0.3 – 1.0	0.2 – 1.3	0.2 – 1.0	0.2 – 1.3

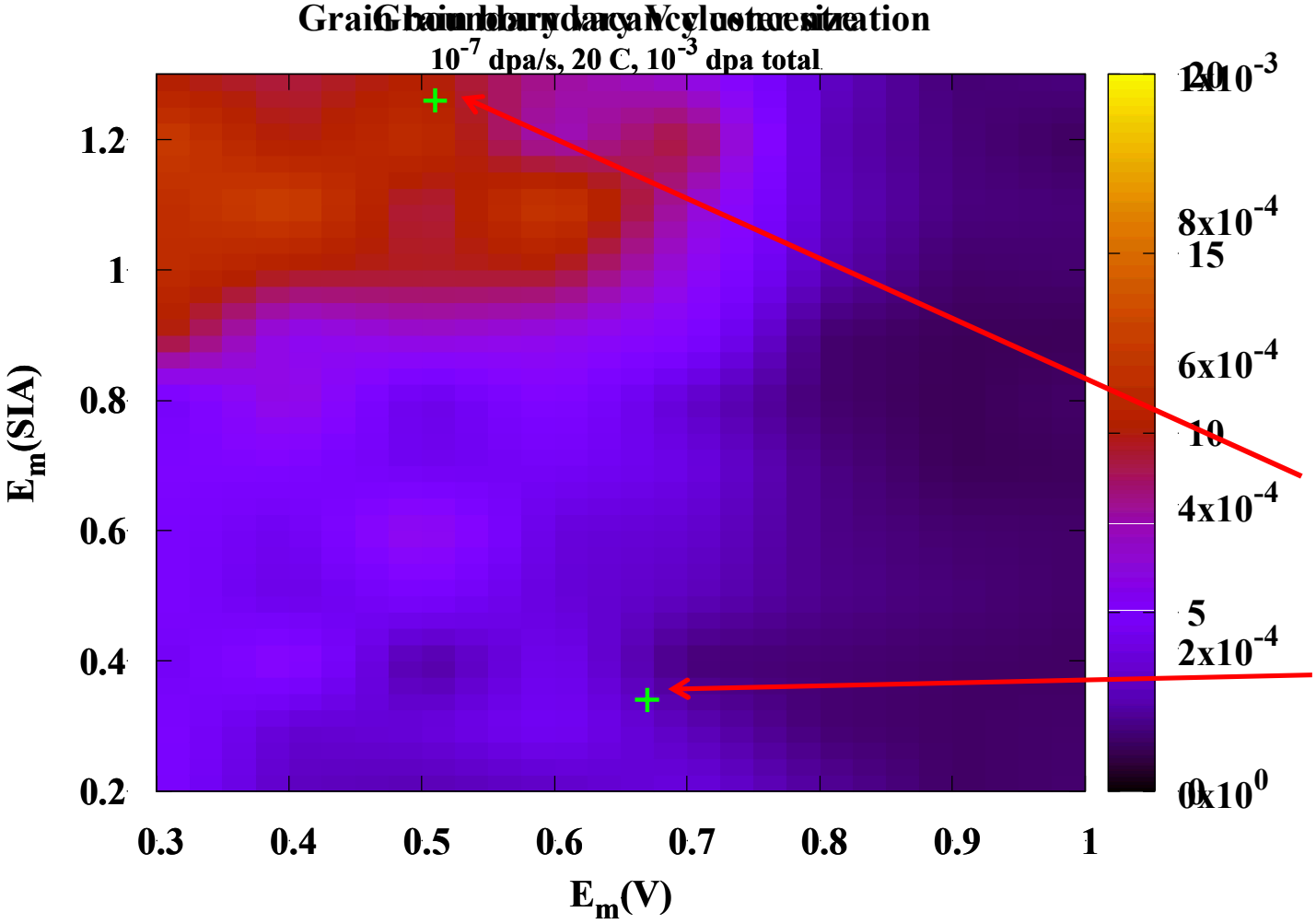
Quantity	E_b(V to V Clusters)	E_b(SIA to SIA Clusters)	E_b(V to GB)	E_b(SIA to GB)
Domain (eV)	0.3 – 3.9	0.8 – 4.4	0.0 – 1.2	0.0 – 2.5

- Vary two parameters while holding others constant. Parameters not varied set to default (bulk) energies

- **Quantities measured:**
  1. Grain boundary vacancy concentration
  2. Grain boundary average vacancy cluster size
  3. Grain boundary sink efficiency η (for vacancies and SIAs)

- **Irradiation conditions:**
  Uniform room temperature implantation of Frenkel pairs into grain
  Total dose of 10^{-3}-10^{-2} dpa
  Dose rate 10^{-7} dpa s^{-1}

Results: Point Defect Diffusion



Varying vacancy and SIA migration energies inside GB

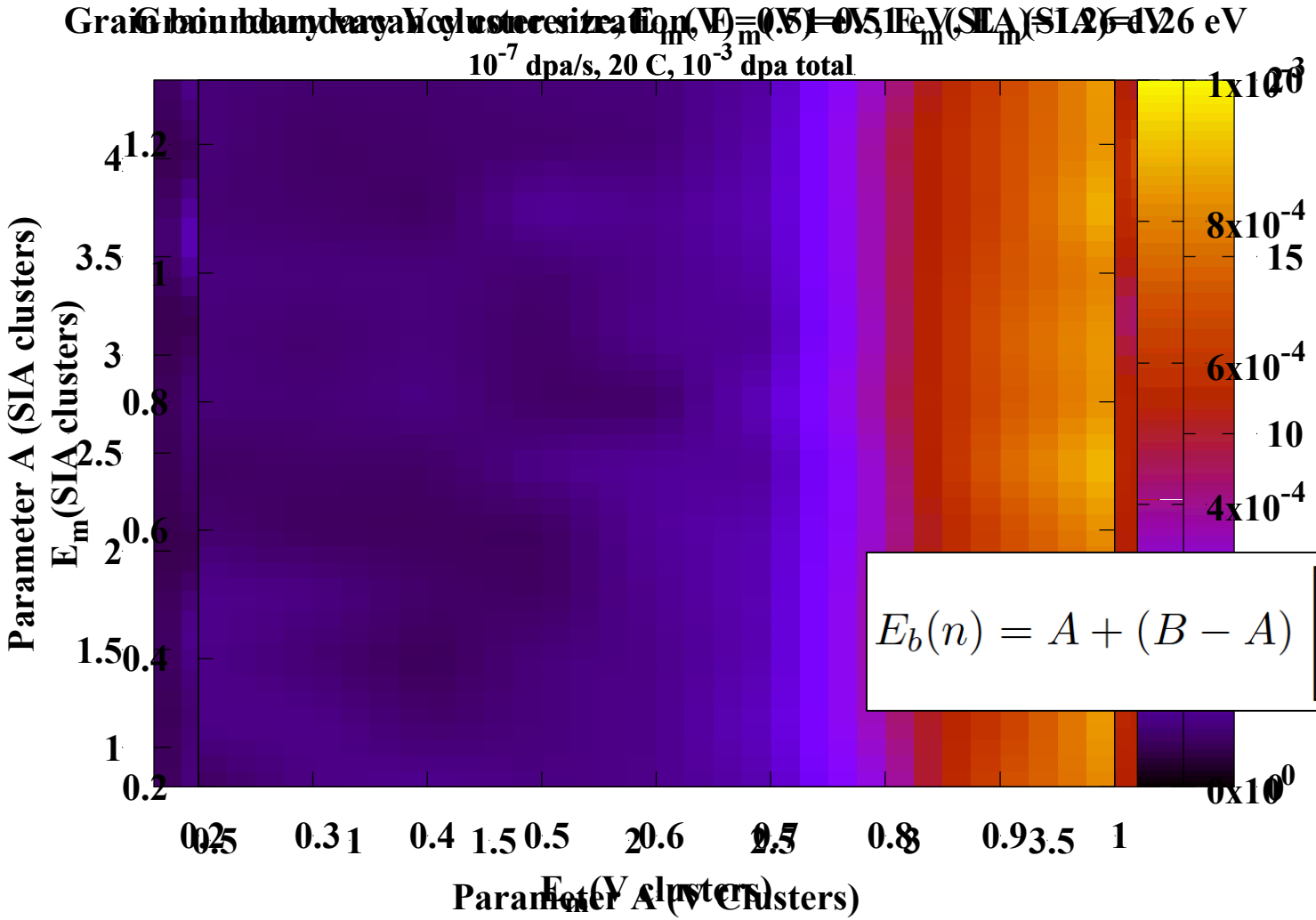
All other GB parameters constant

Σ5 GB: Balluffi and Mehl (1982), Kwok et al. (1984)

Bulk migration energies: Fu et al. (2005)

- Both vacancy and SIA migration energies inside GB strongly influence damage accumulation

Results: Cluster Diffusion and Cluster Binding Energy



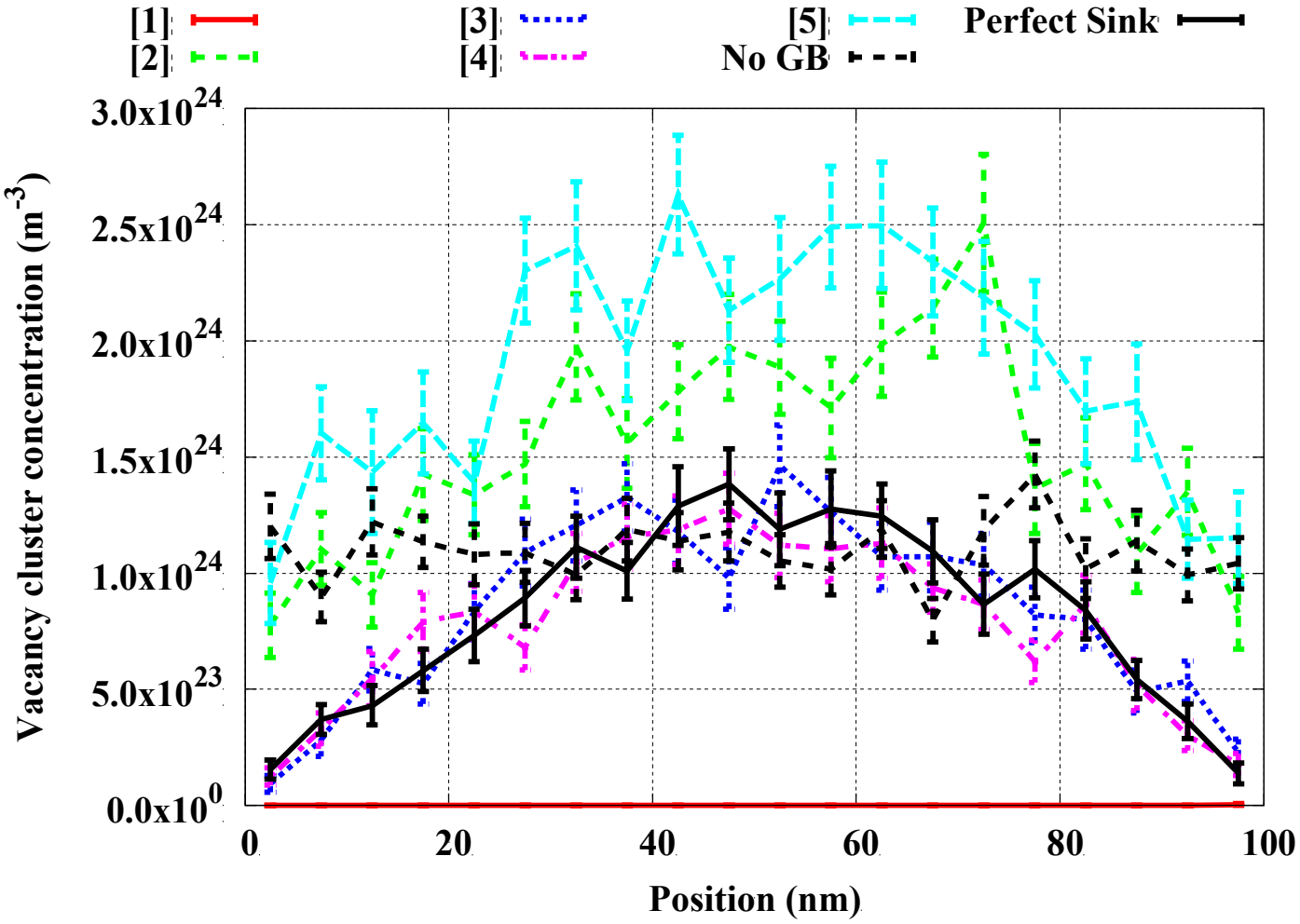
Varying vacancy and SIA cluster migration energies inside GB

Varying parameter A in functional form for binding energy of point defects to clusters inside GB:

$$E_b(n) = A + (B - A)\left[\frac{n^{\frac{2}{3}} - (n-1)^{\frac{2}{3}}}{2^{\frac{2}{3}} - 1}\right]$$

- Vacancy cluster migration energy strongly influences damage accumulation, SIA cluster migration energy, V and SIA cluster binding energies less significant

Results: Grain Boundary Binding Energy



Vary binding energies of point defects to GB

Marked points indicate computed binding energies by Tschopp et al. (2012)

Investigated defect content in grain interior using marked values for binding energies

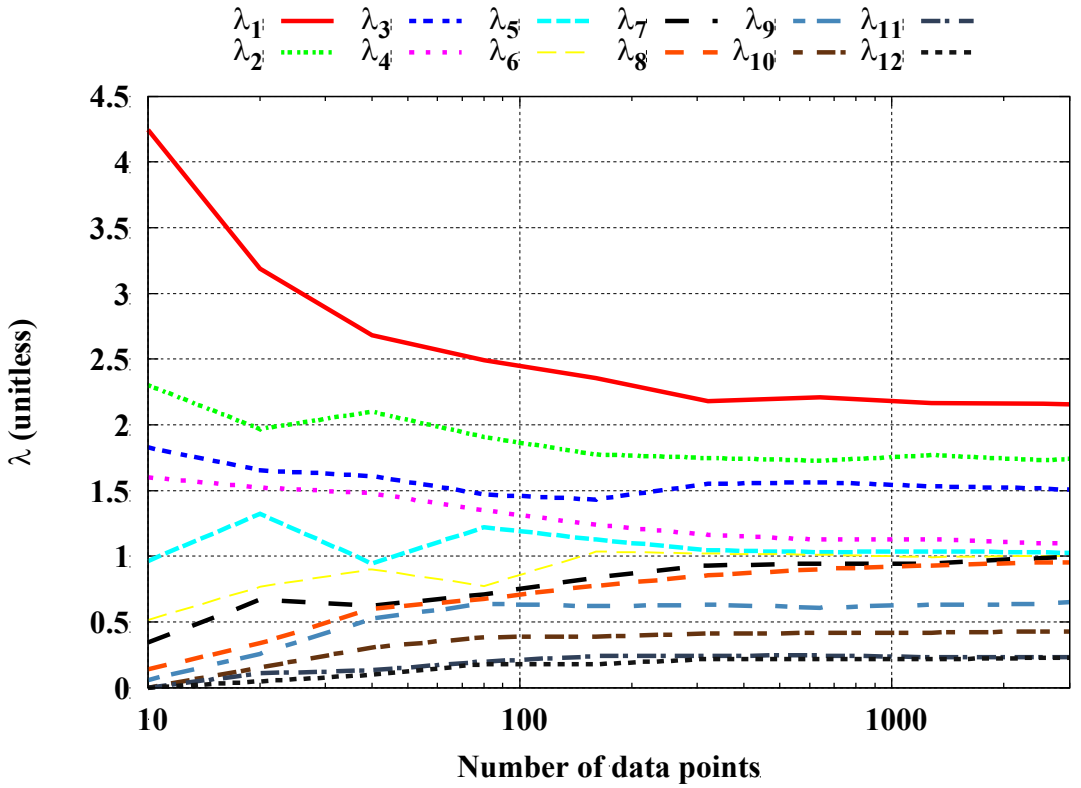
- Different vacancy accumulation behavior depending on the binding energy of point defects to grain boundary
- Damage accumulation ranging from no defects in grain interior [1] to perfect sink behavior [3], [4] to an increase in vacancy content in the grain interior [2], [5]

Principal Component Analysis

Quantity	E_m(V)	E_m(SIA)	E_m(V Clusters)	E_m(SIA Clusters)
Domain (eV)	0.3 – 1.0	0.2 – 1.3	0.2 – 1.0	0.2 – 1.3

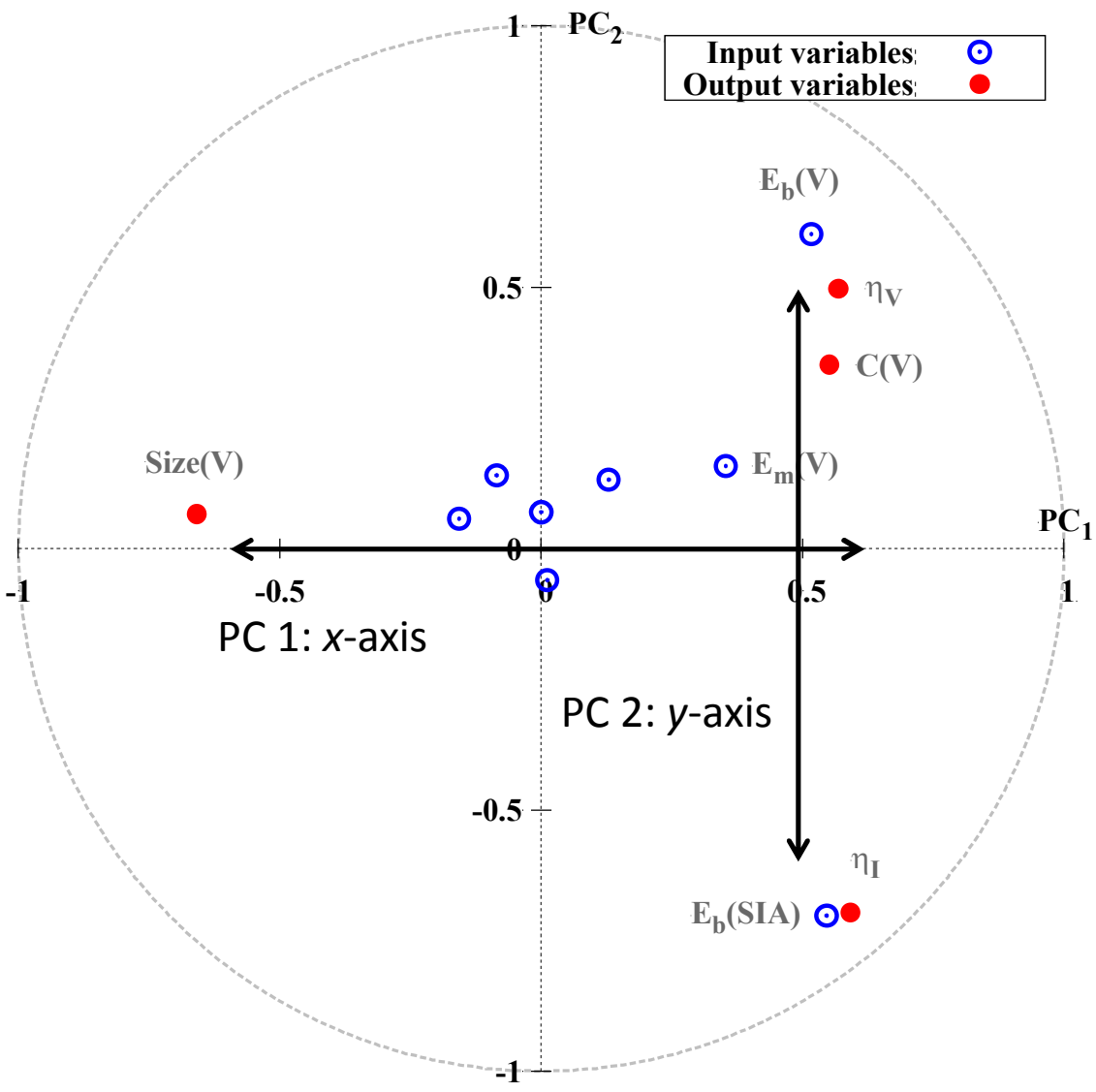
Quantity	E_b(V to V Clusters)	E_b(SIA to SIA Clusters)	E_b(V to GB)	E_b(SIA to GB)
Domain (eV)	0.3 – 3.9	0.8 – 4.4	0.0 – 1.2	0.0 – 2.5

- Random choice of each input parameter during each simulation (see chart above)
- Measure C(V), Size(V), η(V), η(SIA)
- **Correlation matrix**: gives correlations between varied parameters and measured quantities
- Eigenvalues of correlation matrix show stability after 3000 simulations



Principal Component Analysis: Results

- **Principal components**: eigenvectors of correlation matrix
- 77-87% of variation in measured variables explained by four principal components
- **Circle of correlation:** visualization method for principal component analysis
- **Agreement with previous results:** most important variables are single defect diffusion and binding energy to grain boundary



Conclusions

1. Experimental trends relating grain size to defect content reproduced by treating grain boundary as a perfect sink
2. Developed framework for investigating influence of grain boundary defect behavior on damage accumulation / sink efficiency
3. Variables that most strongly influence damage accumulation: single defect diffusion, vacancy cluster diffusion, and binding of defects to grain boundaries
4. Future work: pair with atomistic studies to predict damage evolution near specific grain boundaries

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