ATOMIC-SCALE MODELING FOR FUSION MATERIALS RESEARCH

Fusion Materials Strategic Planning Meeting

UCSB, Santa Barbara CA

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Kinetic Monte Carlo

KMC and Rate Theory

KMC supplements rate theory and other larger scale modeling techniques by

- Quantitatively describing phenomena at time and length scales where the mean field approximation may be invalid
- Supplying source terms (concentrations and interaction characteristics of defects) for rate theory
- Determining the conditions under which mean field rate theory applies

Kinetic Monte Carlo for Microstructure Evolution under Irradiation

- KMC models the evolution of the defect population and microstructure within a limited volume over macroscopic times.
- The properties, positions, migration, and interactions of each defect are treated explicitly, and the evolution of the system is modeled stochastically, representing realistic doses and dose rates .
- There is no single KMC model. Like rate theory, KMC can model only the processes contained in it. KMC must contain an explicit description of each of the defects and processes it follows, including their relative probabilities of happening.
- The more complicated and detailed, the smaller the amount of time and space the KMC model can describe.

Kinetic Monte Carlo

- Is an “ad hoc” method for examining specific issues within a limited space and time, e.g. annealing defects from a single cascade
- Treats defect migration and interactions at length and time scales inaccessible by MD (well beyond sub-micron and sub-nanosecond scales)
- Can examine the sensitivity of results to the values of unknown or unmeasurable parameters (e.g. the lifetime of 1-D SIA clusters or the sink strengths of extended defects)
- Is an essential element for modeling microstructure evolution

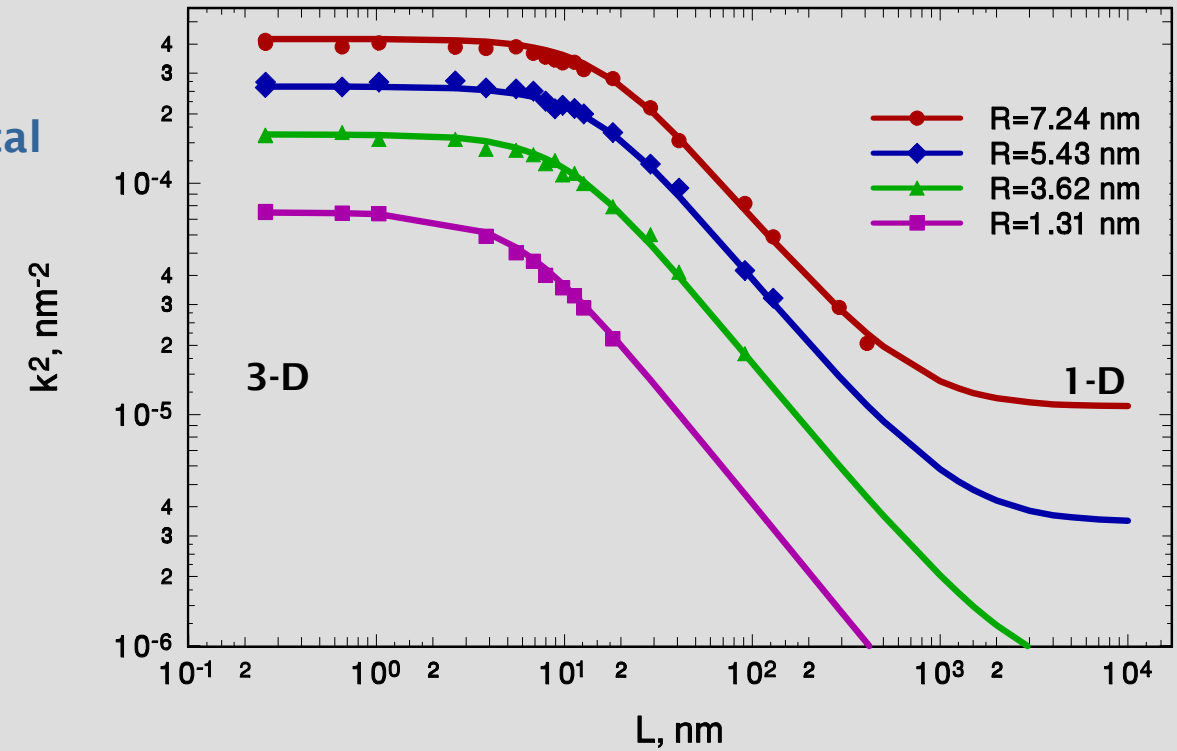
SINK STRENGTH AS A FUNCTION OF 1D PATH LENGTH: ANALYTICAL EXPRESSION AND KMC RESULTS

$$k_m^2 = 0.5\, k_1^2 \{ 1 + \sqrt{1 + 4/(L^2 k_1^2/4 + k_1^4/k_3^4)} \}$$

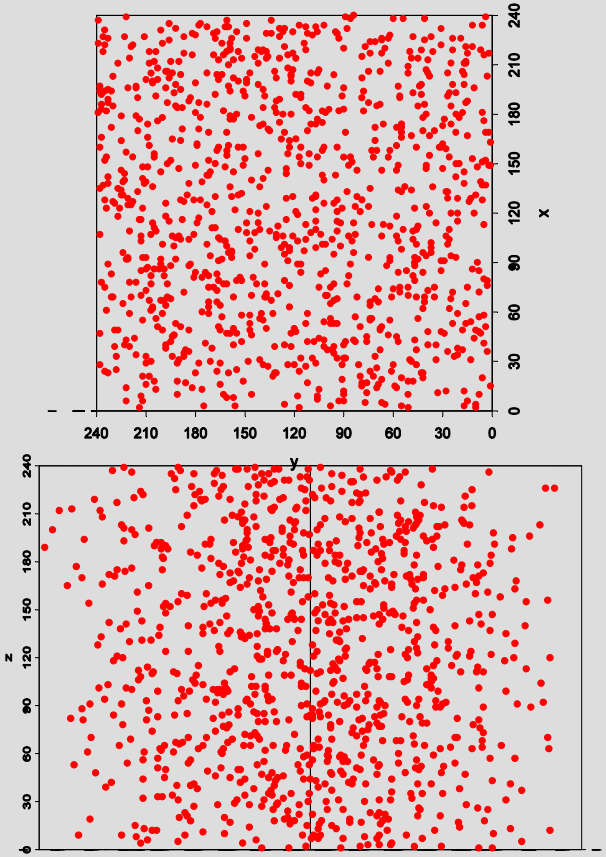
The KMC "thought experiments" are perfectly described by a new analytical theory describing reaction kinetics from 1-D to 3-D.

The new reaction kinetics is being incorporated into the Production Bias Model of microstructure evolution

(Singh, Woo, Trinkaus, Foreman, Golubov)



Formation of a Void Lattice

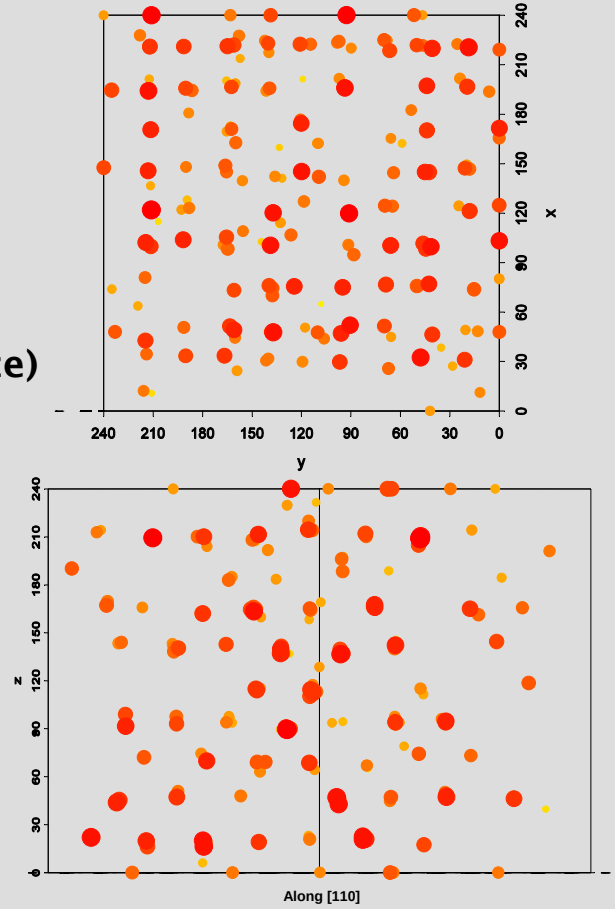


1000 small voids,
randomly arranged

600k SIA clusters

(Ndc=20k, L=box size)

500k VAC clusters



Defect Science in Support of KMC and Rate Theory

Methods

- First principles
- Molecular dynamics
  - potentials: EAM, MEAM, other?
- Transition state theory (Dimer)

The Dimer Method

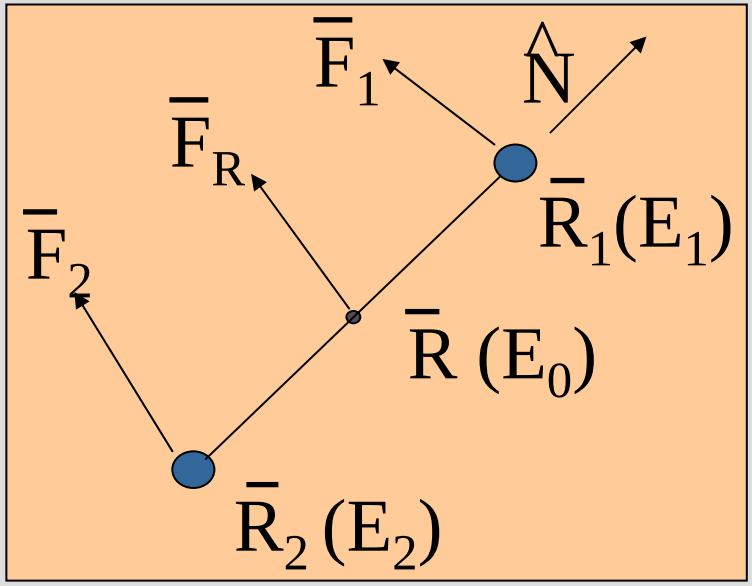
For finding saddle points using only first derivatives

- The Dimer method follows the system from one minimum energy configuration, over a saddle point, to another minimum, without previous knowledge of the final state
- The Dimer consists of two images of the system separated by a short distance from their common midpoint. At each position along the path the dimer can be rotated in response to the forces there to find the minimum curvature mode

Dimer Method

- Dimer: A pair of atomic images separated from $\bar{R}$ by a distance $\Delta\bar{R}$.

$$\begin{cases} \bar{R}_1 = \bar{R} + \Delta R\hat{N} \\ \bar{R}_2 = \bar{R} - \Delta R\hat{N} \end{cases}$$



- E_0 – Energy of $\bar{R}$

$$E_0 = \frac{E}{2} + \frac{\Delta R}{4}(\bar{F}_1 - \bar{F}_2) \bullet \hat{N}$$

- The potential curvature along the dimer $(\partial^2 V(r)/\partial^2 N_i)$:

$$C = \frac{(\bar{F}_1 - \bar{F}_2) \bullet \hat{N}}{2\Delta R} = \frac{E - 2E_0}{(\Delta R)^2}$$

- $\bar{F}_R$ – force at the point $\bar{R}$

$$\bar{F}_R = (\bar{F}_1 + \bar{F}_2)/2$$

Dimer Method

Rotate the dimer in a single iteration towards the minimum energy configuration by finding N along which the dimer has the lowest energy configuration

The rotation angle $\Delta\Theta$ can be found from the force F and its derivative F'=dF/dΘ

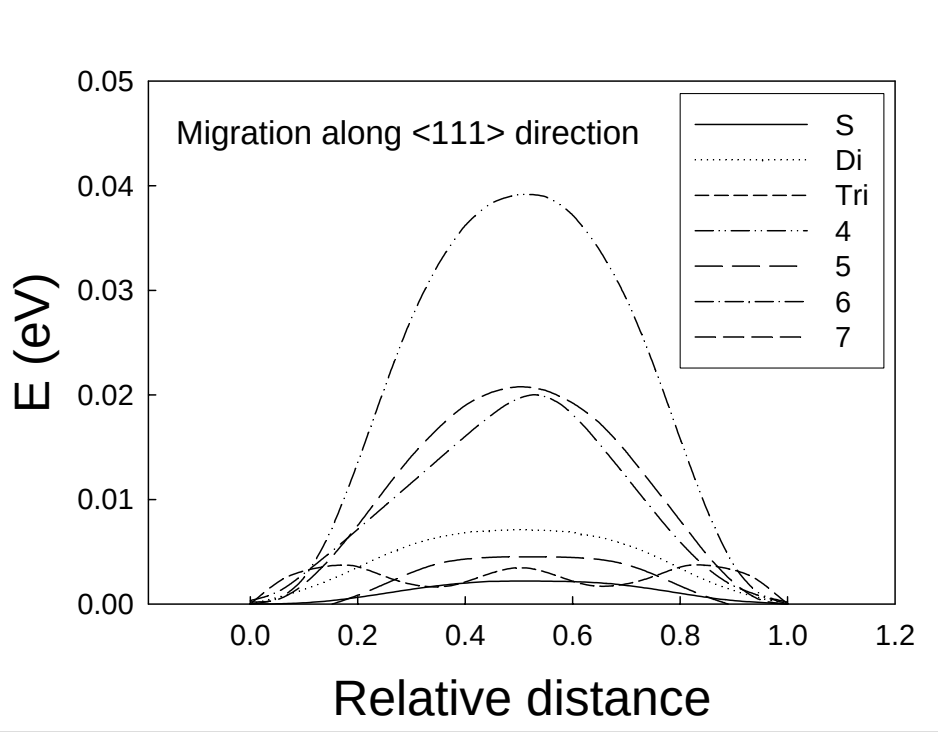
$$\Delta\theta = \theta_0 = -\frac{1}{2}\arctan\left(\frac{2F}{F'}\right)$$

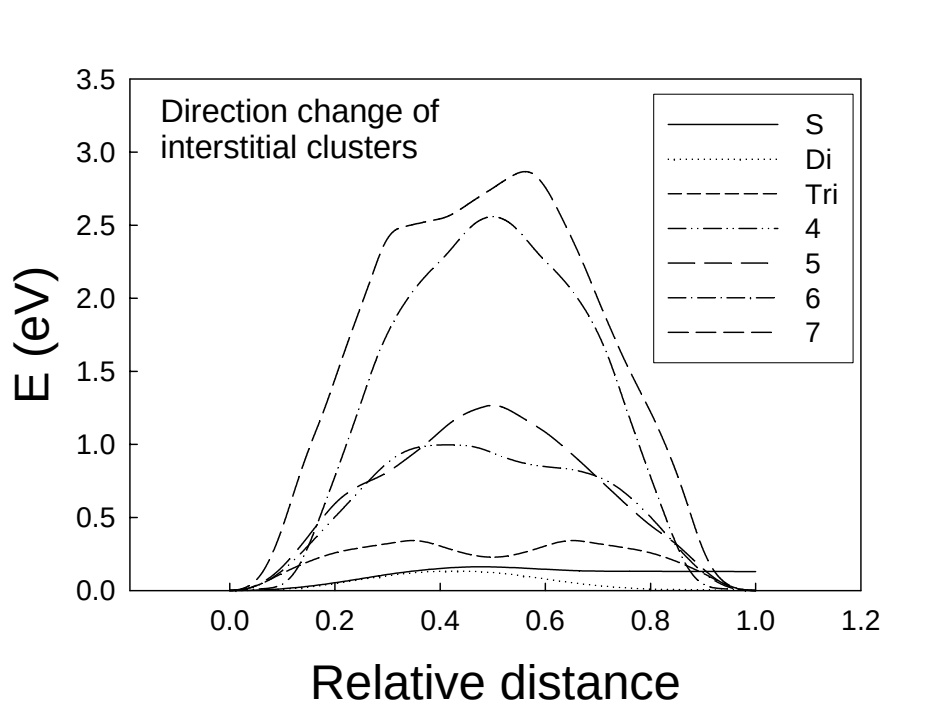
Translate the dimer towards the saddle point

$$\Delta r = \frac{(\overline{F}^{+} \bullet \hat{N} - \overline{F}^{+*} \bullet \hat{N}^{*})}{-2F^{+}{}'}$$

Interstitial clusters (>3)

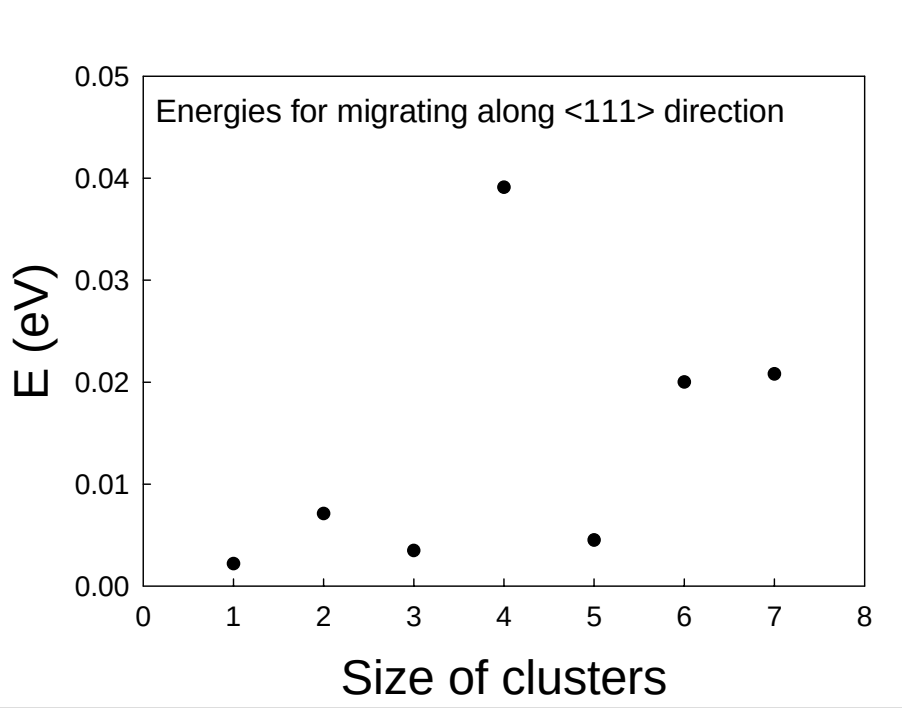
Migration along <111> direction and direction change

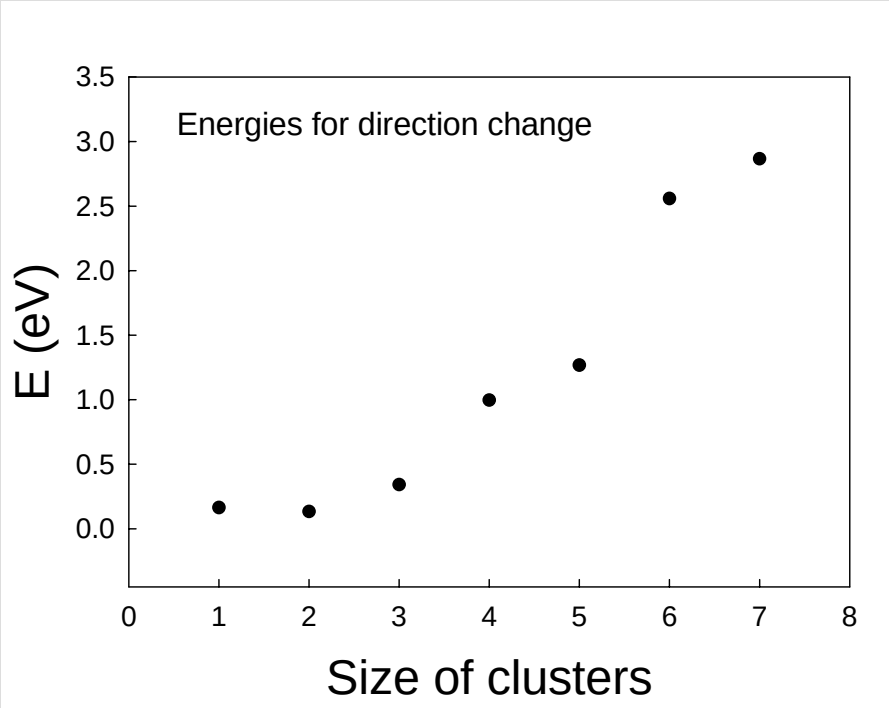




Interstitial clusters (>3)

Energies for migration and direction change





- Energy for direction change increases with increasing cluster size.
- There is a large increase between size 3 and 4, and size 5 and 6.
- Migration energy along <111> direction varies with cluster size (0.0022 – 0.039 eV).

Defect Properties

SIA (crowdion) Clusters

cluster size dependence of

- **stability**
- **mobility – including direction changes**
- **interactions among SIA**

Vacancy Clusters

- **stability**
- **mobility**

Defect Interactions

Defect cluster interactions with

- **other clusters**
- **dislocations**
- **grain boundaries**
- **impurities**

The Importance of Understanding SIA Clusters

Specific properties of the clusters

- Anisotropy in the stress field around the cluster
- Long range interactions along the cluster glide prism
- High mobility in 1-D

Properties of SIA clusters and vacancies can lead to segregation of the vacancy and SIA microstructures

How the reactions of an SIA affect

- The defect balance
- Changes in its own properties
- Defect accumulation

Some Particular Reactions

- SIA cluster – cluster (SIA cluster growth)
- SIA cluster – cluster, -dislocation, -GB, etc. (segregation of V and SIA)
- SIA cluster – vacancy, -vacancy cluster (immobilization, direction change; V-SIA balance)
- SIA cluster – precipitates (sink for SIA, “recombination center”)
- Thermally activated rotation (mobility, kinetics)

Some Things We Already Know

Cluster-cluster interactions (orientation dependent)

- **Large clusters can form immobile complexes**
- **Small clusters can lead to direction changes**
- **Parallel clusters can form rafts**

Some Things We Already Know

Cluster – point defect interactions

- **Vacancy may immobilize SIA cluster (temporarily, depending on T) or annihilate at the cluster edge (small cluster) or change glide direction**
- **Impurity may immobilize or slow down cluster**

Cluster – dislocation interactions

- **Dislocation decoration (can be described by theory, corroborated by atomistic modeling)**

Realistic “Complications”

Effects of stress on defect

- formation
- stability
- mobility
- interactions

Effects on cascades due to presence of

- stress
- grain boundaries
- dislocations
- other defects

Impurities and Alloys

- all of the above

Effects of Helium

- Migration of He-vacancy complexes as a function of size
- Migration of He interstitial clusters as a function of size
- Binding of He-vacancy and He interstitials
- Interaction of He clusters and dislocations; He trapping at dislocations and interfaces
- He effects on displacement cascades: cluster characteristics
- He-solute atom (e.g. Cr) interactions

Elastic Displacement Fields

- Elastic representation of atomistic defect displacement fields
- Enables elastic calculations of interaction energies and forces between point defects (or defect clusters) and other defects (dislocations, grain boundaries, interfaces)
- especially useful in higher scale models such as dislocation dynamics

Atomistic Modeling Priorities

- Crowdion clusters
- Vacancy clusters
- He-vacancy complexes
- Stress effects (exploratory)
- Dilute binary alloy (exploratory)