Role of Kinetic Microstructural Models: Rate Theory and Monte Carlo

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Rate Theory Models -1

Place in multiscale model hierarchy

- longest time scale, seconds to years
- largest length scale, a few nm to mm
- input parameters from atomistic models such as molecular dynamics, ab initio
- results can provide input to mechanical property models, FEM
- perhaps least computationally intensive

Features

- spatially-averaged, mean-field description of microstructure
- suffers from need to determine numerous parameters
- computed microstructural results can be directly compared with experiments

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Summary of primary damage studies relevant to kinetic radiation damage models

- **MD cascade simulation energies have reached energies relevant fast neutron irradiation conditions, maximum equivalent neutron energy ~5.1 MeV**
- **energy dependence of surviving defect fraction and point defect clustering fractions can be expressed using simple functions obtained by least-squares fitting of results up to 100 keV**
- **Simulations have been completed in sufficient numbers to statistically evaluate the effects of cascade energy and irradiation temperature, database has been reanalyzed using a single set of visualization tools**
- **Above ~10 keV, subcascade formation dominates the details of defect formation.**
- **Impact of subcascade formation suggests that neutron energy spectrum effects are probably weak when comparing fission reactor irradiations with DT fusion, thus fission reactor data should be relevant to <u>displacement component</u> of fusion environment**
- **Small clusters <111> crowdions (nascent interstitial loops) are highly glissile, E_m~0.1 eV**
- **More work is underway to:**
  - -- verify predictions of EAM-type potentials with ab initio calculations and development of more detailed potentials
  - -- evaluate impact of MD-based primary damage parameters in kinetic models

Rate Theory Models -2

Reaction rate equations used to describe defect processes such as production, diffusion, absorption at sinks, and microstructural evolution

$$\frac{dC_{i,v}}{dt} = \eta(1 - f_{i,v})G_{dpa} - \alpha C_i C_v - D_{i,v} C_{i,v} S^T_{i,v}$$

- equation shown is for mobile mono-interstitials or vacancies
- similar equations can be written to track the distribution and fate of other defect species of interest:
  - -- a family of interstitial and vacancy clusters (either mobile or not)
  - -- mobile gases such as helium
  - -- defect solute clusters, e.g. He-vacancy
- evolution of extended defects can be modeled the same mean-field framework
  - -- cavities, bubbles and voids
  - -- dislocation structure

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Investigations of radiation-induced microstructural evolution: Current results, status, and planned using from rate theory

- **Most extensive development of rate theory models took place between late 1970s and 1980s**
  - -- demonstrated primary role of radiation-induced microstructural evolution in void swelling and irradiation creep, co-evolution of dislocation structure and cavities
  - -- importance point defect and helium partitioning
  - -- highlighted role of helium and residual gases in driving void swelling by promoting conversion of gas-stabilized bubbles into voids
  - -- good agreement between model predictions and a broad range of data was obtained
  - -- model limitations compensated for by use of “effective” material parameters in some cases
- **Recent and ongoing activities follow from:**
  - -- use of models to predict behavior in irradiation special purpose irradiation experiments
  - -- results of atomistic calculations reveal physical mechanisms not accounted for in earlier models, notably high fraction of in-cascade interstitial clustering and interstitial cluster mobility
  - -- computational advances permit development and application of more detailed kinetic models
  - -- issues related to effects of transmutant helium, helium-vacancy clustering, helium partitioning

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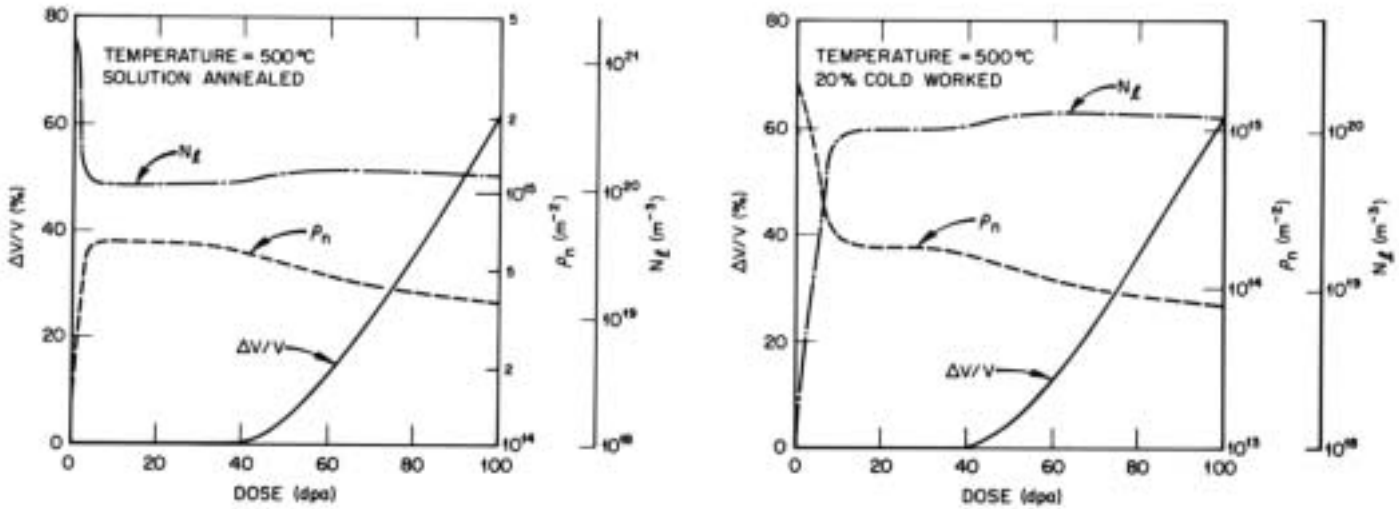
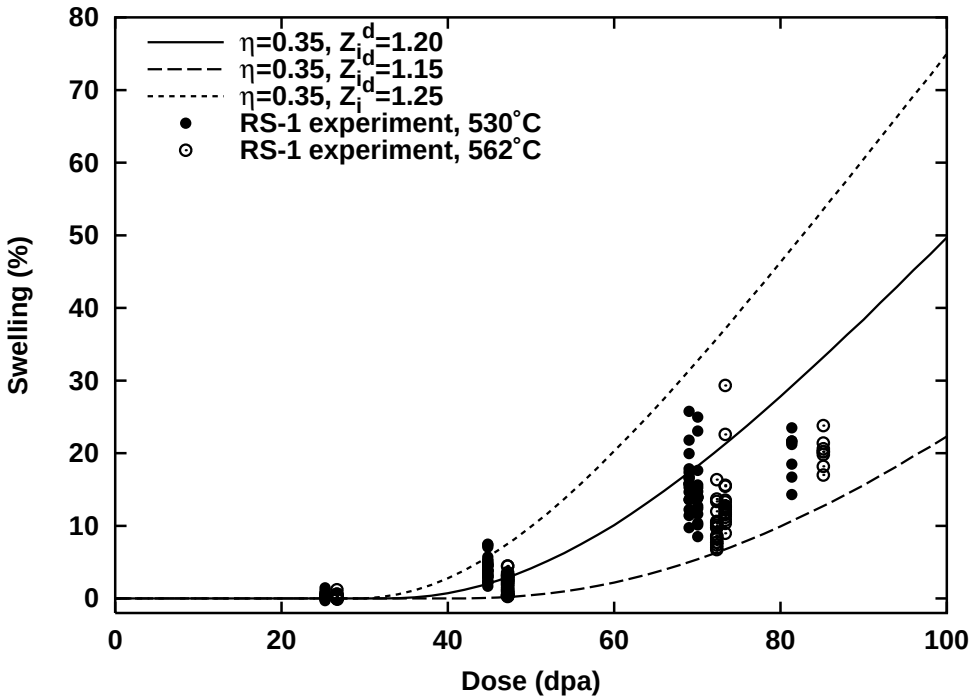
Typical example of results from coupled void swelling - dislocation evolution model

- void incubation time determined by helium partitioning
- co-evolution of different microstructural components observed
  - cavities, dislocation looks and dislocation network



Sensitivity of model predictions to parameter variations can help determine "reasonable" parameter range with input from more basic models

- evaluation of MD-based defect production parameters and dislocation bias



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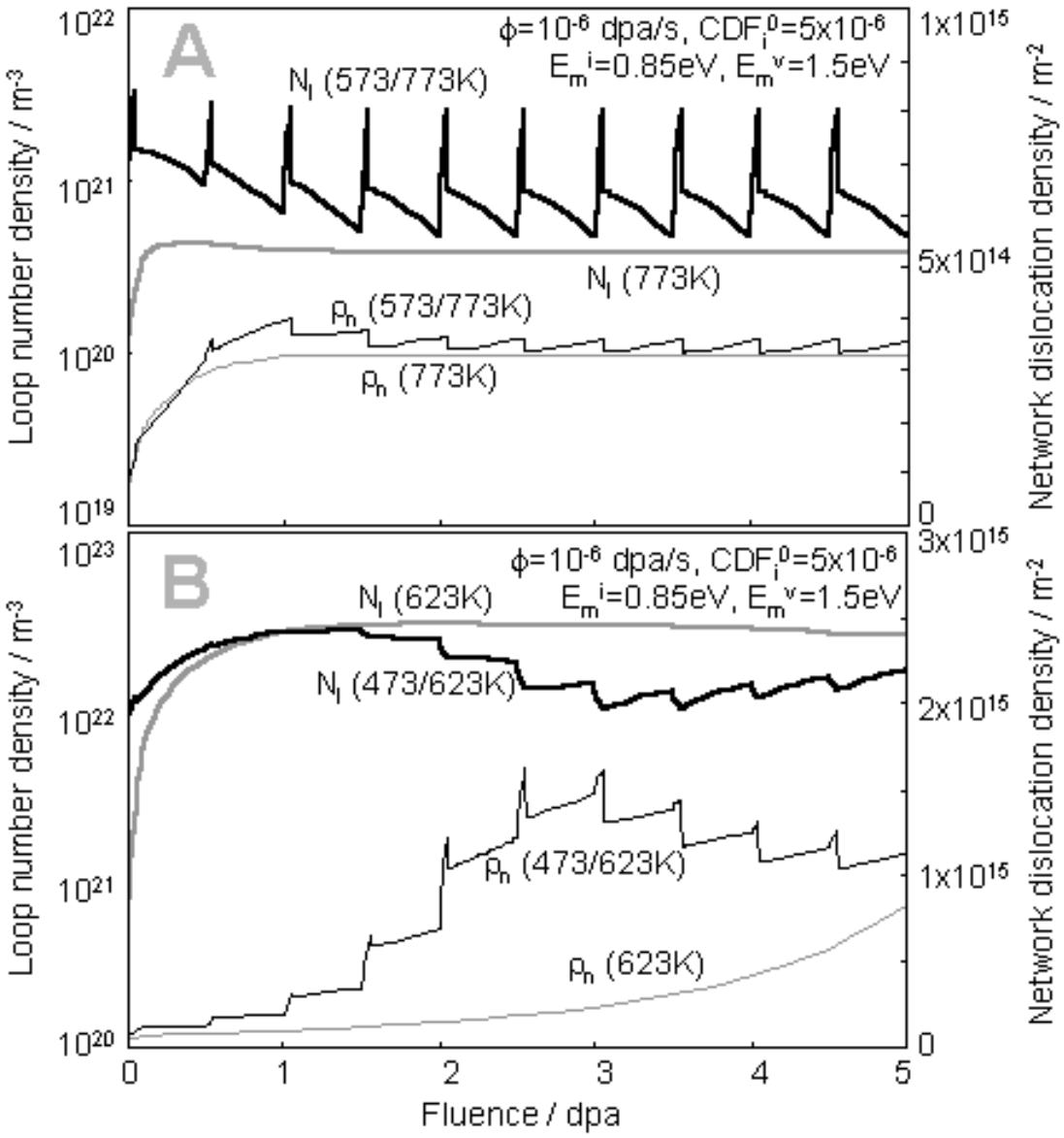
Point defect transients lead to increased nucleation of small interstitial loops and thereby higher network dislocation densities



Overall effect is modest, predictions generally consistent with limited data currently available from experiment

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Helium-effects issues relevant to current fusion program needs

- **Helium diffusion and transport mechanisms**
- **Helium trapping and partitioning between different microstructural sinks**
  - -- Bubble nucleation in matrix, on precipitates and grain boundaries
  - -- Helium flow to grain boundaries
- **Bubble growth and evolution of size distribution, swelling**
- **Grain boundary bubble growth under stress**
- **Creep rupture**

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Bubble Growth & Size Evolution in Steels

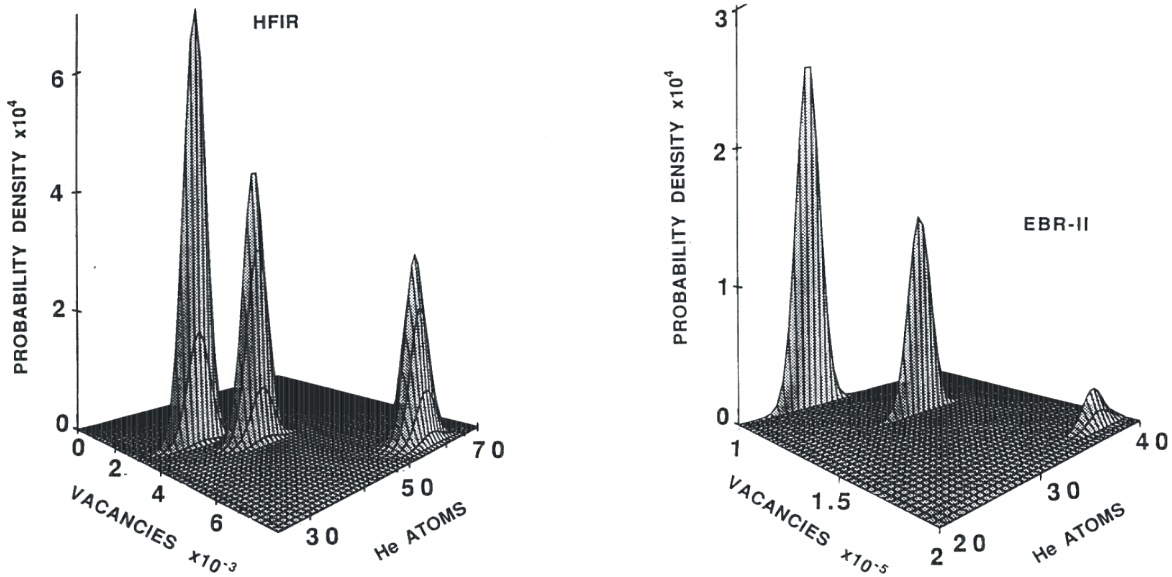

Fig. (2): Computed non-equilibrium vacancy-helium cluster size distributions under low (left), and high (right) helium generation rates.

Rate Theory Work:

Status and Future Directions

- Current models are generally successful at predicting radiation-induced microstructural evolution in the most-studied materials
  - -- temperature and dose dependence of void swelling in austenitic stainless steels
  - -- radiation-induced hardening in reactor pressure vessel steels
- Additional model development should be focused on the rate theory has not been strong in the past
  - -- exploit new computational tools, e.g. by developing more detailed defect clustering (i.e. point defects, solutes, He, ...) models to improve description of <u>nucleation</u>
  - -- develop <u>thermodynamic</u> models to account for solute and precipitate effects more explicitly, e.g. for application to ODS ferritic alloys (capitalize on work in RPV steels)

- Other areas of development
  - -- expanding range of materials, requires interacting with experimentalists to develop microstructural database for model verification
  - -- incorporating insights obtained from MD simulation of damage production mechanisms (while validity of these mechanisms are being examined)
  - -- evaluating impact of MD and MC-based primary damage parameters
  - -- improved description of helium partitioning, obtain guidance from atomistic simulations

- Interact with experimentalists to evaluate both models and experiments, e.g.
  - -- role of irradiation variables, irradiation temperature, displacement rate, helium-to-dpa ratio
  - -- helium diffusion and accumulation mechanisms