Synchronous Parallel kinetic Monte Carlo: Diffusion in Heterogeneous Systems

Enrique Martinez, Jeffery Hetherly and Alfredo Caro

EFRC, MST-8 – LANL

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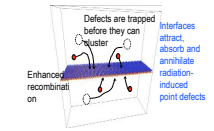
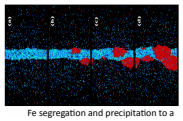
We present a new algorithm that is the key component of our project aiming at a massively parallel off-lattice kinetic Monte Carlo code for heterogeneous systems that will extend the time scale limits of MD to study diffusion at interfaces in concentrated alloys

Motivation

Point defects - interface interactions

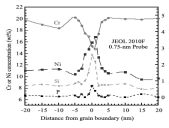


Segregation and precipitation at dislocations



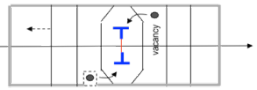
Fe segregation and precipitation to a screw dislocation in Cu

Radiation Induced segregation



Bruemmer SM, et al. J. Nucl Mater 274:299-314

Diffusional Creep



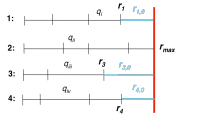
Vacancy diffusion makes dislocations to climb

Technological Issues

- Finding possible events.
  - In crystalline structures, localization of the walkers will help in finding the transition paths.
  - For highly heterogeneous systems, tools like ART (activation-relaxation technique), TAD (temperature accelerated dynamics) or the dimer method may have to be explored.
- Calculate their rates accurately.
  - To achieve it, the right number for the pre-exponential factor and for the activation barrier will have to be calculated.
- Massive Parallelization.
  - kMC is tricky to parallelize. Synchronous parallel kMC.

Synchronous Parallel kinetic Monte Carlo Algorithm

Now, for parallel kMC, perform K (4) domain partitions and construct *frequency lines*:



The $r_{i,0}$ are the 'dummy' rates (no event) that ensure **synchronicity**:

$$r_{max} = r_i + r_{i,0}$$

$$R_{tot} \le \sum_i (r_i + r_{i,0}) \le K r_{max}$$

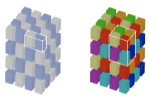
$$\left.\begin{aligned} \delta t' &= -\frac{\ln \xi}{r_{max}} \\ \delta t' &= -\frac{\ln \xi}{R_{tot}} \end{aligned}\right\} \delta t' \le K \delta t'$$

Parallel timestep is ideally K times the serial timestep: **time is advanced the same amount in each domain**

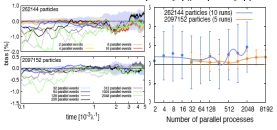
For optimum scalability, perform domain decomposition subject to the following constraint:

$$\min\left[\sum_i r_{i,0}\right]$$

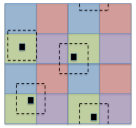
Sectoring-Coloring to avoid boundary conflicts

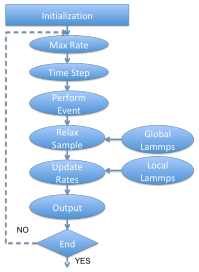


Error Calculation: $bias = \langle m(\sigma_s) \rangle_n - \langle m(\sigma_c) \rangle_c$

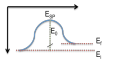


Coupling MD Lammps – Synchronous parallel kMC





- Set of possible events.
- Harmonic transition state theory.
- Particle rate: $\Gamma = \nu \exp(-E_{SP}/kT)$; $E_{SP} = E_0 + (E_f - E_i)/2$

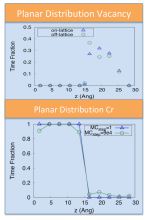


Different Available Models

- Lattice kMC. We can use a perfect rigid lattice.
- Distorted Lattice kMC: The lattice is rigid but it contains some distortion due to the presence of defects in the sample (e.g. dislocations).
- 0K-Off-Lattice kMC: The lattice evolves at each step performing a global conjugate-gradient minimization.
- Off-Lattice kMC: Fully Molecular Dynamics steps follow a kMC event.

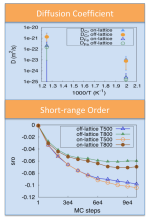
Case Studies

001 Coherent Interface Fe-Cr



System tends to the equilibrium configuration

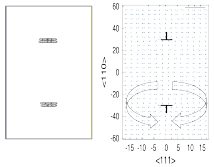
Short-Range Order kinetics in Fe-Cr



Significant difference in the Short-Range Ordering kinetics.

Diffusion in the presence of strain fields

Vacancy Flux around an edge dislocation dipole



Vacancies are less probable to be in regions under tension than in regions under compression

Roadmap

The development of this algorithm will allow us to study the following processes:

1. Absorption and recombination of point defects at interfaces
2. Morphological and chemical stability of interfaces
3. Interface-driven mechanical response

-First objective: treatment of thermodynamics and displacements in the presence of incoherent interfaces.

-Second objective: Implementation of self-interstitial diffusion.

- Third objective: Fully parallelization of the code

Conclusions and Current Work

- We have developed a coupled MD-kMC algorithm that allows us to study heterogeneous systems.
- We can reach real times far beyond MD capabilities.
- We can take into account long-range fields (e.g. elastic fields).
- Localization of possible events via Voronoi tessellation.
- First nearest neighbors search for heterogeneous structures using Voronoi cell face sharing.
- Improvement of the physics:
  - Calculation of the barriers on the fly
  - Calculation of the prefactors.

Acknowlegements

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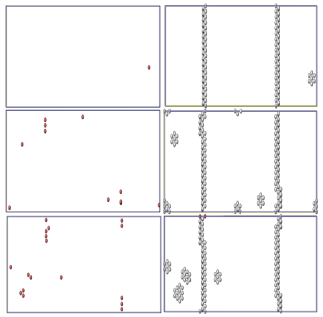
Vacancy Accumulation and Jog Formation on an edge dislocation dipole

Vacancies (red dots) are inserted at a rate of 10^3 V/A^3.s

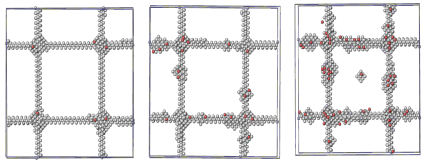


MC steps = 1
T = 2.6x10^{-6} s

MC steps = 4000
T =3.4325x10^{-3} s

MC steps = 10000
T = 5.0032x10^{-3} s

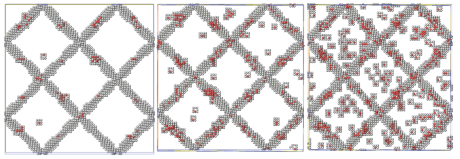
Vacancy Accumulation and Microstructure Evolution on a 2 degrees Twist Boundary in Fe



Dose rate = 10^{-2} V/A^3.s | Dose rate = 3.10^{-2} V/A^3.s | Dose rate = 10^{-3} V/A^3.s

Vacancies accumulate at the dislocation intersections provided that the dose rate is low enough such that they have time to reach those sites

Vacancy Accumulation and Microstructure Evolution on a 2 degrees Twist Boundary in Cu



Dose rate = 10^{-1} V/(A^3.s)
t_s = 1.265e-03 s

Dose rate = 10^{1} V/(A^3.s)
t_s = 4.244e-05 s

Dose rate = 10^{2} V/(A^3.s)
t_s = 8.500e-06 s

Interface dislocations seem to be perfect sinks for vacancies. Vacancies accumulate at the dislocation constrictions but not at the dislocation intersections