Atomic Level Simulation of Morphological Evolution in Multi-Phase Crystalline Systems

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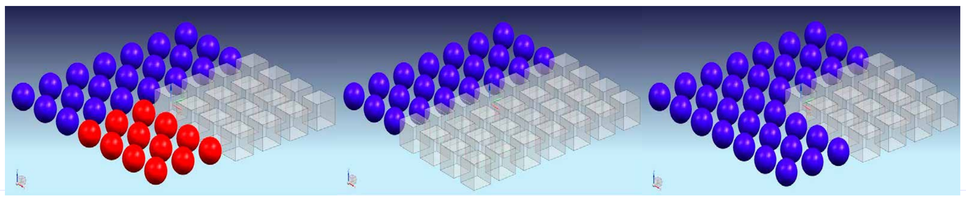
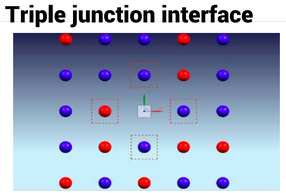
1. Abstract

Computer simulation of microstructure development and evolution during materials processing and service has been of increasing interest. We develop an atomic-level simulation aimed at revealing microstructural features that are closely tied to interfacial energies in materials. Interfacial energies impact several manufacturing processes such as the stability of thin films during semiconductor processing and the nucleation and growth of precipitate particles such as artificial diamonds or other second-phase particles used to enhance mechanical properties. We simulate time dependent atomic jumping (diffusion) on a 1000X1000 square lattice. Input parameters may be tuned to promote mixing of different atom types or maintain distinct chemical phases

2. Problem Statement

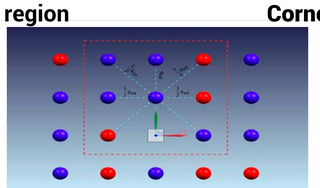


Triple junction interface



Possible selections for the jumping atom

Boundary region

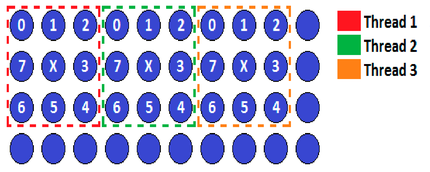


Corner

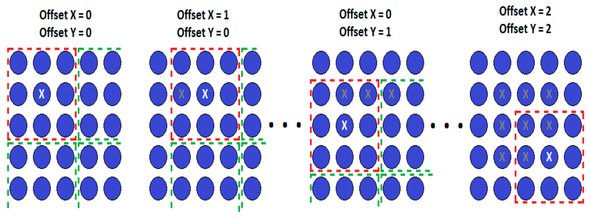
Affected area for jumping atoms. Each non-jumping atom contributes to overall ΔE based on atom type, and atom location

3. Parallel Algorithm.

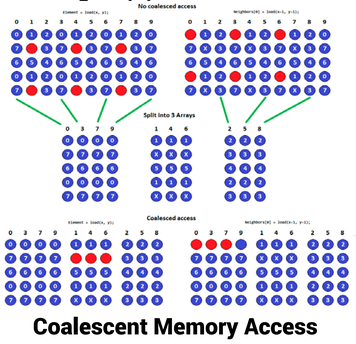
CPU using multiple threads of control to operate on data simultaneously. Each thread chooses one random pixel, checks if it meets the criteria for moving, and moves it if it does meet the criteria. With multiple threads running, it is possible for them to perform conflicting actions. Therefore a series of locks are used to prevent conflicts. When a thread selects a pixel to process, it acquires the lock or locks that cover the pixel and all the neighboring pixels that can affect the outcome of the computation. The sizes of the squares of pixels associated with each lock can be tuned. We found that having about 100 locks per active thread minimizes conflicts while not creating too much overhead.



Atom are affected by a 3x3.
Each thread computes the jump of an atom at the center of the grid (X).



Horizontal and vertical displacement to calculate atoms jumps

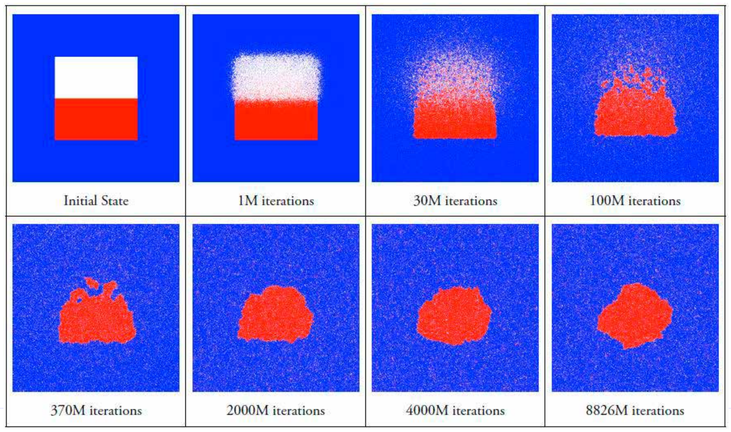


Coalescent Memory Access

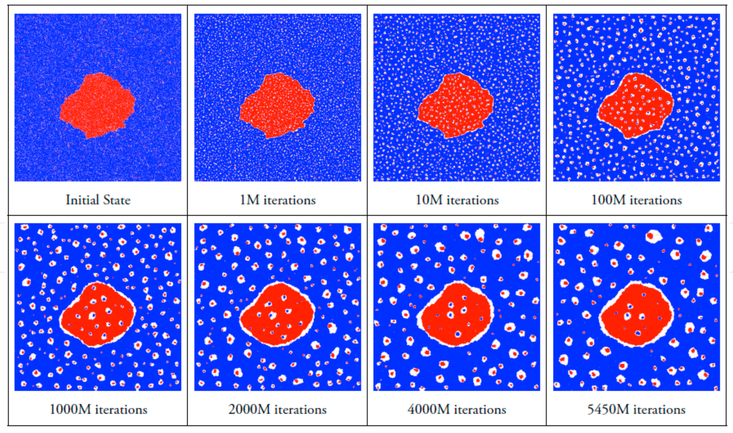
Threads (4 core cpu)	Speedup
1	1
2	1.94
4	3.82
6	4.84
8	5.78
12	2.23
16	1.24

Threads blocks (Nvidia K20 GPU)	Speedup

Results



temperature equivalent to $k_B T = \varphi_{AA} = \varphi_{BB} = 5\varphi_{AB}$. initial state a 250 X 500 array of red atoms embedded within a matrix of blue atoms, the white area in the image corresponds to a void in the material. Initially, red and blue atoms near the void surfacebreak free from the array (1M); the less color dense region simulates a vapor phase (1M/30M). Some roughening of the red/blue interface is observed (30M) since the attraction between red and blue atoms is not as strong as that between like atoms, the vapor phase is lost (100M). This results in a coalescence of red atoms with red atoms and blue atoms with blue atoms where the vapor phase was originally located, and ultimately the smaller red regions join with the original red phase (370M/2000M) *via* a dissolution and re-precipitation mechanism. Indeed some evolution in the morphology of the red phase occurs as the simulation proceeds, and perhaps there is a preference for interfaces oriented along the diagonal directions of the lattice.



Lower temperature equivalent to $2k_B T = \varphi_{AA} = \varphi_{BB} = 5\varphi_{AB}$ using the final state from the high-temperature simulation as our starting point. Equivalent to inducing a sudden cooling to an experimental specimen, and one observes the immediate formation of a very fine dispersion of voids and red particles from the initially supersaturated state. Similarly, voids and blue particles precipitate inside the central red particle.
As the simulation ensues, the particles coarsen (driven by a reduction in $\int \gamma \, dA$), and shape evolution of the central red particle continues. Since the attraction between red and blue atoms is week, they prefer to remain detached from one another, separated by a band of vapor. The stochastic nature of the simulation leads to continual variations in the shapes of these particles, and larger particles are required to discern the features of an equilibrium morphology. The central red particle, as well as the surrounding blue/void interface, still appear to exhibit a tendency toward diagonal interfaces. Ultimately, at least two of the phases (red, blue, and vapor) should evolve to become contiguous bodies.

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