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Analyzing Grain Boundary Dynamics via Kinetic Monte Carlo Simulation

I. Introduction & Research Motive

Monte-Carlo simulations have long been a fundamental tool for Materials Science analysts, due to their impressive ability to capture long time dynamics within complex systems. By manipulating a physical input via random number generation, each simulation captures a potential outcome for a provided system.

By repeatedly running simulations of a given thermal system, in this case, a pure Fe system doped with trace amounts of Cu impurity atoms, one can make conclusive statements pertaining to the grain boundary dynamics under a given set of conditions.

The intention of this research venture is to expand on the current knowledge of the impurity drag effect, and other parameters that effect grain boundary dynamics within metal structures.

KMC Simulation → Improved time range; Random-number fed; Improved vacancy shift

II. Experimental Methods & Analysis

There are five variables accounted for within the python algorithm that are tested to determine their relationship to the velocity of a grain boundary. They are as follows:

- -Temperature
- -Impurity Concentration
- -Order Energy
- -Applied Stress
- -Segregation Energy

The primary means of driving the Grain Boundary is through the applied stress due to the shear-coupling effect. The figure below attempts to explain said effect:

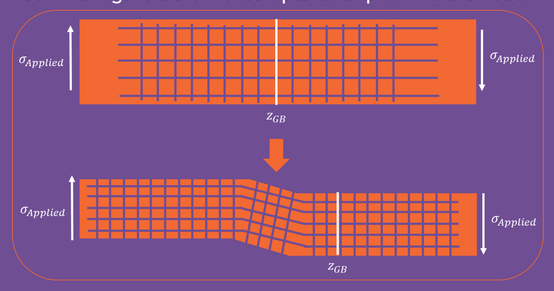

Figure 1. Description of the Shear-Coupling Effect

III. The Energy Landscape & KMC Loop

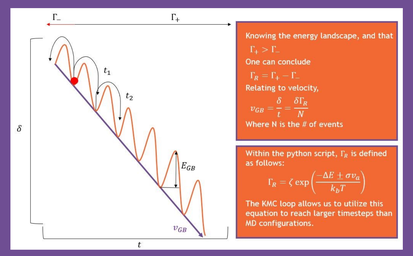

Figure 2. Description of the Simulation's Energy Landscape

The foundation of the algorithms calculations determine whether or not the current state has reached a cutoff energy to drive GB displacement. A description of the rate equation is given in Figure 2.

1. The activation energy to move the GB is accounted for by determining the composition at the boundary
2. If the energy is beyond the cutoff, move the GB in the positive z-direction
3. If the energy is beyond the cutoff but working in the negative direction, move the GB in the negative z-direction

```
if ((rnd < partialSumRates[e]) and (e < z1)):
    typeNei = type[vacNeigh[e]]
    if(typeNei == 2):
        x = lattice[vacNeigh[e],0]
        y = lattice[vacNeigh[e],1]
        z = lattice[vacNeigh[e],2]
        planeX[x] -= 1
        planeY[y] -= 1
        planeZ[z] -= 1
        x = lattice[idv,0]
        y = lattice[idv,1]
        z = lattice[idv,2]
        planeX[x] += 1
        planeY[y] += 1
        planeZ[z] += 1
    type[idv] = typeNei
    idv = vacNeigh[e]
    type[vacNeigh[e]] = 0                                   1
    break
elif ((rnd < partialSumRates[e]) and (e == (nevents-2))):
    zGB -= a0*0.5
    if(zGB < 0): zGB += prdz                                2
    break
elif((rnd < partialSumRates[e]) and (e == (nevents-1))):
    zGB += a0*0.5
    if(zGB >= prdz): zGB -= prdz                            3
    break
```

Figure 3. Segment of Python script with accompanying description

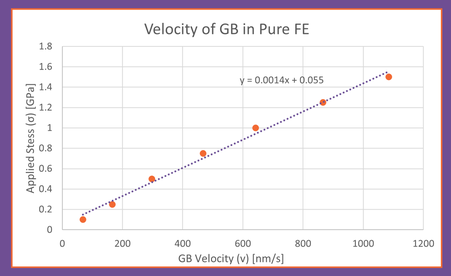

Figure 4. Pure FE Simulation Results

It is impossible to speculate as to the effect of adding impurity to a specimen without first understanding the dynamics of a pure sample. Therefore, various trials were conducted to establish a reference state from which more results could be compared. The data initially follows a linear trend that gradually decays as the velocity reaches a critical value.

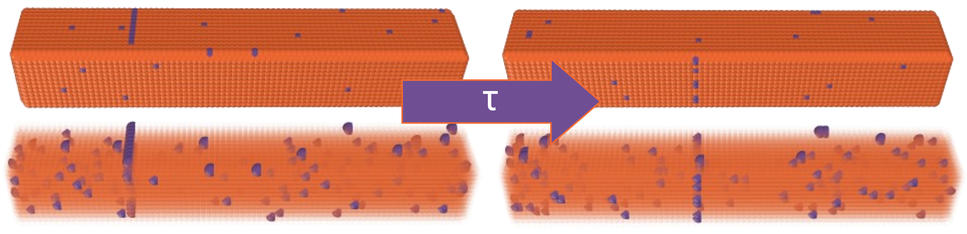

Figure 5.
Atomic composition sample of BCC Fe (Orange) doped with impurity Cu atoms (Purple). The break demonstrates how the GB has moved after timestep τ.

IV. Results

A select set of GB velocity plots as provided by the python code are included within the plots below:

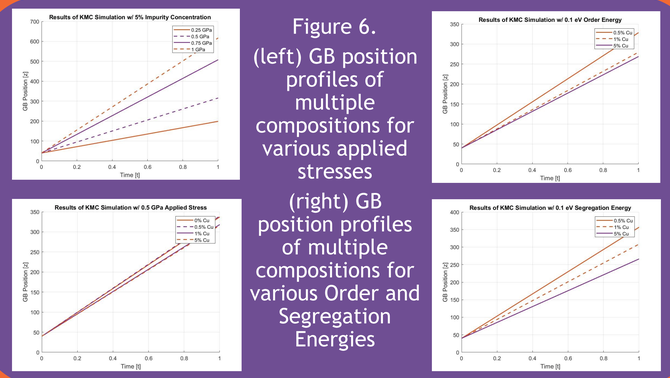

Figure 6.
(left) GB position profiles of multiple compositions for various applied stresses
(right) GB position profiles of multiple compositions for various Order and Segregation Energies

Table 1 serves to map the varable dependence of GB velocity.

Variable	Temperature		Applied Stress		Concentration		Segregation Energy		Order Energy	
Variable Trend	↑	↓	↑	↓	↑	↓	↑	↓	↑	↓
GB Velocity Response	↑	↓	↑	↓	↓	↑	↓	↑	↓	↑

Table 1.
GB Velocity Dependence Map

V. Conclusion

By conducting multiple trials at varied composition, one is able to clearly visualize the impurity drag effect as it applies to grain boundary motion. From the contents of Figure 6, one notes how the GB translates more slowly as the composition of impurity atoms increases. This is because the impurity atoms have a higher magnitude of energy interactions with the grain boundary, slowing its translation across the sample. As this research project is ongoing, all steps moving forward can be visualized below:

Relate findings on impurity drag effect to published academic work → Generate conclusive results defining all previously mentioned variables → Contact lmyhill@clemson.edu → Write and publish a scholarly article detailing all findings within a relevant academic journal

VI. Acknowledgements

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