Kinetics and transition pathways in metastable crystalline alloys

OVERVIEW: Fe alloys that are supersaturated in carbon (~1 wt.%) are structurally metastable but exhibit impressive mechanical strength for applications such as bearings. This compositional metastability enables unique kinetic pathways towards thermodynamic equilibrium that can lead to material failure, especially at elevated temperature and stress. Thus, it is of great interest to understand, simulate, and predict defect evolution and failure in such metastable crystalline alloys.

OBJECTIVES:

• Utilize multiscale modeling principles to develop, explain, and predict kinetics and transitions in the Fe-C system
• Attempt to explain effect of mechanical loading on driving metastable systems to equilibrium

RESULTS:

Work is currently being conducted to extend formation energies of defect clusters in iron previously tabulated using DFT to find transition pathways and transition energies.

![Figure 4. Selected defect formation energies at 160°C in Fe at equilibrium with Fe₃C [1].](image)

<table>
<thead>
<tr>
<th>Defect Species</th>
<th>Formation Energies (in eV)</th>
<th>Defect Species</th>
<th>Formation Energies (in eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C Out</td>
<td>0.58</td>
<td>2Va + 100</td>
<td>3.83</td>
</tr>
<tr>
<td>1Va</td>
<td>2.02</td>
<td>2Va + 1 C1</td>
<td>3.49</td>
</tr>
<tr>
<td>1C + 1Va</td>
<td>3.91</td>
<td>2Va + 2 C1</td>
<td>3.31</td>
</tr>
<tr>
<td>2C + 1Va</td>
<td>1.96</td>
<td>2Va + 11 1</td>
<td>3.85</td>
</tr>
<tr>
<td>3C + 1Va</td>
<td>1.93</td>
<td>2Va + 1 C1</td>
<td>3.66</td>
</tr>
</tbody>
</table>


APPROACH: Use complementary computational approaches (density functional theory [DFT], molecular dynamics [MD], kinetic Monte Carlo [kMC]) to probe relevant length and time scales with the resolution and detail that these modern techniques can afford. Each method will be used to inform and provide information required or inaccessible to the others, compared to experimental data where possible, and integrated to predict the kinetic pathways and mechanical consequences of metastability in Fe-C alloys.

RESEARCH ASSISTANT PROFILE

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Interesting fact: I have a strong interest in Mediterranean civilizations in the time frame of 3000 B.C. to A.D. 400.

References: