Defect Interactions with STGBs in Bi-crystalline FCC Nickel

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Introduction

Understanding defect interactions with grain boundaries is crucial for developing radiation-tolerant materials. In nuclear reactors, neutron irradiation degrades steels and reduces reactor lifespan.

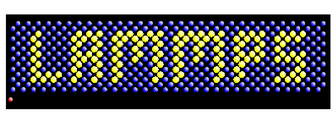
By engineering grain boundaries in alloys, self-healing mechanisms can be introduced to mitigate radiation damage. This study employs atomic-scale simulations to investigate defect evolution in Ni, a model system for FCC steels commonly used in reactors.

Methods

This computational study made use of the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [2] to accurately model the bi-crystalline structure and defect dynamics.

The interatomic interactions were parametrized using the Embedded Atom Method (EAM) [3] interatomic potential where the total energy E_i of the atom i is given by:

$$E_i = F_\alpha\left(\sum_{j\neq i}\rho_\beta(r_{ij})\right) + \frac{1}{2}\sum_{j\neq i}\phi_{\alpha\beta}(r_{ij})$$



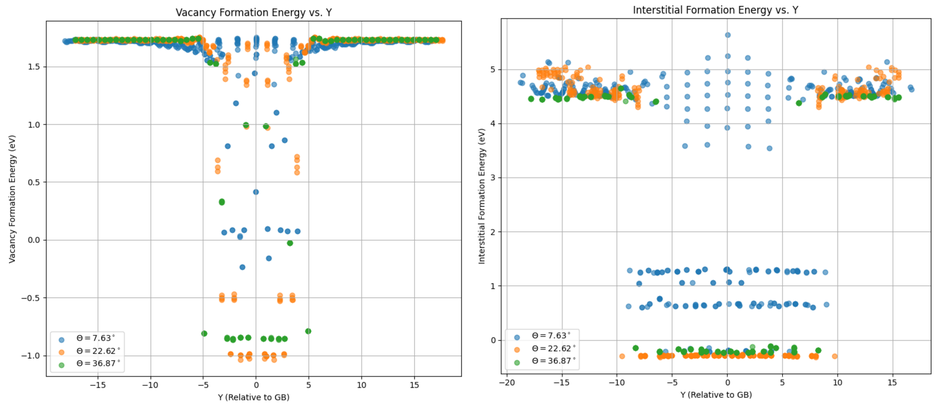


Figure 1. Point defect formation energies plotted against relative distance from the grain boundary (GB) along the y-axis. The three misorientation angles, $\theta_1 = 7.63°, \theta_2 = 22.62°$, and $\theta_3 = 36.87°$ colored in blue, orange, and green respectively correspond to the $(15\bar{1}0)[001]\sum 113$, $(5\bar{1}0)[001]\sum 13$, and $(3\bar{1}0)[001]\sum 5$ STGBs. Variations in point defect formation energies at similar relative distances suggest the presence of lower-energy defect configurations, explored in Figure 2.

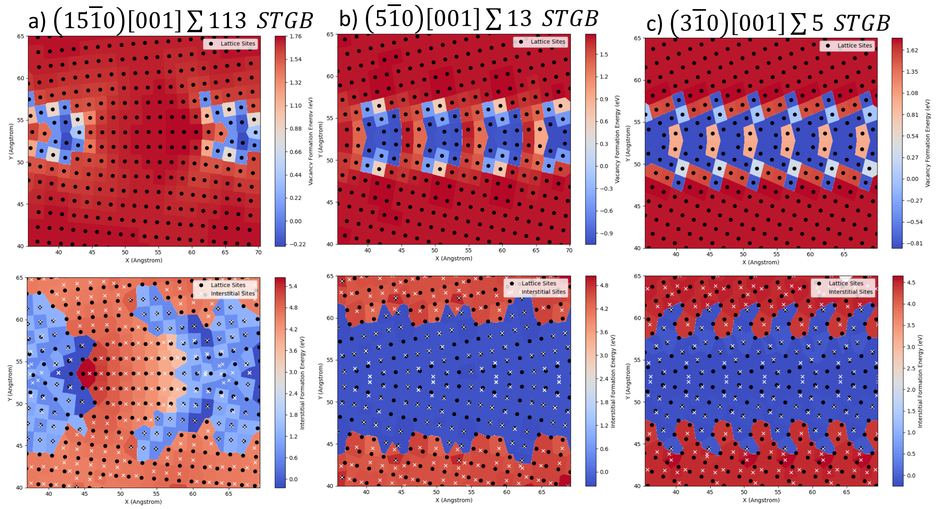


Figure 2. Point defect formation energies around Symmetric Tilt Grain Boundaries (STGBs) in FCC Nickel described by their Coincident Site Lattice (CSL) theory parameters. The point defect formation energies were calculated by sequential addition of point defects (vacancies and ⟨100⟩ self-interstitials) followed by minimization of the resulting structure.

Results

In FCC structures, defect annihilation near the STGB follows a 'chain-like' mechanism similar to that observed in BCC materials. The calculated defect formation energies and the spatial distribution of lower-energy sites suggest a potential correlation with self-healing mechanisms.

Discussion & Conclusion

The intricate defect formation energy patterns reveal the need to consider atomic-scale interactions, as classical rate theory underestimates their complexity. These patterns influence defect diffusion and sink availability, emphasizing the importance of optimizing grain boundaries to enhance defect trapping and improve radiation tolerance.

Acknowledgements

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References

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