Tailoring of Atomic-Scale Interphase Complexions for Mechanism-Informed Material Design

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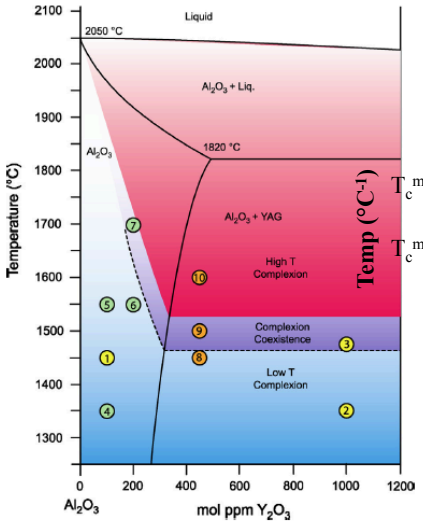
Carnegie Mellon

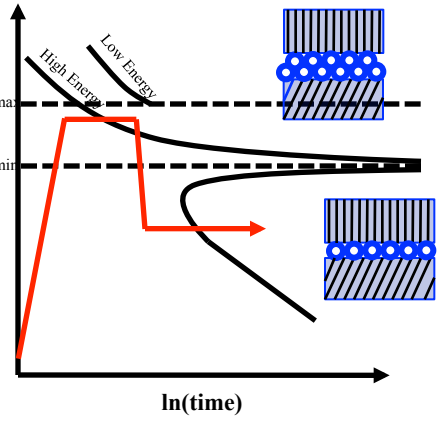
S&T OBJECTIVES

- Establish a unifying scientific framework for the understanding of grain boundaries and their properties in materials using concept of interphase complexions (ICs).
- Exploit the fundamental understanding of role of ICs in existing strategic materials for enhanced processing and improved properties.
- Apply the IC concept to the design and synthesis of bulk nanocrystalline materials and entirely new classes of materials with unique combinations of properties.
- Develop complexion diagrams and TTT complexion diagrams akin to bulk phase diagrams and TTT diagrams for understanding and application of ICs for practical applications.

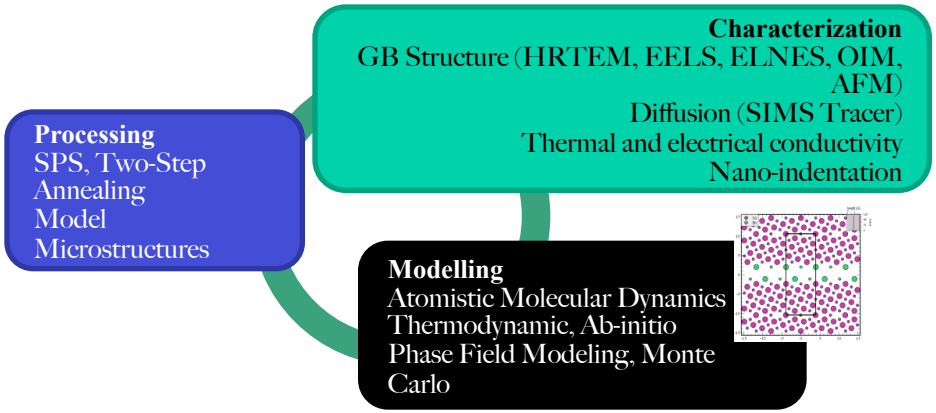
Equilibrium Complexion Diagram



TTT Complexion Diagram



APPROACH



Scientific and Naval Impact/Results

•We have elucidated the critical role of ICs in liquid metal embrittlement in Ni-Bi alloys. We have determined for the first time the exact nature of the atomic ordering of bismuth in nickel grain boundary planes, and shown it to be consistent with reconstruction models for bismuth on nickel surfaces. This new understanding provides guiding principles for mechanism-informed materials design by complexion engineering.

•We are developing equilibrium complexion diagrams and TTT complexion diagrams. These diagrams can be used as engineering tools to tailor microstructure development and macroscopic materials properties.

•We are exploring the role of ICs on the stabilization of bulk nanocrystalline materials. This research focus will provide new perspective on the stabilization mechanisms in this class of materials.