Freitas Research Group

Emergent microstructure physics of materials

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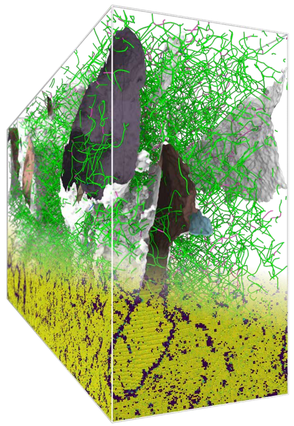
What we do

We are a computational materials science research group based in the Department of Materials Science and Engineering at MIT. Our work is focused on the investigation of mechanisms of microstructural evolution for systems of relevance in materials science broadly construed. We employ a combination of computational, theoretical, and data-driven techniques to perform physics-based modeling of materials.



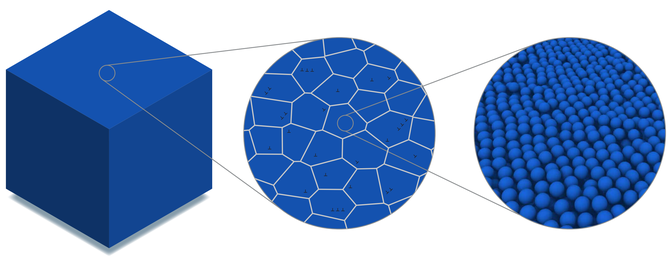
Microstructure { predictive models of materials properties

we bridge this gap

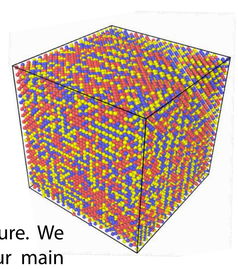
Atoms { most detailed level of materials simulations

Cross-scale atomistic simulations

Numerical modeling of materials is performed at its most accurate level when each atom is accounted for individually. When atomistic simulations contain a large number of atoms – typically more than 10^6 atoms – they enable the investigation of unique materials properties not accessible at small scales. Such simulations are known as cross-scale simulations because they allow the investigation of materials properties across multiple length scales.

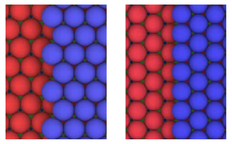


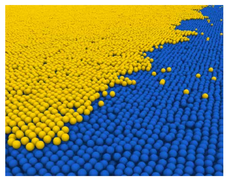
Most materials properties can only be calculated with the use of cross-scale simulations. At these increased length scales, crystalline materials present structural defects that involve a very large number of atoms, such as grain boundaries, dislocations, surface steps, and interfaces among different phases (e.g, solid electrolyte interphase). The collection of all such defects is often referred to as the materials' microstructure. We employ cross-scale atomistic simulations as our main tool in the investigation of materials properties.



Uncovering microstructural elements in cross-scale simulations with Machine Learning

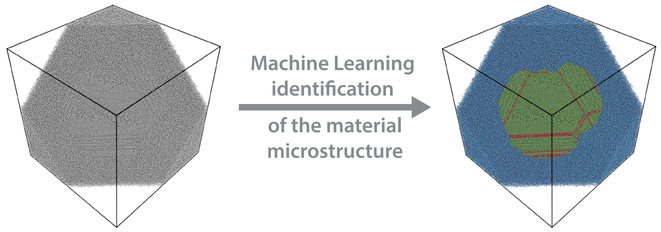
Materials form patterns at many different length scales, but some patterns are only apparent when observing a very large number of atoms; we refer to those as the material microstructure. Cross-scale simulations are unique in their capability of accounting for microstructural elements when calculating materials properties.





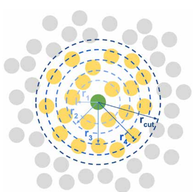
It is difficult to identify the material microstructure in cross-scale simulations because of their spatial complexity. This problem renders cross-scale simulations unsuitable for simple human inspection, severely limiting the amount and quality of scientific information that can be extracted from them.

We develop Machine Learning frameworks for the recognition of microstructural elements in cross-scale simulations and the analysis of their temporal evolution. Our approach aids the interpretation of cross-scale simulations and lends itself easily to the calculation of materials properties while accounting for all mesoscale elements present in the material.

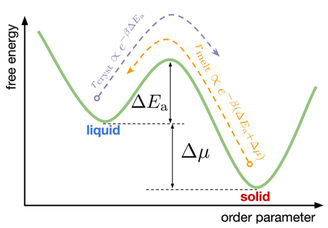


Physics-based modeling with Machine Learning

We perform physics-based modeling of materials by blending prevailing scientific methods with Machine Learning frameworks, producing physically-consistent models and conceptual knowledge. By leveraging Machine Learning as an aid to augment human intuition we facilitate the computation of quantities of practical importance in materials science – such as activation energies, kinetic coefficients, free energies, and growth rates.



The algorithms developed in our research group aim to analyze atomistic simulations with unprecedented sophistication. Our goal is to disentangle the contribution of each atomistic kinetic event leading to microstructural evolution in order to uncover the emergence of structure-property relationships.



$$F(N,V,T;\lambda) = -k_{\mathrm{B}}T\ln\left\{\int \exp\left[H(\mathbf{x};\lambda)\right]\mathrm{d}\mathbf{x}\right\}$$

$$r(T,\mathbb{S}) = k(T,\mathbb{S})\left\{1-\exp\left[-\beta\Delta\mu(T,\mathbb{S})\right]\right\}$$

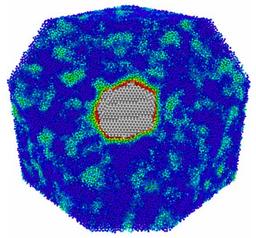
$$S = k_{\mathrm{B}}\ln\Omega \qquad \mathbf{f} = (\boldsymbol{\sigma}\cdot\mathbf{b})\times\boldsymbol{\xi}$$

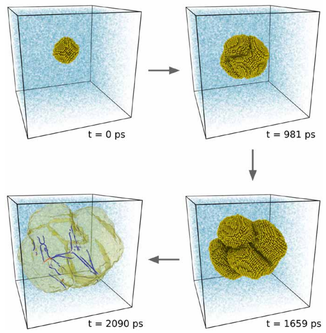
$$\alpha_i = \frac{1}{N}\sum_{j=1}^{N}\boldsymbol{\xi}_i\cdot\boldsymbol{\xi}_j$$

$$\gamma A = -k_{\mathrm{B}}T\ln\left\{\int \exp[-\beta\mathcal{H}(\mathbf{R})\mathrm{d}\mathbf{R}\right\}$$

Solidification and crystal growth

Solidification from the melt is a pervasive process in industry, from metal casting for structural applications to the Czochralski process for semiconductor wafer growth for electronics. It is important to control and understand the crystal growth process because it is at this stage that the material's microstructure morphology is formed, which in turn defines the material's mechanical, transport, and thermal properties.



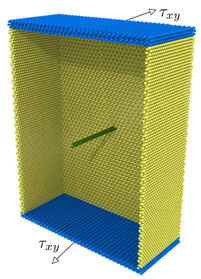


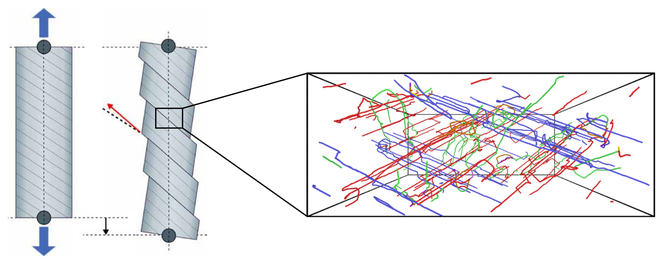
We aim to develop models of crystal growth that are predictive and account for the nonequilibrium and multiscale behavior of materials during solidification. Our approach is derived from atomistics principles and contains a physics-based description of microstructural elements.

Mechanical and transport properties

Microstructural elements (such as dislocations, grain boundaries, etc.) are of significant fundamental interest and also of practical importance due to their impact on mechanical and thermal properties of metals and ceramics.

We investigate the thermodynamics, kinetics, and mechanics of microstructural evolution in high-entropy alloys and ionic conductors. Our goal is to understand how macroscopic materials properties emerge from the underlying physics of microstructural evolution.





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