Microstructural Instabilities in Phase Transformation Materials

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ABSTRACT

Our research is centered on the observation that the delicate interplay between microstructural patterns, material instabilities, and material constants can have dramatic effects on a material's physical properties. We seek to understand and predict how this interplay affects material behavior and how these patterns can be designed to create materials with enhanced properties. In today's talk, I will present two lines of research highlighting our efforts:

First, I will share our recent findings on the origins of hysteresis in soft magnetic alloys. In 1914, a magnetic alloy (now known as the Fe-Ni permalloy) with unusually high magnetic permeability and low hysteresis was discovered at the Bell Telephone Laboratories. Several researchers have attributed this unusual behavior of the permalloy to the small anisotropy constant, however, there are several outliers (e.g., Fe-45Ni has small hysteresis despite large anisotropy constant, similar observation is noted for Sendust alloys), and this theory that dot not explain the complete story of magnetic hysteresis. In a departure from prior work, we hypothesize that a combination of a large local disturbance (needle microstructure) and material constants (e.g., anisotropy, magnetostriction) contributes to the drastic decrease in hysteresis in magnetic alloys. We recently developed a nonlinear framework based on the micromagnetics theory to test this hypothesis, and our findings provide insights into the longstanding permalloy problem and suggest a new mathematical relationship between material constants for which magnetic hysteresis is minimum [1].

Second, I will present our ongoing efforts to mitigate chemo-mechanical degradation in intercalation materials (used as electrodes in lithium batteries). These materials undergo structural transformations (of up to ~10% lattice strains) during intercalation, which expands the material and nucleates microcracks that eventually lead to material failure. By contrast, shape memory alloys—another material—undergo structural transformation without volume changes despite also having large lattice strains. This is because shape memory alloys form microstructures that adapt to the material shape and can be reversibly cycled many times. We seek to mimic shape-memory-like microstructures in intercalation materials to mitigate it's volume changes and interfacial stresses. To this end, we are developing a variational framework to investigate the coupled interplay between crystallographic texture, lithium diffusion, and electrochemical operating conditions. Our findings identify lattice transformation pathways and material kinetics that are conducive to the formation of shape-memory-like microstructures in intercalation materials [2].

References
[1] Balakrishna, A. R. & James, R. D. (2022). Design of soft magnetic materials. npj Computational Materials, 8(1), 4.
[2] Zhang, D. & Balakrishna, A. R. (2023). Designing shape-memory-like microstructures in intercalation materials. Acta Materialia, 118879.

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