Combinatorial Exploration of Phase Transformation in NiTi-Based Shape Memory Alloys

Ni-Ti based shape memory alloys (SMAs) “remember” their shape via a reversible martensitic phase transformation (PT). In the last 70 years, they have found widespread use and continue to be a topic of intense investigation. This is because improving their functional stability remains a key quest as they are sensitive to compositional variations. Tuning their lattice parameters, transformation temperature and thermal hysteresis ($DT$) by alloying with ternary and quaternary elements, therefore, is a challenging materials exploration effort. Combinatorial materials science streamlines synthesis, characterization, and data management processes from multiple high-throughput techniques. To probe a substantial composition space under identical conditions, thin film libraries of Ni-Ti-X ($X = \text{Co, Hf, Pd, V}$) and Ni-Ti-Cu-Y ($Y = \text{Co, Fe, Pd, V}$) alloys were prepared by magnetron co-sputtering. Composition-dependent PT temperature and microstructure were investigated using high-throughput wavelength dispersive spectroscopy (WDS), temperature-dependent resistance $R(T)$, and synchrotron x-ray diffraction (XRD) measurements. Through case studies, I will discuss unsupervised machine learning for phase determination. I will also show how composition-structure-property maps allow us to correlate functional properties with composition and local microstructure. Finally, I will discuss how we can use this methodology to advance the discovery, development, and deployment of materials for emerging technologies. My work was supported by the National Science Foundation Graduate Research Fellowship Program under Grants DGE 1322106 & 1840340.

Naila Al Hasan is a postdoctoral researcher at the National Renewable Energy Laboratory in the photovoltaic reliability and performance group. She defended her dissertation in November 2020 from the department of Materials Science and Engineering at the University of Maryland, College Park. Her doctoral research was focused on developing shape memory alloys for solid-state refrigeration and thermal energy storage applications. She was advised by Dr. Ichiro Takeuchi, a leading expert on synthesis of combinatorial thin film libraries and rapid characterization methodology to develop new electronic, magnetic and smart materials. Her research was awarded the Silver Graduate Student Award at the Materials Research Society Fall 2019 Conference in Boston, MA.

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