ROLE OF NANOSCALE COHERENT PRECIPITATES ON THE THERMO-MECHANICAL RESPONSE OF MARTENSITIC MATERIALS

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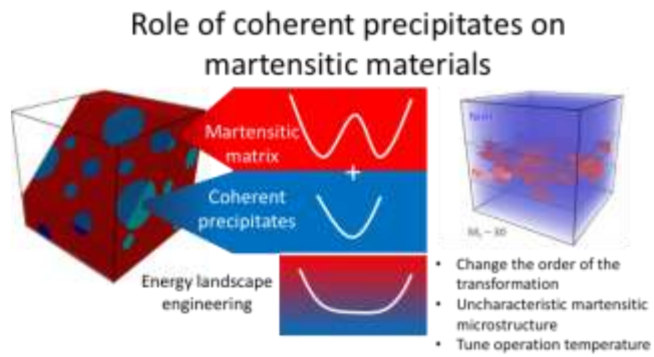
Martensitic phase transitions are first order, diffusionless, solid-to-solid, transformations that underlie shape memory, superelasticity, and strengthening in modern steels, impacting a wide range of technologies. While shape memory and superelasticity in traditional alloys are well understood from a mechanistic point of view, recent unexpected results by our group and others indicate a much richer set of phenomena yet to be fully characterized and with significant potential to result in improved or tunable properties. Specifically, martensitic materials with coherent second phases or nanoscale variations in composition have been shown to exhibit uncharacteristic, and some unprecedented, properties.

I will discuss recent work in our group that combines theory with high-fidelity atomistic simulations to demonstrate that a tailored, coherent second phase can modify the free energy landscape that governs the martensitic transformation and achieve notable changes in response, see Figure on the right. We demonstrated that a coherent second phase can reduce the energy barrier that separates the martensite and austenite phases and reduce the hysteresis of the transformation.[1] More importantly, we demonstrated ultra-low stiffness metallic alloys with high strength.[2] We predicted Young's moduli as low as 2GPa, a value typical of soft materials, in full density metallic nanomaterials. This remarkable result is possible by the stabilization of a thermodynamically unstable state with negative stiffness via interfacial stresses caused by the coherent second phase. MD simulations further revealed how the size and shape of the second phase affects the hysteresis and temperature of the phase transition as well as the martensitic microstructure.[3] In addition, we showed that coherency stresses from an appropriately chose second phase can also change the nature of the martensitic transformation in metallic alloys from first order (discontinuous transitions) to second order or continuous transformations. Large scale MD simulations showed a remarkable change in the character of the martensitic transformation in Ni-Al alloys near the critical point. We observed continuous transformation, uncharacteristic martensitic microstructures, and scaling behavior described by power-law exponents compatible to those of similar second-order transitions.



White lines represent the free energy as a function of lattice parameter in the martensitic phase and in the coherent precipitates. Their combined landscapes (bottom) can exhibit properties not achievable otherwise.

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[2] Reeve, S. T., Belessiotis-Richards, A. & Strachan, A. Harnessing mechanical instabilities at the nanoscale to achieve ultra-low stiffness metals. *Nat. Commun.* 8, 1137 (2017).
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