Superelasticity generated by instability

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Fe-based shape memory alloys (SMAs) are a promising class of smart materials; their low cost and large reversible strain—driven by martensitic phase transformation (MPT) and twinning-detwinning processes—make them suitable for diverse applications. The key areas of use are civil engineering and infrastructure, due to their significant stress-strain hysteresis and compatibility with structural steel, as well as high-strength aerospace components designed for compact, hydraulic-free actuation. Despite their excellent damping and positioning capabilities, Fe-based SMAs exhibit a functional decrease in superelasticity (SE) resulting from dislocation activity, martensite-variant cross-blockage, and residual deformations.

Experiments performed on austenitic steels show that strain front mobility is achieved through the junction of the hard-to-deform (111) orientation and the compliant (110) orientation [1, 2]. To transfer this effect to Fe-based SMAs, a molecular dynamics (MD) simulation was performed. The application of a modified embedded atom method (MEAM) interatomic potential [3] revealed that the martensitic phase transformation (MPT) starts within elastic eigen-subspaces on both sides of the boundary; however, due to energetic advantages, martensite propagates primarily within the (110)-oriented part of the SMA bicrystal under tension. The (111) component serves as a trigger area, resulting in the formation of large reversible strains. This process is driven by the reduction of the Gibbs free energy of the unstable, traveling martensite-austenite interface as it returns toward the coherent (111) || (110) junction. To further investigate this instability-driven SE, additional bicrystals featuring coherent boundaries were analyzed. The underlying mechanisms identified in this work offer a pathway toward mitigating functional fatigue in Fe-based SMAs.

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