Atomistic modelling of structure and mobility of twin boundaries in NiTi shape memory alloys

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Shape memory alloys (SMAs) possess unique properties that make them suitable for various applications, including energy-efficient actuators, biomedical devices for minimally invasive surgery, and aircraft morphing. Their distinct behaviour involves the recovery of large strains under stress or thermal cycles, and it is well-known that microstructural twinning governs this exotic mechanism. However, it is crucial to understand the structure and mobility of twin systems in martensite microstructures to determine why specific twinning systems arise more frequently than others [1].
In this study [2,3], we demonstrate with the prototypical NiTi SMA that twin interface mobility can strongly influence twin emergence. We employ an integrated methodology that combines crystallographic theory [4], state-of-the-art atomistic modelling, topological model [5], and validation using high-resolution transmission-electron micrographs [6]. Our atomistic model is based on a machine learning Atomic Cluster Expansion (ACE) interatomic potential trained on an extensive density functional theory (DFT) database, and tested on key benchmark properties of B2 and B19' phases in NiTi.
Our atomistic simulations reveal that twinning stress, rather than interfacial energy, determines the occurrence of twins. Moreover, our simulations address long-standing questions by explaining the atomistic structure and propagation mechanisms of twin interfaces at zero and finite temperatures, which established theories of martensite crystallography cannot explain. This mechanistic understanding of the role of interface mobility in twin formation can help predict variant selection and inform the design of SMAs with enhanced functional performance. Moreover, our predictions of twin interface energetics and kinetics can inform higher scale models of microstructure formation (e.g. phase-field).

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