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Deformation physics of shape memory alloys – Fundamentals at atomistic frontier



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ABSTRACT

Application spectrum of shape memory alloys (SMA) is expanding rapidly and proportionately so is the engineering demand for superior materials. An essential prerequisite to developing novel SMAs is a clear perception of the deformation physics underlying their extraordinary shape recoverability. To that end, modern atomistic simulation tools have proffered state-of-the-art models, which usher in new clarifications for SMA deformation properties. It was found, for example, that ab initio energy pathways are at the core of dictating the extent of shear and shuffle for both phase transformation and variant formation at atomic lengthscale. These important revelations are accomplished by addressing inherent solid-state effects, which underpin the natural tendency to seek the energetic ground state. Moreover, empirical potential based models, benefitting from ab initio calculations, have allowed an atomic-resolution view into the phase evolution and the concurrent twinning phenomena relating directly to constitutive properties. Here, we revisit salient examples of these cutting-edge theoretical discoveries regarding SMA deformation along with discussions on pertinent experimental evidences.

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Contents

1. Background	50
1.1. Perspective on SMA literature	50
1.2. Significance of atomistics	52
2. Overview of general deformation behaviors of SMAs	53
3. Case study: equiatomic NiTi SMA	53
3.1. Stability of phases from first principles	53
3.1.1. Energy pathway	53
3.1.2. B19' versus B33	54
3.2. Calculation of elastic moduli	54
3.2.1. Predictions based on single crystal and their significance	54
3.2.2. Modified elastic anisotropy in a twinned lattice	55
3.2.3. Elastic anisotropy of Ni ₄ Ti ₃ precipitate	57
3.3. Energetics of twinning	57
3.3.1. Brief overview of various twinning modes in NiTi	57
3.3.2. Type II twinning in martensite (B19') phase	59

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3.3.3.	Compound twinning in martensite (B19') phase	61
3.3.4.	{201} type twinning in B19' martensite phase	61
3.3.5.	{211} twinning in austenite (B2) phase	63
3.3.6.	{114} twinning in B2 austenitic phase	64
3.4.	Molecular dynamics models	65
3.4.1.	Early endeavors on empirical potential	65
3.4.2.	Recent developments	67
3.4.3.	Promising developments	69
4.	Case study: ferromagnetic Ni ₂ MnGa SMA	70
4.1.	Empirical observation of structure-property relations	70
4.2.	Atomistic investigation from first principles	70
4.2.1.	Energetics-tetragonality relationships in austenite and martensite phases	72
4.2.2.	Shearing energetics of martensite variants	73
5.	Case study: ferromagnetic Ni ₂ FeGa SMA	73
5.1.	A rationale for martensite modulation	73
5.2.	Implications for deformation reversibility	74
5.3.	Devising potential strategies for alloy improvement	74
6.	Case study: Co-Ni-Al SMA	75
7.	Case study: Ti-Nb based SMAs	75
7.1.	Atomistic mechanism of transformation	76
8.	Case study: Fe-Mn-Si based SMAs	78
8.1.	Transformation mechanism and avenues for atomistic modeling	78
9.	Case study: Fe-Mn-Ni-Al SMA	79
9.1.	Transformation mechanism	80
9.2.	Experimental evidence of similar mechanism	80
10.	Other emerging studies: Ni-Ti-Hf, Ti-Ni-Cu, Ni-Mn-Sn SMAs	80
10.1.	Ni-Ti-Hf based alloys	80
10.2.	Ti-Ni-Cu based SMAs	81
10.3.	Ni-Mn-Sn based SMAs	81
11.	Concluding remarks	81
	Acknowledgement	82
	References	82

1. Background

1.1. Perspective on SMA literature

Nowadays shape memory alloys are finding diversified applications in a wide array of industries (e.g. biomedical, aerospace, automotive) owing to their extraordinary deformation recoverability [1–3]. The mechanical healing ability of an SMA-made component (e.g. a cardiovascular stent) is principally rooted upon reversible martensitic transformations at microstructural level [4]. Deformation micro-mechanisms, however, could be rather complex, involving internal twinning, precipitation, intermediate phase nucleation, etc. [5–8]. Variables across multiple spatial scales (ranging from sub-nanometer quantum forces within a single grain to micron-level multi-grain interactions) collectively contribute to the overall inter-crystal transformability. Given their technological importance, predicting SMA behavior remains a dedicated discipline, currently employing theoretical tools spanning atomistics to continuum [9,10]. This article provides an overview of the atomic lengthscale mechanisms pertaining to molecular dynamics and density functional theory studies. More discussions follow on these two approaches. Fig. 1 puts the current topics into perspective.

The extent of SMA research, both experimental and theoretical, is vast. It is instructive to categorize them lengthscale-wise, as illustrated by Fig. 2, to develop a proper perspective. It follows that the majority of studies concerns continuum scale behaviors, namely, thermodynamics [11], constitutive modeling [12–14], finite element simulations [15–18]; experimentally, thermo-mechanical characterizations and component performance assessment remain the primary emphases [19,20]. At the mesoscale (i.e. grain level), digital image correlation (for measuring strain localizations [21,22]), X-ray diffraction (for phase identification [23–25]), electron microscopy (for studying microscopic defects [26]) and electron backscatter diffraction (for texture determination [27]) are the common experimental techniques for microstructure characterization. On the other hand, theorization of mesoscale variables (e.g. roles of grain size, texture, precipitates) is approached commonly with phenomenological assumptions [28–32]. Such models are tied back-to-back with empirical observations from which are extracted the requisite material constants i.e. the fitting parameters essential for accurate prediction of macroscale constitutive responses [33]. Phase field models consider the evolution of the martensitic phase in terms of free energy functionals [34–36] (per the Ginzburg-Landau theory [37]). The advent of molecular dynamics [38] in the SMA context is a recent development (over last decade) as a promising mesoscopic tool, capable of addressing sub-micron phenomena within a single grain. The quantum lengthscale tools include density functional theory based predictions of sub-nanometer physics [39],

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