Progress in Materials Science 88 (2017) 49–88

Contents lists available at ScienceDirect

Progress in Materials Science

journal homepage: www.elsevier.com/locate/pmatsci

Deformation physics of shape memory alloys – Fundamentals at atomistic frontier

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ARTICLE INFO

Article history:
Received 13 January 2017
Received in revised form 21 March 2017
Accepted 24 March 2017
Available online 27 March 2017

Keywords:
Shape memory
Martensitic transformation
Phase reversibility
Density functional theory
Molecular dynamics

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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http://dx.doi.org/10.1016/j.pmatsci.2017.03.003
0079-6425/

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],