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An origin of functional fatigue of shape memory alloys

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ABSTRACT

Functional fatigue (FF) during thermal and mechanical cycling, which leads to the generation of macroscopic irrecoverable strain and the loss of dimensional stability, is a critical issue that limits the service life of shape memory alloys (SMAs). Although it has been demonstrated experimentally that such a phenomenon is related to microstructural changes, a fundamental understanding of the physical origin of FF is still lacking, especially from a crystallographic point of view. In this study, we show that in addition to the normal martensitic phase transformation pathway (PTP), there is a symmetry-dictated non-phase-transformation pathway (SDNPTP) during phase transformation cycling, whose activation could play a key role in leading to FF. By investigating crystal symmetry changes along both the PTPs and SDNPTPs, the characteristic types of defects (e.g., dislocations and grain boundaries) generated during transformation cycling can be predicted systematically, and agree well with those observed experimentally in NiTi. By analyzing key materials parameters that could suppress the SDNPTPs, strategies to develop high performance SMAs with much improved FF resistance through crystallographic design and transformation pathway engineering are suggested.

1. Introduction

Since its discovery [1], shape memory alloys (SMAs) have found many advanced applications in medical and engineering devices [2–5]. However, one of the critical issues limiting the application of SMAs is functional fatigue (FF) during repeated actuation through either thermal or load cycling (i.e., transformation cycling). It is reported that macroscopic irrecoverable strain (also called open-loop strain) can be accumulated in commercial SMAs, resulting in the loss of dimensional stability [6–18]. Even though such FF dictates the functionality, durability and service life of SMAs, its physical origin is far from clear and, thus, a systematic way to characterize and control it is still lacking. This is reflected partly by the various loose terminologies introduced in the literature to describe the phenomenon over the years, including "functional fatigue" and "low temperature creep" [6,7]. Fatigue is commonly associated with crack initiation and propagation during cyclic loading while creep is related to time-dependent deformation at elevated temperatures, and neither of them is necessarily related to phase transformations. In contrast, FF found in SMAs is associated exclusively with structural phase transformations. Even though it is similar to fatigue and creep with regard to irrecoverable deformation caused by external loads below the yield strength, it is transformation-cycle-dependent rather than just stress-cycle- or time-dependent and does not necessarily happen at elevated temperatures. Keeping these differences in mind we formulate in this study a new theoretical framework based on crystallographic theory of structural phase transformations to reveal a unique physical origin and distinctive features of FF in at least some SMAs. However, to keep consistency with existing literature we continue to use the term "functional fatigue".

Ample experimental results have shown that a considerable amount of crystalline defects are generated during load- or temperature-cycling in a number of typical SMA systems [6–8,16–19]. In comparison with what happens in conventional dislocation plasticity, defect generation during FF has several distinctive features. As observed in experiments [14–18], the irrecoverable strain can be accumulated during thermal cycling around the martensitic transformation (MT) temperature with a bias-load much lower than the yield stress, and the total irrecoverable strain depends strongly on the number of cycles. This suggests a strong correlation between defect generation and accumulation and transformation cycling. More interestingly, in addition to the generation of dislocations, grain refinement (without apparent

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recrystallization) and formation of special grain boundaries (Σ boundaries) have been observed during the transformation cycling [19]. These recent observations imply not only a crystallographic origin of the defects, but also a unique generation mechanism, different from that in conventional dislocation plasticity. At a higher level, these results suggest a fundamental relationship between FF and the unique structural change (i.e., symmetry change) during phase transformation cycling.

Several crystallographic studies have attempted to understand defect generation during MTs. Bhattacharya et al. [20] proposed that if the symmetry groups of the parent and product phases cannot be included in a common finite group, dislocations are inevitably generated. On the other hand, if a group-subgroup relationship exists, the martensitic transformation should be fully reversible and no other lattice defects such as dislocations should be generated, assuming that local stresses produced by the MT would not cause plastic yielding. However, for the most widely used commercial SMA, the NiTi system, even if it undergoes a B2 to B19′ MT that satisfies the group-subgroup relationship and self-accommodation among 12 martensitic variants can be accomplished by 192 twinning modes, defect generation is still widely observed during thermal cycling especially under a biased-load that is much lower than the yield stress [6,7,11–14]. On the other hand, another crystallographic criterion called the “cofactor condition” was proposed recently for the design of SMAs, and Zn-Au-Cu and Ni-Ti-Cu alloys have been identified for enhanced reversibility using (or partially using) this criterion [21,22]. However, such a criterion is rather strict and only the lattice parameters of specific systems can satisfy coincidentally the cofactor condition. Furthermore, to study the FF phenomenon, the effect of biased load on the generation of defect structures has to be considered.

In this article, the physical origin of FF is investigated by phase transformation pathway (PTP) and symmetry-dictated non-phase-transformation pathway (SDNPTP) analyses. It is demonstrated that during transformation cycling, defects including both dislocations and special grain boundaries are generated due to symmetry breaking along the SDNPTPs that are easily activated by either internal or external stresses. By investigating the symmetry change along the SDNPTPs in NiTi, the types of defects induced by the transformation cycling are predicted systematically, revealing <100>{011} type dislocations and Σ grain boundaries, which agree with the experimental observations [19]. Through the PTP and SDNPTP analyses, key material parameters are identified and strategies to improve FF resistance of SMAs are developed. A systematic way of designing SMAs with improved FF resistance is also discussed from the crystallographic point of view.

2. Crystallographic origin of defect generation during martensitic transformation with group-subgroup relationship

As a classical description of the energetics of phase transformations with symmetry breaking in Landau theory, the free energy landscape is represented by a Landau polynomial in which the free energy of nearby low symmetry states (referred to as the Ericken-Pitteri Neighborhood (EPN) [23,24]) are described by a series expansion with respect to the high symmetry parent phase state. In particular, when the order parameter characterizing the structural change during the phase transformation is chosen as the uniform lattice distortion (i.e., inelastic strain), the PTPs described by the Landau polynomial could be taken as *localized* deformation pathways. On the other hand, because of the translational symmetry of a crystal that leads to an infinite symmetry group (i.e., space group), there are infinite numbers of ways of lattice invariant deformations. As a consequence, there are infinite numbers of deformation states describing the same lattice in the deformation space, and all of these states are connected by *non-localized* deformation pathways (lattice invariant deformation) dictated by the crystal symmetry, leading to an infinite pathway network in the deformation space [20]. In general, all the above non-localized deformation pathways are intrinsic features of a given crystal lattice, not necessarily involved in any phase transformation. Even though both PTPs and NPTPs are in the deformation space, they are usually treated independently in the literature, which is a good simplification when the deformation caused by phase transformation is much smaller than the lattice invariant deformation. However, if the lattice distortion associated with a phase transformation is large enough (i.e., in most SMAs), the PTPs and NPTP could be interconnected and hence new pathways may appear, which has to be taken into account in analyzing domain and defect structures. Here we refer to the new pathways as SDNPTPs in order to distinguish them from either PTPs or the deformation pathways related to conventional dislocation and twinning plasticity.

To illustrate the interconnection between the PTPs and SDNPTP as well as the connection between SDNPTPs and FF in SMAs at the intuitive level, a simplified 2D example is presented. For MT from a rectangular lattice (α austenite, point group: *2mm*) to a parallelogram lattice (β martensite, point group: *2*), the transformation mechanism could be described as a simple shear deformation (Fig. 1). As a result, each atom in the α lattice corresponds to an atom in the β lattice, which establishes a lattice correspondence between the two lattices as illustrate by the red frames in Fig. 1. If the absolute value of the shear strain is smaller than 0.5, the free energy landscape among the parent phase structural state and the two nearby crystallographically equivalent and energetically degenerate martensitic structural states (i.e., β-1 and β-2 deformation variants [25]) can be described by a Landau polynomial with the transformation strain (shear strain) being the order parameter (Fig. 1).

However, such a description of PTPs is local and the non-localized lattice-invariant deformation pathways are not captured

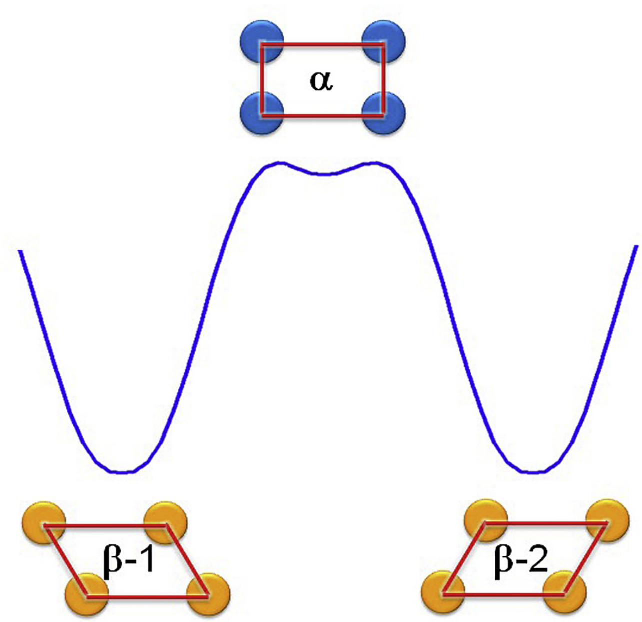

Fig. 1. Schematic drawing of a rectangle to parallelogram transformation in 2D and the local energy landscape as described through a Landau polynomial. (The lattice correspondence is shown by the red frames.). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)