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# The evolution of microstructure during twinning: Constitutive equations, finite-element simulations and experimental verification

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ABSTRACT

In this work, we develop a rate-dependent, finite-deformation and crystal-mechanics-based constitutive theory which describes the twinning in single-crystal metallic materials. Central to the derivation of the constitutive equations are the use of fundamental thermodynamic laws and the principle of micro-force balance [Fried, E., Gurtin, M., 1994. Dynamic solid–solid transitions with phase characterized by an order parameter. Physica D 72, 287–308]. A robust numerical algorithm based on the constitutive model has also been written and implemented in the ABAQUS/Explicit [*Abaqus reference manuals*, 2007. SIMULIA, Providence, R.I.] finite-element program.

Physical experiments in compression, cyclic tension-compression, plane-strain compression and three-point bending have been conducted on an initially-martensitic shape-memory alloy single crystal. In order to determine the material parameters in the constitutive model, the stress–strain result from a finite-element simulation of the single crystal in simple compression was fitted to the corresponding result determined from the physical experiment. With the material parameters determined, we show that the stress–strain and force–displacement curves for the other aforementioned experiments were predicted to be in good accord by our constitutive model. Our calculations show that the overall stress–strain responses and the microstructure evolution exhibited by the single crystal shape-memory alloy during the twinning process is highly dependent on the initial microstructure, crystal orientation and the loading conditions e.g., tension vs. compression etc.

Finally, we show that by suitable augmentation of the free energy density with a gradient energy, the sensitivity of the

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calculated twin plane interface thickness to the density of the finite-element mesh can be minimized. This makes the tracking of the twin plane interface during the twinning process possible without the aid of jump conditions.



## 1. Introduction

Under suitable driving forces, twinning in metallic materials occur due to the motion of atoms such that the atoms on one side of a twin boundary mirrors the atoms on the other side. The coordinated movement of these atoms will cause a reorientation of a part of the crystal. For many technologically-important metallic materials, twinning can be the most dominant mechanism for accommodating inelastic deformations e.g., low-symmetry crystals at low homologous temperatures (Magnesium, Titanium), compound semiconductors (GaAs), martensitic shape-memory alloys etc. Recently, martensitic single-crystal shape-memory alloys (SMA) have been shown to be a very promising candidate for actuator and sensor applications. These SMA alloys mentioned above make good actuation devices due to the low stress requirements to cause twinning (and actuation). Some examples of these SMAs (also known as ferromagnetic SMAs) include the NiMnGa, FePd and CoNiAl alloys. Of these different alloys, the near-Heusler NiMnGa systems are the currently most popular SMA for the aforementioned applications.

The macroscopic manifestation of twinning can be explained by using a shape-memory alloy as an example. Before doing so, it is important to describe the different microstructures that can exist in a shape-memory alloy. Under zero stress and at temperatures above the *austenitic finish temperature*, a shape-memory alloy exists in the *austenite* phase. Cooling the austenitic SMA to temperatures below the *martensitic finish temperature* will cause the SMA to transform from an austenitic phase to a *martensitic* phase. The martensite plates which nucleate from the austenite phase will consist of martensite twin variants (or *variants*) i.e., equal energy configurations of martensite single crystals which are differently oriented. Each single crystal martensite is twin-related to the other martensitic single crystals.

Taking the example of the ferromagnetic SMAs mentioned above, the transformation from a single crystal austenite to a single crystal martensite results in a conversion from a cubic crystal structure to a tetragonal crystal structure (see Fig. 1). Since this conversion of crystal structure can take place in 3 different ways, there will be a total of 3 martensitic variants identified by variant 1, variant 2 and variant 3. With all indices henceforth given with respect to the cubic crystal basis, martensite variant 1, variant 2 and variant 3 have their $c$-axes aligned along the [1 0 0], [0 1 0] and [0 0 1]-directions, respectively.

To explain twinning under the application of mechanical loads, we are aided by the schematic stress–strain diagram for a martensitic SMA as shown in Fig. 2. Starting with the material being under zero load and no deformation (point $a$), the material fully consists of a single-crystal martensite variant $i$. Under the application of deformation, the material will first deform elastically. At a critical stress level, the conversion from martensite variant $i$ to martensite variant $j$ will start to occur due to the nucleation and propagation of a twin plane interface between variant $i$ and variant $j$. Continuous deformation will result in the further conversion from variant $i$ to variant $j$. At any point $b$ on the stress plateau, the material will consist of a mixture between variant $i$ and variant $j$. At point $c$, the material fully consists of a single-crystal variant $j$. Further deformation beyond point $c$ will cause the material to deform elastically. Reverse loading from point $c$ to point $d$ will result in the material being elastically unloaded to a state of zero stress. However, there is a residual inelastic deformation in the material as a result of the prior motion of the twin interface. This residual inelastic deformation is also termed as a *transformation* or *twinning* strain.

Further reversal of the deformation will cause variant $i$ to grow at the expense of variant $j$ at a critical stress level through the motion of the twin plane interface in the reverse direction. Continued reversal of deformation will result in the further conversion from variant $j$ to variant $i$. At any point