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Dislocation slip stress prediction in shape memory alloys

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ABSTRACT

We provide an extended Peierls–Nabarro (P–N) formulation with a sinusoidal series representation of generalized stacking fault energy (GSFE) to establish flow stress in a Ni_2FeGa shape memory alloy. The resultant martensite structure in Ni_2FeGa is $L1_0$ tetragonal. The atomistic simulations allowed determination of the GSFE landscapes for the $(1\,1\,1)$ slip plane and $\frac{1}{2}[\bar{1}\,0\,1]$, $\frac{1}{2}[\bar{1}\,1\,0]$, $\frac{1}{6}[\bar{2}\,1\,1]$ and $\frac{1}{6}[1\,1\,\bar{2}]$ slip vectors. The energy barriers in the $(1\,1\,1)$ plane were associated with superlattice intrinsic stacking faults, complex stacking faults and anti-phase boundaries. The smallest energy barrier was determined as 168 mJ/m^2 corresponding to a Peierls stress of 1.1 GPa for the $\frac{1}{6}[1\,1\,\bar{2}](1\,1\,1)$ slip system. Experiments on single crystals of Ni_2FeGa were conducted under tension where the specimen underwent austenite to martensite transformation followed by elasto-plastic martensite deformation. The experimentally determined martensite slip stress (0.75 GPa) was much closer to the P–N stress predictions (1.1 GPa) compared to the theoretical slip stress levels (3.65 GPa). The evidence of dislocation slip in Ni_2FeGa martensite was also identified with transformation electron microscopy observations. We also investigated dislocation slip in several important shape memory alloys and predicted Peierls stresses in Ni_2FeGa, NiTi, Co_2NiGa, Co_2NiAl, CuZn and Ni_2TiHf austenite in excellent agreement with experiments.

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1. Introduction

1.1. Background

Shape memory alloys with high temperature (Chumlyakov et al., 2008; Hamilton et al., 2006a,b, 2007; Hartl et al., 2010; Oikawa et al., 2003; Omori et al., 2004; Santamarta et al., 2006; Sutou et al., 2004) and magnetic actuation capabilities (Arndt et al., 2006; Brown et al., 2002; Kokorin et al., 1992; Planes et al., 1997; Pons et al., 2005; Ullakko et al., 1996; Zheludev et al., 1996) have generated considerable recent interest. The development of such alloys has traditionally relied on processing of different chemical compositions, making polycrystalline ingots, and then taking the expensive route of making single crystals. Then, the alloys have been tested under temperature or stress cycling, and in the case of ferromagnetic shape memory alloys under applied magnetic fields (Ullakko et al., 1996). Additional tests may be necessary to establish the elastic constants, lattice constants and to determine the twinning stress and the slip stress of the austenite and martensite phases. There are numerous advantages to establishing the material performance in advance of the lengthy experimental procedures with simulations to accelerate the understanding of these alloys and to establish a number of key properties. Therefore, rapid assessment of potential alloys can be ascertained via determination of twinning, slip and phase transformation barriers, the stability of different phases (austenite and martensite), their respective elastic constants, and lattice constants. In this paper

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we focus on the slip stress determination with simulations and compare the results to experiments. We combine the ab-initio calculations with a modified mesoscale Peierls–Nabarro based formulation to determine stress levels for slip in close agreement with experiments.

We utilize the Ni_2FeGa as an example system to illustrate our methodology and then show its applicability to the most important SMAs. The Ni_2FeGa alloys are a new class of shape memory alloys (SMAs) and have received significant attention because of high transformation strain magnitudes (>12% in tension and >6% in compression) and low temperature hysteresis. They also have the potential for magnetic actuation and high temperature shape memory (Hamilton et al., 2007; Omori et al., 2004). The magnetic actuation requires twinning at low stress magnitudes, and high temperature shape memory can only occur in the presence of considerable slip resistance. These alloys are proposed to be a good alternative to the currently studied ferromagnetic Ni_2MnGa-based SMAs due to their superior ductility in tension (Barandiarán et al., 2008; Oikawa et al., 2002; Sutou et al., 2004; Yu et al., 2009). There are several crystal structures identified in Ni_2FeGa (Hamilton et al., 2006a, 2007; Whang et al., 1998), which exhibits martensitic transformations from $L2_1$ cubic austenite to intermediate 10M/14M modulated monoclinic martensites, and finally to the $L1_0$ tetragonal martensite (Efstathiou et al., 2008; Hamilton et al., 2008; Masdeu et al., 2005; Sutou et al., 2004). However, one can get a single stage transformation from $L2_1$ to $L1_0$ as temperature is increased (Hamilton et al., 2007), also in the case of nano-pillars (Ozdemir et al., 2012), and upon aging treatment (Chumlyakov et al., 2012). Therefore, a study on the $L1_0$ martensite is both scientifically interesting and technologically relevant. The phase transformation of Ni_2FeGa has been experimentally observed and theoretically investigated using atomistic simulations (Efstathiou et al., 2008; Hamilton et al., 2006a; Martynov, 1995; Segui et al., 2005; Sehitoglu et al., 2012). The results show that the $L2_1$ austenite requires high stress levels for dislocation slip while undergoing transformation nucleation at much lower stress magnitudes (Sehitoglu et al., 2012). However, the plastic deformation of $L1_0$ martensite via dislocation slip has not been fully understood, although it is very important in understanding the shape memory performance.

Fig. 1 shows a schematic of the stress–strain curve of Ni_2FeGa at temperatures in the range 75° C to 300 °C where $L2_1$ can directly transform to $L1_0$. These temperatures are significantly above the austenite finish temperature. The initial phase of Ni_2FeGa is $L2_1$ and it transforms to $L1_0$ when the stress level reaches the transformation stress. The transformation occurs at a near plateau stress followed by elastic deformation of martensite. With further deformation, dislocation slip (of $L1_0$) takes place at a critical stress designated as σ_{slip}. This stress is much higher than the transformation stress. During unloading, the reverse phase transformation occurs with plastic (residual) strain remaining in Ni_2FeGa as part of the deformation cannot be recovered.

It is well known that plastic deformation occurs via dislocation glide; and at the atomic level, dislocation glide occurs upon shear of atomic layers relative to one another in the lattice. At the dislocation core scale, quantum mechanics describe the atomic level interactions and the forces exerted on atoms; while at the mesoscale level, elastic strain fields of defects address the interactions (Kibey, 2007). The ensemble of dislocations and their interactions with the microstructure define the continuum behavior.

With atomistic simulations one can gain a better understanding of the lattice parameters and the unstable fault energies of $L1_0$. Therefore, atomistic simulations in this case will provide additional insight into material's behavior and the deformation mechanisms (Ezaz et al., 2011). Fig. 2 shows the different length scales associated with plasticity of transforming Ni_2FeGa alloys. The generalized stacking fault energy (GSFE) surface (γ-surface) at the atomic level (via atomistic simulations using density functional theory (DFT)) is shown at the lowest length scale. Of particular interest is the (1 1 1) plane, and from

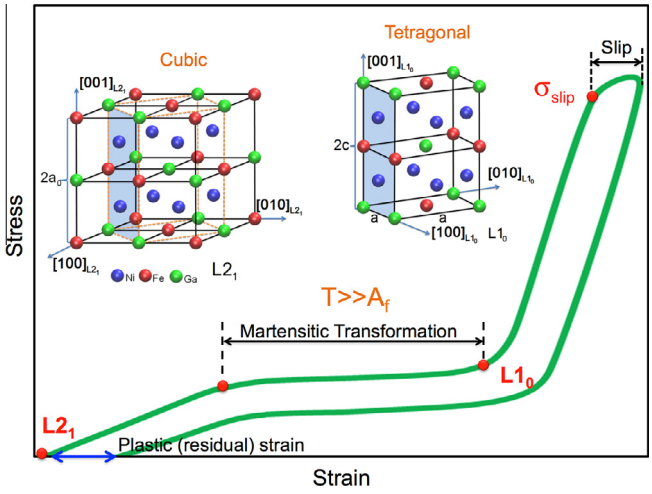

Fig. 1. Schematic illustration of the stress–strain curve showing the martensitic transformation from $L2_1$ to $L1_0$, and the dislocation slip in $L1_0$ of Ni_2FeGa at elevated temperature. After unloading, plastic (residual) strain is observed in the material as deformation cannot be fully recovered.

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