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A model coupling plasticity and phase transformation with application to dynamic shear deformation of iron

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We dedicate this paper to Alain Molinari on the occasion of his 65th birthday for his contributions to many areas of mechanics of materials, particularly to dynamic deformation and adiabatic shear localization.

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Plasticity
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ABSTRACT

A simple model that brings together well-established thermo-mechanical models of plasticity with those of martensitic phase transformation into a single thermodynamic framework is proposed. The presentation is in one space dimension, but the framework is general so that the model may be extended to higher dimensions. The model is used to study recent experiments on the $\alpha \Longleftrightarrow \epsilon$ martensitic phase transformation of pure iron under dynamic, shear-dominant loading conditions. It is shown that the model fitted to established thermodynamic data and selected experiments is able to reproduce the experimental observations in a wide range of loading rates ranging from quasistatic to $10^4\ s^{-1}$ as well as a wide range of phenomena ranging including overall rate hardening and thermal softening. In doing so, the model also provides new insight into the $\alpha \Longleftrightarrow \epsilon$ phase transformation in iron.

1. Introduction

The mechanical properties of pure iron have been extensively studied in the past decades mostly in the context of its response at high strain-rates and pressures (see for example Follansbee, 1989; Jia et al., 2000; Klepaczcko, 1969; Mason and Worswick, 2001; Nicolazo and Leroy, 2002; Ostwaldt et al., 1997; Watson, 1970; Weston, 1992). The high pressure is applied either in a quasi-static way using a diamond anvil press, or using shock wave for example in plate-impact experiments of a very short duration (Clifton and Klopp, 1985; Murr and Esquivel, 2004; Rosenberg et al., 1980). Since the shock wave techniques are more accessible than the quasi-static experiments, a major part of the literature reports results obtained using shock experiments (Bancroft et al., 1956; Kalantar et al., 2005; Millett et al., 1997; Ostwaldt et al., 1997; Sano et al., 2003; Yaakobi et al., 2005).

One of the main points of interest is the existence of an allotropic α (BCC) $\Longleftrightarrow$ ε (HCP) phase transition in this material (Ahrens et al., 2002). This phase transformation, discovered by Bancroft et al. (1956), is known to be reversible, and occurs at large pressures, starting at 13 GPa and completing around 23 GPa in high pressure compression experiments. While much of the literature considered hydrostatic pressure as the trigger for the phase transformation, Jones and Graham (1968) pointed out the role of shear that is inherent in high pressure experiments (see also direct measurements by Millett et al. (1997)). So, recent work has focused on the role of shear stresses in determining the critical pressure for the onset of the phase

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transformation. Specifically, Von Barge and Boehler (1990) have shown that shear stresses in the pressure transmitting medium systematically affect the transformation pressure and hysteresis loop observed upon unloading. Further, atomistic calculations have shown the significant contribution of the shear strain, even of modest magnitude, to the $\alpha \iff \varepsilon$ transition (Caspersen et al., 2004; Lew et al., 2006). Still, the experimental literature on direct observations of the phase transition, or on the role of shear on its occurrence, is still scarce (Kalantar et al., 2005; Sano et al., 2003). For example, real-time diffraction experiments like those of Kalantar et al. (2005), who confirmed the existence of the phase transition, do not address the role of shear in the phase transformation process.

Rittel et al. (2006) conducted a comprehensive series of dynamic shear experiments on pure iron using the shear-compression specimen (SCS) in a split Hopkinson (Kolsky) pressure bar. Due to the reversibility of the phenomenon, those authors could not provide a direct evidence of phase transformation, but several indirect observations supported the likelihood of the claim. Specifically, it was observed that at very high strain rates (of the order of 8000 s^{-1}), pure iron would exhibit a negative strain-hardening response from the onset of yielding. Further, the measured value Taylor–Quinney factor (Taylor and Quinney, 1934) (which describes the amount of plastic work that is converted to heat) would exceed unity thereby suggesting that some latent heat was injected into the system.

In this paper, we develop a simple model that combines martensitic phase transformations with plasticity, and uses it to study the experiments of Rittel et al. (2006). The model builds on the formulation of rate-dependent thermoplasticity proposed by Rosakis et al. (2000) and that of martensitic phase transformations by Sadjadpour and Bhattacharya (2007). We introduce internal variables to describe the phase transformation and plasticity, place them on a consistent thermodynamic setting and prescribe appropriate evolution laws – stick slip style for the phase transformation and Johnson–Cook for the plasticity. We then specialize the model to a homogenous, adiabatic, constant strain rate setting as is appropriate for the experimental setting. We fit the model to well-known thermodynamic properties of iron, as well as selected experimental observations, and show that the model is capable of capturing the entire range of experimental observations. While the development of such a model is not conclusive in establishing that allotropic phase transition actually occurs in iron as a result of shear loading, it nevertheless adds to the growing evidence establishing its feasibility.

Various authors have studied the coupling between plasticity and martensitic phase transformation. Much of this work is motivated by transformation induced plasticity (TRIP) in steels where a non-transforming ferritic matrix contains transforming inclusions and the transformation in the transforming grains leads to plastic deformation in both the grains and the surrounding matrix (e.g. Fischer et al., 2000; Cherkaoui et al., 2000; Turteltaub and Suiker, 2005; Leblond et al., 1989; Leblond, 1989; Levitas et al., 1998). This work seeks to understand the nature of the plastic deformation, as well its effect on overall properties. There is also an emerging literature how martensitic laths contribute ductile fracture (Shanthraj and Zikry, 2013), and the interplay of plasticity and phase transformations in shape-memory alloys (Richards et al., 2013). These do not address the α–ϵ transformation in iron. Barton et al. (2005) developed a continuum model (in a crystal plasticity type setting) for this transformation and used it to study shock-induced transformation and texture evolution. Similarly, Caspersen et al. (Caspersen et al., 2004; Lew et al., 2006) developed a multiscale model for this phenomena. However these models are quite involved. In contrast, the model we present is limited in scope, but simple. Yet, it retains enough physics to enable us to analyze the shear-dominant experiments described above and to provide insights into the transformation and the thermomechanical coupling.

The paper is organized as follows. Section 2 introduces the model and describes its thermodynamic setting. In Section 3 we fit the model to experimental observations and then study the response of the material under a number of strains-controlled tests. We conclude in Section 4 with a brief discussion.

2. A thermo-mechanical model

In this section we develop and discuss our phenomenological constitutive model within a continuum thermodynamic framework. The model builds on the formulation of rate-dependent thermoplasticity proposed by Rosakis et al. (2000) and martensitic phase transformations by Sadjadpour and Bhattacharya (2007).

2.1. Kinematics

We work in the one dimensional setting. We denote by $u(x,t)$ the displacement at particle x at time t and by $\varepsilon(x,t)$ the strain. We assume that the strain can be additively decomposed into elastic, transformation and plastic strains:

$$\varepsilon(x,t) = \varepsilon_e(x,t) + \lambda(x,t)\varepsilon_m(x,t) + \varepsilon_p(x,t), \quad (1)$$

where ε_e is the elastic strain, λ is the volume fraction of martensite, ε_m is the transformation strain associated with the martensite and ε_p is the plastic strain. Note that we are in the coarse-grained setting on a length scale of multiple grains so that we do not resolve the details of the martensitic microstructure and grains. Thus, $\lambda(x,t)$ is the volume fraction averaged over a representative volume element (RVE) associated with the particle x at time t while ε_m is the average transformation strain of every subregion of martensite in the RVE. Consequently, they satisfy the constraints

$$\lambda \in [0,1] \quad \text{and} \quad \varepsilon_m \in [\varepsilon_m^-, \varepsilon_m^+], \quad (2)$$

where the parameter $\varepsilon_m^- < 0 < \varepsilon^+0$ depends on the crystallography and texture of the material. Further, the total transformation strain of the RVE is $\lambda\varepsilon_m$ (Sadjadpour and Bhattacharya, 2007).