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Interfacial energy and dissipation in martensitic phase transformations. Part II: Size effects in pseudoelasticity

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ABSTRACT

This paper is a continuation of the Part I (H. Petryk, S. Stupkiewicz, Interfacial energy and dissipation in martensitic phase transformations. Part I: Theory. J. Mech. Phys. Solids, 2010, doi:10.1016/j.jmps.2009.11.003). A fully three-dimensional model of an evolving martensitic microstructure is examined, taking into account size effects due to the interfacial energy and also dissipation related to annihilation of interfaces. The elastic micro-strain energy at microstructured interfaces is determined with the help of finite element computations and is approximated analytically. Three interface levels are examined: of grain boundaries attained by parallel martensite plates, of interfaces between austenite and twinned martensite, and of twin interfaces within the martensite phase. Minimization of the incremental energy supply, being the sum of the increments in the free energy and dissipation of the bulk and interfacial type at all levels, is used as the evolution rule, based on the theory presented in Part I. An example of the formation and evolution of a rank-three laminated microstructure of finite characteristic dimensions in a pseudoelastic CuAlNi shape memory alloy is examined quantitatively.

1. Introduction

Martensitic phase transformation is essentially a multi-scale phenomenon. Even within a single grain of a given size, two other characteristic dimensions typically appear, namely the spacing of martensite plates and the twin spacing within a single martensite plate composed of two variants of martensite. Such microstructures are quite common in shape memory alloys, cf. the book by Bhattacharya (2003) and the references therein. The set of possible martensite plate orientations and compositions can be found from the classical crystallographic theory of martensite (Wechsler et al., 1953; Ball and James, 1987) when neglecting the effect of actual stress. Quasi-static and isothermal evolution of stress-induced three-dimensional (3D) microstructures in the form of rank-one or rank-two laminates has been modelled *including dissipation* but without size effects, e.g., by Stupkiewicz and Petryk (2002, 2004, 2006), Kružik et al. (2005), Bartel and Hackl (2008), and Kouznetsova and Geers (2008).

Our goal here is to incorporate size effects by including the interfacial energy and the related dissipation. There are several limitations of the scope of this work. First, within a more general theoretical framework presented in Part I of this paper (Petryk and Stupkiewicz, 2010), the attention in the present Part II is essentially focused on the pseudoelastic behaviour of shape memory alloys, although the results of Section 2 are applicable more generally. Second, we examine here isothermal quasi-static transformations only and assume that the dissipation is fully rate-independent. Next, to

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simplify the model, geometric nonlinearity is neglected (strains are reasonably small here) and elastic homogeneity and isotropy are assumed; these assumptions are only relaxed when calculating the elastic micro-strain energy at austenite–twinned martensite interfaces for a CuAlNi alloy (for which anisotropic elastic constants are known for both phases, cf. Sedlak et al., 2005). Moreover, effects observed in the case of nano-sized grains are not considered (cf. Waitz et al., 2007; Sun and He, 2008).

Interfaces occur in martensitic microstructures at various levels. The lowest level is that of fully coherent interfaces between two twin-related variants of martensite. Such interfaces are atomistically sharp and planar (cf. Christian and Mahajan, 1995) except in vicinity of other interfaces; the related twin branching phenomenon (cf. Kohn and Müller, 1992; James et al., 1995) is not examined here. Phase interfaces between austenite and internally twinned martensite are more complex (Bhattacharya, 2003); we call them 'microstructured interfaces' as the material at one side has its own microstructure.[1] As the material phases have freedom to adapt during transformation, those interfaces are in addition corrugated rather than planar on the scale of twin spacing (e.g., Knowles and Smith, 1981; Hÿtch et al., 1999). In turn, the interface between a martensite–austenite laminate in one grain and another grain in a polycrystal is also microstructured on the higher scale of spacing of martensite plates. A unifying feature of the microstructured interfaces is that there is incompatibility of eigenstrains across the interface on the scale of the corresponding material microstructure (although *averaged* eigenstrains may be compatible), which results in residual stresses and elastic micro-strains in vicinity of the interface. One of the aims of this paper is to examine the elastic micro-strain energy at such microstructured interfaces, cf. Section 2.

It is well known that the competition between the interfacial energy and the energy of elastic micro-strains introduces a size scale in laminated microstructures (Khachaturyan, 1983; Ball and James, 1987). Estimations of the energy part due to atomic scale interactions can be found in the materials science literature (e.g., Porter and Easterling, 1992; Howe, 1997), while the elastic micro-strain energy at microstructured interfaces is to be determined. The frequently used approach, i.e. introducing energy due to non-locality or strain gradients (cf. Barsch and Krumhansl, 1984; Kohn and Müller, 1992; Bhattacharya and James, 1999; Ren and Truskinovsky, 2000; Sun and He, 2008), does not seem to be directly applicable to 'sharp' microstructured interfaces. We use another approach, announced in Part I of the paper and elaborated below in more detail. In particular, within the linear elasticity framework with shear eigenstrains and with the help of finite element analysis, we determine the energy of a transition layer at a planar boundary of laminated domains and express it by an analytic formula with a single adjustable parameter. The ratio of the layer energy divided by the interface area is interpreted as a microstructural part of the interfacial energy density at a grain boundary at a higher level. It is combined with our recent results of the analysis of the elastic micro-strain energy at corrugated interfaces between austenite and internally twinned martensite in CuAlNi (Maciejewski et al., 2005; Stupkiewicz et al., 2007). In these works, unlike in papers where the interface shape was prescribed *a priori* (Sridhar et al., 1996; Roytburd, 1998; Waitz et al., 2007), the morphology of the interfacial layer was determined by energy minimization with respect to free shape parameters.

The next question to be examined is the dissipation related to annihilation of interfaces. The energy release due to annihilation of interfaces can hardly be reverted into the bulk free energy and, consequently, provides a contribution to the total dissipation during evolution of martensitic microstructures. As proposed in Part I of the paper, we use a simple assumption that a specified fraction (close to unity) of the interfacial energy is dissipated when an interface disappears. The fraction may depend on the interfacial energy components and hence be different for interfaces on different scales. Those dissipation contributions from interfaces on different scales are summed up and added to the usual dissipation term proportional to the assumed threshold value $f_c \geq 0$ for the Eshelby driving force on a moving phase transformation front.

Assuming for simplicity that f_c is a constant of the same value for forward and reverse austenite-to-martensite transformation, we obtain the simplest formula $\Delta\overline{\mathcal{D}}_v = f_c|\Delta\eta|$ for the bulk dissipation density. It is proportional to the increment $\Delta\eta$ in the volume fraction of martensite provided the transformation is *one-way*. In accord to Section 5 of Part I, minimization of the first-order incremental energy (free energy plus dissipation) without interfacial energy effects leads to the local transformation criterion (either forward or reverse), cf. Section 5.2 in Part I, in the form

$$|f|-f_c \leq 0, \quad (|f|-f_c)\Delta\eta = 0, \quad \Delta\eta|f| = f|\Delta\eta| \quad \text{(no interfacial energy)}, \tag{1}$$

where $\Delta\eta$ is the volume fraction of a thin (in the theory infinitely thin) transformed layer and f is the Eshelby (1970) driving force acting on the layer boundary. The thermodynamic criterion of rate-independent martensitic phase transformation defined by (1) coincides with that obtained from Rice's (1975) theory and used earlier (e.g., by Stupkiewicz and Petryk, 2002) without reference to the incremental energy minimization. On neglecting a difference between f_c above and f_c^v in formula (42) of Part I, formula (1) can also be applied to sudden formation of a product phase layer with creation or annihilation of interfaces.

The main goal of this paper is to combine the earlier approach based on size-independent criterion (1) with the interfacial contributions to energy and dissipation, to arrive at a model where characteristic dimensions of the microstructure are well-defined. As discussed in Part I, a general evolution rule is needed for determining the changes in microstructure upon loading. One possibility would be to exploit the *first-order* energy minimization principle to derive the

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[1] Microctructured interfaces here have somewhat different meaning than 'structural interfaces' examined in a different context in the literature, cf. Bigoni and Movchan (2002).