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Study of the *cofactor conditions*: Conditions of supercompatibility between phases

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ABSTRACT

The *cofactor conditions*, introduced in James and Zhang(2005), are conditions of compatibility between phases in martensitic materials. They consist of three subconditions: (i) the condition that the middle principal stretch of the transformation stretch tensor $\mathbf{U}$ is unity ($\lambda_2 = 1$), (ii) the condition $\mathbf{a} \cdot \mathbf{U}\mathrm{cof}(\mathbf{U}^2 - \mathbf{I})\mathbf{n} = 0$, where the vectors $\mathbf{a}$ and $\mathbf{n}$ are certain vectors arising in the specification of the twin system, and (iii) the inequality $\mathrm{tr}\mathbf{U}^2 + \det \mathbf{U}^2 - (1/4)|\mathbf{a}|^2|\mathbf{n}|^2 \geq 2$. Together, these conditions are necessary and sufficient for the equations of the crystallographic theory of martensite to be satisfied for the given twin system but for any volume fraction f of the twins, $0 \leq f \leq 1$. This contrasts sharply with the generic solutions of the crystallographic theory which have at most two such volume fractions for a given twin system of the form f^* and $1-f^*$. In this paper we simplify the form of the cofactor conditions, we give their specific forms for various symmetries and twin types, we clarify the extent to which the satisfaction of the cofactor conditions for one twin system implies its satisfaction for other twin systems. In particular, we prove that the satisfaction of the cofactor conditions for either Type I or Type II twins implies that there are solutions of the crystallographic theory using these twins that have *no elastic transition layer*. We show that the latter further implies macroscopically curved, transition-layer-free austenite/martensite interfaces for Type I twins, and planar transition-layer-free interfaces for Type II twins which nevertheless permit significant flexibility (many deformations) of the martensite. We identify some real material systems nearly satisfying the cofactor conditions. Overall, the cofactor conditions are shown to dramatically increase the number of deformations possible in austenite/martensite mixtures without the presence of elastic energy needed for coexistence. In the context of earlier work that links the special case $\lambda_2 = 1$ to reversibility (Cui et al., 2006; Zhang et al., 2009; Zarnetta et al., 2010), it is expected that satisfaction of the cofactor conditions for Type I or Type II twins will lead to further lowered hysteresis and improved resistance to transformational fatigue in alloys whose composition has been tuned to satisfy these conditions.

1. Introduction

This paper gives a precise derivation and implications of the cofactor conditions (James and Zhang , 2005), defined briefly in the abstract. These conditions are appropriate to a material that undergoes an austenite to martensitic phase transformation having symmetry-related variants of martensite. The cofactor conditions represent a degeneracy of the

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equations of the crystallographic theory of martensite (Lieberman et al., 1955; Bowles and Mackenzie, 1954a, 1954b), under which this theory possesses solutions with any volume fraction $0 \le f \le 1$ of the twins (James and Zhang , 2005).

For the special cases $f=0$ and $f=1$ the equations of the crystallographic theory reduce to the equations of compatibility between austenite and the appropriate single variant of martensite. Hence, as also can be seen from the conditions themselves (in particular, the condition $\lambda_2 = 1$), the cofactor conditions imply perfect compatibility between austenite and each single variant of martensite. The solutions of the crystallographic theory for the intermediate volume fractions $0 < f < 1$ imply the existence of the standard low energy transition layers between austenite and finely twinned martensite.

The main result of this paper is that in many cases, the cofactor conditions imply that the transition layer can be eliminated altogether, resulting in the coexistence of austenite and twinned martensite with zero elastic energy. Examples are shown in Figs. 2(right), 3, 4, 6 and 7. These include macroscopically curved austenite/martensite interfaces and natural mechanisms of nucleation (Figs. 6, 7). The latter are continuous families of deformations in which the austenite grows from zero volume in a matrix of martensite, or the martensite grows in a matrix of austenite, all having zero elastic energy. Said differently, while the crystallographic theory implies that the energy due to elastic distortion can be reduced as close to zero as desired by making the twins finer and finer, the elastic energy in the cases studied here is eliminated at all length scales. From a physical viewpoint, the only remaining energy is then a small interfacial energy. We describe explicitly the cases in which the transition layer can be eliminated in Section 4.

The value of λ_2 can be modified by changing composition, and the special case $\lambda_2 = 1$ (up to experimental error in the measurement of lattice parameters) has been achieved in many systems. As reviewed in detail below, satisfaction of only the condition $\lambda_2 = 1$ has a dramatic effect on hysteresis and transformational fatigue (Cui et al., 2006; Zhang et al., 2009; Zarnetta et al., 2010; Delville et al., 2009; Srivastava et al., 2010; see also Buschbeck et al., 2011; Meethong et al., 2007; Louie et al., 2010; Srivastava et al., 2011). A theory for the width of the hysteresis loop that predicts this sensitivity was given in Zhang et al. (2009), Knüpfer et al. (2011), and Zwicknagl (2013). It is based on the idea that transformation is delayed, say on

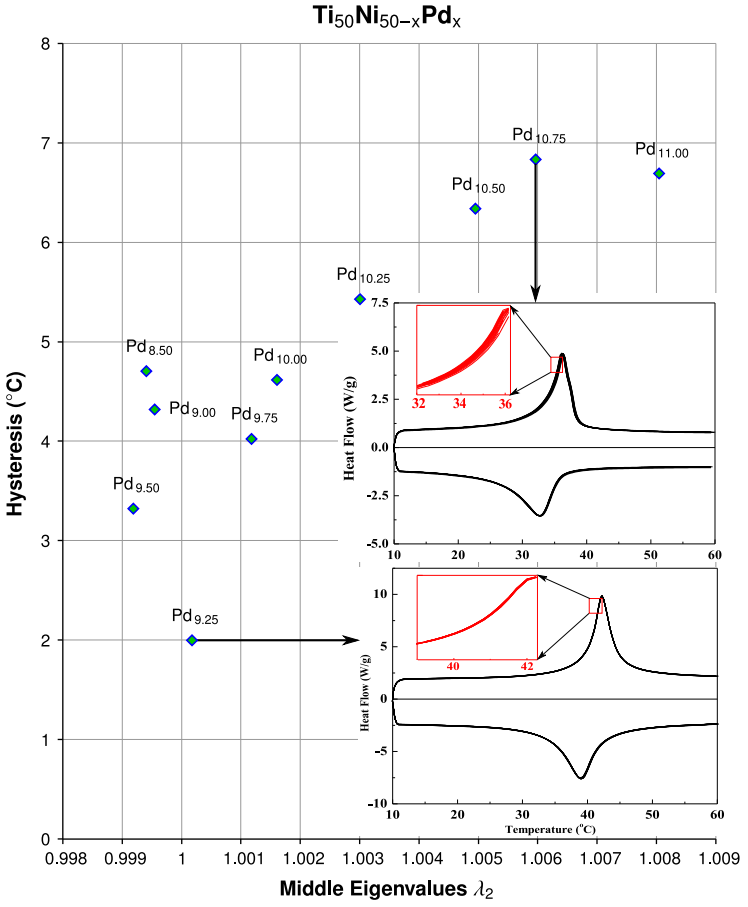

Fig. 1. Reduced hysteresis of $Ti_{50}Ni_{50-x}Pd_x$ alloy system as the composition is tuned to achieve $\lambda_2 = 1$. A thermal hysteresis of 2 °C is obtained at $x=9.25$. The insets show a comparison of thermal hysteresis under repeated cycling through the transformation (30 cycles) measured by differential scanning calorimetry at $x=9.25$ vs. $x=10.75$. A careful comparison of these graphs shows an average migration of transformation temperature of 0.16 °C/cycle at $x=10.75$ is reduced to 0.030 °C/cycle at $x=9.25$. These values should be contrasted to ordinary TiNi which exhibits an average migration over 30 cycles of about 0.6 °C/cycle.

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