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Determination of the stretch tensor for structural transformations

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ABSTRACT

Structural transformations in crystalline solids are increasingly the basis of the functional behavior of materials. Recently, in diverse alloy systems, both low hysteresis and reversibility of phase transformations have been linked to the satisfaction of the non-generic conditions of compatibility between phases. According to the Cauchy–Born rule, these conditions are expressed as properties of *transformation stretch tensor*. The transformation stretch tensor is difficult to measure directly due to the lack of knowledge about the exact transforming pathway during the structural change, and the complicating effects of microstructure. In this paper we give a rigorous algorithmic approach for determining the transformation stretch tensor from X-ray measurements of structure and lattice parameters. For some traditional and emerging phase transformations, the results given by the algorithm suggest unexpected transformation mechanisms.

1. Introduction

Structural transformations increasingly underlie the unusual behavior of emerging functional materials designed for sensors/actuators (Otsuka and Wayman, 1999; Li et al., 2003; Kaufmann et al., 2010), solid-state refrigerators (Liu et al., 2012; Cui et al., 2012), batteries (Kang and Ceder, 2009; Louie et al., 2010), thermoelectrics (Ikeda et al., 2009) and direct energy conversion devices (Srivastava et al., 2011; Song et al., 2013a). These applications rely on the change of crystal structure. The resulting change of lattice parameters, together with sensitivity of magnetoelectric properties to lattice parameters, inspires an approach to the discovery of new functional phase-transforming materials (Cui et al., 2006; Zarnetta et al., 2010; Srivastava et al., 2010; Song et al., 2013b). However, the formation of microstructure during phase transformation introduces elastic distortion at phase interfaces due to lattice misfit, which in turn leads to functional degradation. Recent studies of morphological interface compatibility for phase-transforming materials shed light on the effect of lowering and even eliminating this distortion by tuning composition so that the lattice parameters satisfy strong conditions of compatibility (Chen et al., 2011, 2013). These conditions are restrictions on the form of the *transformation stretch tensor* (Ball and James, 1987; Bhattacharya, 2003) and the point groups of the two phases. The reversibility, thermal hysteresis, and resistance to cyclic degradation of functional materials have been dramatically linked to properties of the transformation stretch tensor and symmetries (Zarnetta et al., 2010; Chen et al., 2011; Song et al., 2013b; Chluba et al., 2015; James, 2015). Here we propose an algorithmic approach for the determination of the transformation stretch tensor based on X-ray

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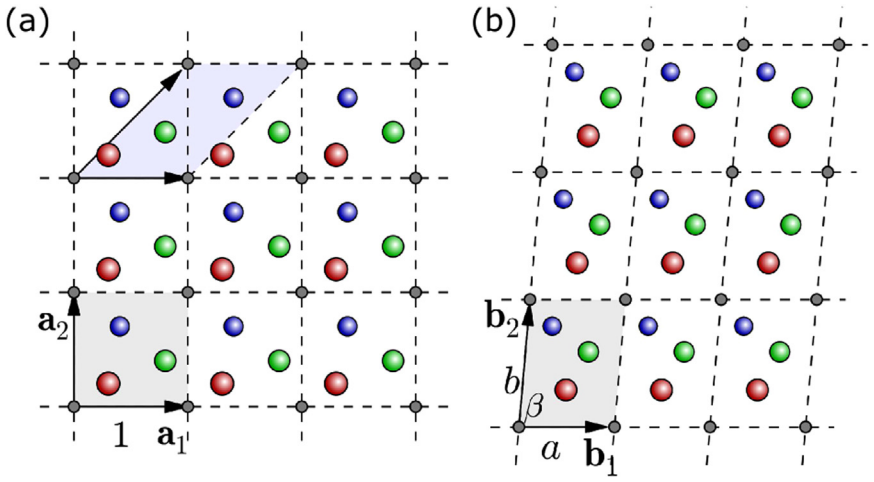

Fig. 1. Non-uniqueness of Cauchy–Born deformation gradient from a (a) square lattice to (b) oblique lattice due to lattice invariant deformations. Red, blue and green balls represent different atomic species. Gray dots define the periodicity. In this example both lattices are chosen as primitive, for simplicity. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

measurements, and we give a rigorous proof of its validity. The results below reveal some unexpected transformation mechanisms in traditional and emerging phase-transforming materials.

In principle, the determination of the transformation stretch tensor $\mathbf{U}$ is straightforward: simply observe where each atom goes during transformation and deduce the macroscale deformation gradient $\mathbf{F}$ associated to this motion. The stretch tensor associated to this macroscale deformation gradient (via the polar decomposition $\mathbf{F}=\mathbf{QU}$, $\mathbf{Q}\in \mathrm{SO}(3)$, $\mathbf{U}=\mathbf{U}^T$ positive-definite) should be the main quantity that is relevant to the stressed transition layers between phases that underlies improvements of reversibility discussed above.

In practice, however, determination of this macroscale deformation gradient is surprisingly subtle. First, not every atom is convected with this macroscopic deformation gradient. Rather, *some sublattice* of the parent (austenite) phase is transformed into *some sublattice* of the transformed (martensite) phase. The atoms within the unit cell of the chosen austenite sublattice are not generally deformed by this macroscale deformation gradient, but rather undergo independent movements called *shuffling*. Fix the lattices of austenite and martensite. It is easily seen that, by taking larger and larger sublattices of austenite and suitable choices of corresponding sublattices of martensite, the associated deformation gradient can be made arbitrarily close to the identity. Thus, the choices of sublattice are important.

Fortunately, there are guidelines for choosing the sublattice. The deformation gradient has been measured directly by macroscopic methods in a few cases by the so-called "two-surface analysis" (Kurdjumov et al., 1961; Duggin and Rachinger, 1964; Otsuka and Shimizu, 1974). This consists of scratching an austenite single crystal on two nonparallel surfaces, transforming the crystal to martensite by cooling, detwinning the crystal by stress to remove the inevitable microstructure that forms, carefully removing the stress, and measuring suitable lengths and angles associated to the scratches to get $\mathbf{F}$. In all of these cases of which we are aware it is found that relevant martensite sublattice is a primitive lattice of martensite.[1] The austenite sublattice is generally not primitive.

While the algorithm given below works in more general cases, it is here written *to find the sublattice of austenite that is closest in a certain norm to the primitive lattice of martensite*. The distance chosen is a measure of strain having certain algorithmic advantages. Besides being frame-indifferent, it also has certain advantages with regard to symmetry, i.e., lattices of different variants of the martensite phase have the same distance to the austenite sublattice. The idea of minimizing strain has a long history in martensite originating from the work of Bain (1924).

A second consideration for the determination of $\mathbf{F}$ is well-known. This is the presence of *lattice-invariant deformations*. Referring to Fig. 1, suppose sublattice vectors of initial and final phases are, respectively, linearly independent vectors $\mathbf{a}_i$ and $\mathbf{b}_i$ for $i=1, 2, \ldots, d$, where d is the dimension of the lattice. A nonsingular linear transformation $\mathbf{F}$: $\mathbb{R}^d \to \mathbb{R}^d$ can be defined uniquely by

$$\mathbf{F}\mathbf{a}_i = \mathbf{b}_i, \quad i=1, 2, \ldots, d. \tag{1}$$

The notation $\mathbf{a}_i \to \mathbf{b}_i$ denotes a *lattice correspondence*. In the case of transformation in Fig. 1, one choice of the lattice correspondence can be $\mathbf{a}_1 \to \mathbf{b}_1$, $\mathbf{a}_2 \to \mathbf{b}_2$ where $\mathbf{a}_1=[1, 0]$, $\mathbf{a}_2=[0, 1]$ and $\mathbf{b}_1=[a, 0]$ and $\mathbf{b}_2=[b\cos\beta, b\sin\beta]$ as illustrated in Fig. 1. The alternative set of vectors $\mathbf{a}_1$ and $\mathbf{a}_1+\mathbf{a}_2$ describes the same lattice (a), which results in a different correspondence from (a) to (b). This obviously changes the $\mathbf{F}$ and thus the transformation stretch tensor $\mathbf{U}$. More generally, any two sets of

[1] A *primitive lattice* of martensite is a sublattice of the martensite structure having a unit cell of smallest volume, i.e., it embodies the fundamental periodicity of the martensite lattice, accounting for the crystal structure and species.