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Wavelet analysis of microscale strains

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Abstract

Recent improvements in experimental and computational techniques have led to a vast amount of data on the microstructure and deformation of polycrystals. These show that, in a number of phenomena, including phase transformation, localized bands of deformation percolate in a complex way across various grains. Often, this information is given as point-wise values arrayed in pixels, voxels and grids. The massive extent of data in this form renders identifying key features difficult and the cost of digital storage expensive. This work explores the efficiency of wavelets in storing, representing and analyzing such data on shape-memory polycrystals as a specific example. It is demonstrated how a compact wavelet representation captures the essential physics contained in experimental and simulated strains in superelastic media.

Keywords: Wavelets; Polycrystals; Phase transformation; Microstructure

1. Introduction

Recent developments in material characterization techniques have led to new abilities in determining the microstructure and strain fields of heterogeneous media [1–3], and in particular shape-memory alloys [4,5]. These are often represented as images composed of pixels or voxels. (For a review on the dominant electron microscopy tools and the state of the art X-ray techniques the reader is referred to Ref. [6].) Similarly, improvements in computational methods have enabled accurate full-field simulations for the mechanical fields developing in polycrystalline aggregates [7–9]. Again, such fields are described on grids.

These capabilities bring with them massive amounts of produced information. The digital storage space required can reach terabytes, depending on the grid, time resolution, dimensionality and fields of interest for a single experiment or simulation. To exploit this information, it needs to be stored, retrieved and analyzed efficiently; this has become a challenge [10].

Further, a combination of the heterogeneity, nonlinear behavior and fundamental physics (equilibrium and compatibility) causes the stress and strain in these materials to localize into bands (plates) that percolate in complex patterns through the material. Such patterns are observed in the context of elastic composites with a complex microstructure [12], plastic polycrystalline alloys [13] and shape-memory alloys [14]. An understanding of the properties of the materials requires us to readily identify these bands, to understand their interactions and to infer their consequences. However, as noted above, much of the data generated in experiments is arrayed point-wise, in pixels, voxels and grids. This makes it difficult to identify and analyze such bands.

These observations give rise to the question: *what is a suitable way to represent and analyze strain fields with localized features?*

In this work, we explore the efficiency of wavelets in representing and analyzing strain data. By construction, these

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functions are compactly supported at different length-scales, in both frequency and spatial domains, and are efficient in the representation of heterogeneous fields with localized features. The local multi-scale nature of wavelets is reminiscent of the way in which strain evolves: namely, from small-scale patches to bands. This similarity is the motivation for utilizing wavelet analysis in the representation of microscale strains.

The canvas upon which this concept is presented is that of polycrystals undergoing martensitic phase transformation. Such materials are capable of recovering strains beyond their apparent elastic limit. This phenomena is known as *super-* or *pseudo-elasticity*. Variants of martensite induced by stress, admitting non-zero transformation strains, rearrange to accommodate deformation without application of additional stress. Upon unloading, the variants transform back to austenite, and the strains caused by the rearrangement are recovered [15]. When considering a polycrystal, on top of a kinematic incompatibility of the phase mixtures within each grain, the different orientations of neighboring grains give rise to an additional inter-grain incompatibility. In turn, an intricate evolution of strain, transformation and stress fields emerges [16,17,14]. Transformation, in particular, initiates in local regions at grains which are well oriented with the loading. The inter-granular compatibility constraint dictates non-uniform progression of transformation in confined bands perpendicular to the loading. This extreme heterogeneity of transformation induces extreme heterogeneity of stress, concentrated at misoriented grains.

This work investigates the efficiency of wavelets in representing, storing and analyzing microscale strain fields and, in turn, identifying the relevant information dictating the macroscopic behavior. This notion is examined via experimental data on full-field strains of nitinol under tension, obtained by Daly et al. [17], and using a numerical model derived by Richards et al. [14]. In a way, we treat strains as *images*, and employ tools of image compression in our analysis. To the best of the authors' knowledge, the only studies to use a reminiscent framework are those of Teranishi et al. [10] and Wang and Mottershead [11]. The former developed a scheme based on image compression principles to reduce the microstructure data size, whereas the latter used orthogonal polynomial-based shape descriptors to analyze vibrations and full-field strains in irregular domains.

While we focus on shape-memory polycrystals, we note that this kind of localized deformation is also seen in the context of polycrystalline plasticity and composites. Thus, we believe that the lessons learnt in this work are applicable to a broad class of materials.

The paper is composed as follows. Section 2 provides a basic introduction to wavelets. The efficiency of wavelets in representing experimental data sets is examined in Section 3. Section 4 explores the capability of a compact set of wavelets to characterize the interplay between the strain, transformation and stress fields, and, in turn, the macroscopic stress–strain relation, using a numerical model of a polycrystalline aggregate. We complete the paper by summarizing its main conclusions and observations in Section 5.

2. Wavelet representation

A brief introduction to wavelet representation is given here. For a more comprehensive review, the reader is referred to Mallat [18] and Walnut [19]. Broadly speaking, the main idea of representing a function is twofold. First, the space is partitioned into a nested sequence of scales at different resolutions. The function is then described in terms of its average across the coarse scale and its details across finer scales only in regions where the function is changing. Using this multi-resolution representation, one can focus attention on those specific regions where the interesting features occur and ignore the rest. This is in contrast with Fourier analysis, in which all regions of space are treated equally. This difference is illustrated in Fig. 1.

Rigorously, wavelet representation consists of a mother wavelet function $\psi(x)$ of vanishing integral $\int_{\mathbb{R}} \psi(x)\mathrm{d}x = 0$ and a scaling father function $\phi(x)$ of a unit integral $\int_{\mathbb{R}} |\phi(x)\mathrm{d}x| = 1$, both of which are locally supported. These functions are uniquely related, such that the wavelet function is a linear combination of translations of compressed scaling functions, i.e., $\psi(x) = \sum_{n\in\mathbb{Z}} b_n\phi(2x - n),\ b_n \in \mathbb{R}$. The translations and dilations of $\psi(x)$ and $\phi(x)$ are defined as

$$\psi_{j,k}(x) \overset{\text{def}}{=} 2^{j/2}\psi\left(2^j x - k\right), \quad j,k \in \mathbb{Z}, \tag{1}$$

$$\phi_{j,k}(x) \overset{\text{def}}{=} 2^{j/2}\phi\left(2^j x - k\right), \quad j,k \in \mathbb{Z}. \tag{2}$$

A nested structure of approximation spaces for the square integrable functions is obtained using the function sets introduced in Eq. (2):

$$V_j = \left\{\phi_{j,k}(x),\ k \in \mathbb{Z}\right\}, \{0\} \subset \ldots V_j \subset V_{j+1} \subset \cdots \subset L^2(\mathbb{R}). \tag{3}$$

The orthogonal complement of V_j within V_{j+1} is spanned by $\left\{\psi_{j,k}(x)\right\}$, i.e.,

$$V_{j+1} = V_j \oplus W_j,\ \ W_j = \left\{\psi_{j,k}(x),\ k \in \mathbb{Z}\right\}. \tag{4}$$

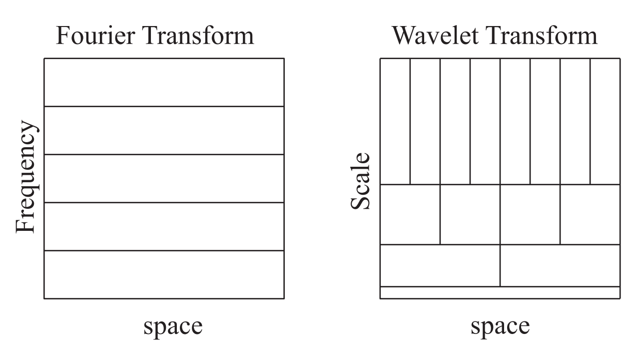

Fig. 1. Illustrative comparison between Fourier and wavelet transforms.