Homology Metrics for Microstructure Response Fields in Polycrystals

Thomas Wanner*
Department of Mathematical Sciences
George Mason University
Fairfax, VA 22030, USA
twanner@gmu.edu

Edwin R. Fuller Jr.
National Institute of Standards and Technology
Materials Science and Engineering Laboratories
Ceramics Division
Gaithersburg, MD 20899, USA
edwin.fuller@nist.gov

David M. Saylor
Food and Drug Administration
Center for Devices and Radiological Health
Office of Science and Engineering Laboratories
Silver Spring, MD 20903, USA
david.saylor@fda.hhs.gov

August 24, 2009

*Thomas Wanner was partially supported by NSF grant DMS-0406231 and the U.S. Department of Energy under Contract DE-FG02-05ER25712.
Abstract

Quantitative homology metrics are proposed for characterizing the thermal-elastic response of polycrystalline materials. Simulations for a calcite-based polycrystal, marble, are used as an illustrative example. The homology metrics are based on topological measurements, such as the number of components and the number of handles of the thermal-elastic response fields for a complex microstructure. These homology metrics are applied to characterize not only the elastic energy density and maximum principal stress response fields in a polycrystal but also the correlated grain-boundary misorientation distributions that influenced the formation of these response fields. It is demonstrated that the topological analysis can quantitatively distinguish between different types of grain-boundary misorientations, as well as between differences in the resulting response fields.

Keywords: homology metrics; microstructures; polycrystals, finite element simulations; thermal expansion anisotropy; residual stress; grain orientation distributions; grain-boundary misorientation distributions

1 Introduction

Natural building stones, such as marble, are widely used in both structural and decorative applications. Yet many marbles show limited and often unpredictable durability [1]. One such deterioration phenomenon is the bowing of marble panels, which, for example, has been observed at the university library in Göttingen [2] and at the Finland Hall in Helsinki [3] — in each case only a few years after completion of the building. This bowing process is accompanied by a reduction of structural durability, and ultimately leads to static failure of the facade with time. A major factor in such degradation phenomena is thermal heating and cooling. Due to the anisotropic thermal expansion of the underlying mineral materials, calcite and dolomite, stresses are created which lead to the formation of microcracks and granular decohesion of the material with time. While environmental factors certainly play a role, the formation of microcracks is mainly driven by residual mechanical forces caused by anisotropies in the fabric of the marble microstructures.

The specific geometric arrangement of the constituent grains in the rock microstructures, i.e., the geometry of the grains and their size, has minimal measurable effect on the thermal-elastic response [4]. In contrast, the other aspect of the polycrystal fabric, the crystallographic arrangement of the grains, has a significant effect [5]. Typically, the grain crystallography is described by the bulk orientation distribution and the correlated grain-boundary misorientation distribution. Using microstructure-based finite element simulations, effects of these distributions on the elastic energy density and the bulk thermal expansion were studied in [5]. While the bulk orientation is widely accepted as an important factor in the thermal-elastic response, the results of [5] demonstrate
that the grain-boundary misorientations play a significant role — potentially even more important than the bulk orientation distribution.

In the current work, we develop quantitative metrics for characterizing both the crystallographic grain arrangement and the resulting thermal-elastic response fields, e.g., the elastic energy density and the maximal principal stress. In contrast to the study in [5], we are interested in quantitatively characterizing the response fields themselves. Upon visual inspection, these fields show very distinct length scales, which seem to have nothing in common with the length scale of the underlying grain geometry. In particular the maximal principal stress fields form networks of regions with high stress, which presumably have direct implications for the formation of microcracks in the material. Our characterization of the response fields uses topological measurements such as the number of components and the number of handles of a complex structure. Such methods have recently been employed in a variety of settings [6, 7, 8, 9, 10, 11], early applications can be found in [12]. The topological measurements are applied to regions where the response field lies above or below a certain threshold level, for varying thresholds. In this way we obtain response signatures which are functions of the threshold, and which in some sense characterize the complexity of the response fields as a function of the response threshold. Similarly, we characterize the grain-boundary misorientations using analogous topological measurements and can point out similarities between them and the response field results.

2 Methods

2.1 Generation of the Grain Geometry and Orientation

The data sets used for this study were generated via microstructure-based finite-element simulations, as described in detail in [5]. We therefore only present a brief description of the procedure. For all data sets we use the same underlying hypothetical grain geometry, as shown in Figure 1. This two-dimensional microstructure consists of 924 grains and was created using the method of [13]. Starting from a random sample of overlapping ellipses, which are generated so as to reflect realistic grain size and shape distributions, a pixel-based continuous nucleation and growth algorithm produced the final microstructure [13, 14].

While the grain geometry is kept fixed for all sample simulations, the grain orientations and grain-boundary misorientations do change. The orientation of a grain can be defined as the rotational relationship between the crystal coordinate system and a fixed sample coordinate system. Even though the primary constituents of natural marbles, calcite and dolomite, have only trigonal symmetry, we make the simplifying assumption that the crystal symmetries are transverse isotropic. This is justified by the fact that for both calcite and dolomite the single crystal thermal-elastic behavior is nearly transverse isotropic, and it allows us to describe the orientation of a grain $g$...
Figure 1: Geometric arrangement of the 924 grains in the hypothetical microstructure used for all simulations of this paper.

by specifying the unit vector \( \hat{n} \) in the laboratory frame parallel to the crystallographic \( c \)-axis, i.e., \( g = g(\hat{n}) \).

As described in [5], the first step in creating the crystallographic grain arrangement consists in choosing orientations for each of the 924 grains based on a given underlying bulk orientation distribution as follows. Let the laboratory reference frame be specified by the \( e_1 \)-direction pointing horizontally across the two-dimensional structure in Figure 1 from left to right, the \( e_3 \)-direction pointing vertically from bottom to top, and the \( e_2 \)-direction pointing away from the viewer. Within this reference frame, the grain orientation is described by three Euler angles \( \alpha \), \( \beta \), and \( \gamma \). Here \( \gamma \) specifies an initial azimuthal angle rotation about \( e_3 \). The polar angle \( \alpha \) specifies the rotation away from \( e_3 \), about the new \( e_1 \)-direction, and the azimuthal angle \( \beta \) specifies the rotation about the new \( e_3 \)-direction. As the crystalline symmetry is assumed to be transverse isotropic, the angles \( \beta \) and \( \gamma \) are inconsequential. For our simulations, the azimuthal angles \( \beta \) and \( \gamma \) are distributed uniformly in the interval from 0 to 2\( \pi \). The polar angle \( \alpha \) is distributed according to a specific March-Dollase distribution [15, 16]. More precisely, we consider a March-Dollase distribution with parameter \( M = 1 \), i.e., the angle \( \alpha \) is distributed with density

\[
f(\alpha) = \sin \alpha .
\]

Once the 924 bulk grain orientations have been chosen according to the above orientation distribution, we assign the orientations to specific grains in three distinct ways which represent three different grain-boundary misorientation distributions, which will be denoted by \( f^H \), \( f^U \), and \( f^L \). For the first of these distributions the grain boundaries prefer high angle misorientations. More precisely, we assign the orientations in such a
way that the misorientation distribution matches the half-normal distribution

\[ f^H(\theta) = \frac{2}{\sigma \pi} \exp \left( -\frac{\theta^2}{\sigma^2 \pi} \right), \quad \text{where } \theta \text{ lies between } 0 \text{ and } \frac{\pi}{2}, \quad (2) \]

as closely as possible. In addition to the distribution \( f^H(\theta) \), we also consider a distribution which prefers low angle misorientations, namely \( f^L(\theta) = f^H(\pi/2 - \theta) \), as well as a uniform distribution \( f^U(\theta) = 2/\pi \) in the range from 0 to \( \pi/2 \). As in [5], these three misorientation distributions are referred to as \( S^H \), \( S^L \), and \( S^U \), respectively.

For the simulations used in this paper, we created five different sets of grain orientations as above, and for each of these sets, we arranged the orientations to match the misorientation distributions \( S^H \), \( S^L \), and \( S^U \) as closely as possible. The resulting fifteen distinct microstructures serve as the basis for the response field calculations. For more details, we refer the reader to [5].

2.2 Computation of the Response Fields

For each of the fifteen hypothetical microstructures described above we then calculated the thermal-elastic response using the microstructure-based finite element program OOF [17]. As a first step, an adaptive mesh procedure was employed to generate a suitable triangular mesh for the grain geometry. The mesh was optimized in such a way that the element edges closely follow the grain boundaries, which resulted in a mesh consisting of 54982 triangles. Since the grain geometry of our hypothetical microstructures remains fixed, the same mesh was used for all of the fifteen microstructures. For the finite element computations using OOF, material properties were then assigned to each of the mesh triangles. These include the thermal expansion coefficients \( \alpha_{ij} \), the elastic stiffness coefficients \( C_{ijkl} \), as well as the grain orientation as described by the Euler angles. For the simulations of this paper we used the material properties of calcite, the corresponding thermal-elastic coefficients can be found in [5].

The program OOF was then used to apply a temperature increase of 100°C to each of the fifteen microstructures and to compute the resulting elastic energy density and maximal principal stress as a function of position. For six of the fifteen hypothetical microstructures these two response fields are shown in Figures 2 and 3, respectively.

2.3 Homological Methods

In order to study quantitatively the response fields described in the last section, we use the OOF software to convert the output of the finite element simulations into 512 × 512 pixel gray-scale images. Colorized versions of these images are shown in Figures 2 and 3. Since areas of high elastic energy density, or high maximum principal stresses, have impact on the formation of microcracks in the material, we are interested in quantitatively studying the sets of positions at which the respective field takes values...
Figure 2: Maps of elastic energy density as a function of position in a set of hypothetical calcite microstructures. Within each row the underlying orientation distribution remains fixed, but the misorientation distribution changes from $S^H$ (left column) to $S^U$ (middle column) and $S^L$ (right column).

larger than a given threshold value. In other words, if the response field is described by a field variable $u = u(x)$ which depends on the spatial variable $x \in \Omega$, and if $\mu$ is a suitable threshold value, then we consider the super-level set

$$X^+ = X^+(\mu) = \{x \in \Omega \mid u(x) > \mu\}.$$  

For the right-most principal stress field in the first row of Figure 3 such a super-level set $X^+$ is shown in the left-most image of Figure 4. In order to only capture the essential geometric topological features of the set, we do not work directly with the fairly noisy original image. Rather, we consider the smoothed version shown in the center of Figure 4. This image was obtained by applying a convolution filter to the original version. Throughout this paper, we use a center-weighted convolution filter, similar to the one described in [22, p. 3391]. In our filter, the convolution kernel is a piecewise affine tent function with square domain, which achieves its maximum at the center of the domain. For our computations, the side length of the square was chosen as
Figure 3: Maps of the maximal principal stress as a function of position in a set of hypothetical calcite microstructures. Within each row the underlying orientation distribution remains fixed, but the misorientation distribution changes from $S^H$ (left column) to $S^U$ (middle column) and $S^L$ (right column).

Figure 4: Thresholded sets derived from one of the fields in Figure 3. The first image shows the original thresholded image, the second one is a smoothed version. The final image is a smoothed version of $X^*$ for a different value of the threshold $\mu$. 
seven pixels. A similarly smoothed version of a set $X^+$ for a different, larger threshold value is shown on the right.

We now turn our attention to assigning quantitative information to the images in Figure 4. Motivated in particular by their network-like structure, we employ methods from algebraic topology for our study. This mathematical discipline has been developed to describe complicated structures in terms of their connectivity properties, and enables one to assign quantitative algebraic information to arbitrary sets. In the mathematical theory, this information is given by the so-called homology groups $H_i(X^+)$, where $i = 0, 1, 2, \ldots$. See for example [18] and the references therein. For our specific application, namely pixel-based black and white images, the information in these groups can be reduced to a set of integers. In fact, one can show that for sets $X^+$ as above we always have $H_i(X^+) = 0$ for $i \geq 2$, and that

$$H_i(X^+) \cong \mathbb{Z}^{\beta_i} \quad \text{for} \quad i = 0, 1,$$

(4)

where $\mathbb{Z}$ denotes the integers and $\beta_i$ is a non-negative integer called the $i$-th Betti number. While the mathematical theory of this construction is fairly involved, the Betti numbers themselves have a straightforward interpretation:

- The 0-th Betti number $\beta_0$ equals the number of components of the set $X^+$,

- the 1-st Betti number $\beta_1$ equals the number of independent loops, or handles, that can be drawn within the set $X^+$, which cannot be shrunk to a point or into one another within $X^+$.

For example, the set shown in the center of Figure 4 has $\beta_0 = 54$ and $\beta_1 = 50$, while the one on the right has Betti numbers $\beta_0 = 44$ and $\beta_1 = 23$. Notice that the first Betti number $\beta_1$ also equals the number of distinct white components, which are completely enclosed by the black region $X^+$.

Betti numbers have been used only rarely in a materials science context before, see for example [6, 19, 12]. In fact, most studies which use topological methods have used the Euler characteristic $\chi$, see for example [7, 8, 9, 10, 11]. The Euler characteristic of a set is easily computable, since it is an additive set functional. Yet, as was pointed out in [6], the set of Betti numbers provides more information than the Euler characteristic alone. In fact, given the Betti numbers, the Euler characteristic is easily computed as their alternating sum, i.e., we have

$$\chi = \beta_0 - \beta_1 + \beta_2 - \ldots.$$

(5)

In contrast, computing the Betti numbers of a set is fairly involved, especially in higher dimensions. For the purposes of this paper, we use the freely available software CHomP [20]. An elementary introduction to homology and the underlying algorithms can be found in [18].
Using the Betti numbers rather than the Euler characteristic has additional benefits. Particularly, we can use Betti numbers to distinguish between boundary and bulk effects in materials. To see this, consider again the set \( X^+ \) as above, and denote its Betti numbers by \( \beta_i^+ \). Similarly, we can introduce the sub-level set
\[
X^- = X^-(\mu) = \{ x \in \Omega \mid u(x) \leq \mu \},
\]
and let \( \beta_i^- \) denote its Betti numbers. Then one can easily see that the number \( \beta_{\text{int}}^+ \) of internal components of \( X^+ \) is given by
\[
\beta_{\text{int}}^+ = \beta_1^-,
\]
and the number \( \beta_{\text{bnd}}^+ \) of components of \( X^+ \) which touch the boundary is given by
\[
\beta_{\text{bnd}}^+ = \beta_0^+ - \beta_1^-.
\]
Analogous formulas hold for the set \( X^- \) as well. For the center image in Figure 4 we have \( \beta_0^- = 59 \) and \( \beta_1^- = 43 \), which implies \( \beta_{\text{int}}^+ = 43 \) and \( \beta_{\text{bnd}}^+ = 11 \). Similarly, for the right-most image in Figure 4 we have \( \beta_0^- = 29 \) and \( \beta_1^- = 34 \), which implies \( \beta_{\text{int}}^+ = 34 \), as well as \( \beta_{\text{bnd}}^+ = 10 \). This simple observation will allow us to assess the influence of the boundary on our characterizations.

3 Results and Discussion

3.1 Topology of the Grain-Boundary Misorientations

We begin our homological analysis by characterizing the grain-boundary misorientations. In order to capture the grain boundaries as well as the misorientation across them, the following procedure is employed. First, we superimpose a \( 1024 \times 1024 \) square grid over the original grain topology shown in Figure 1. (Throughout our computations, only this square grid was used.) For each point \( p \) in the grid, the unit normal vector \( \hat{n}_p \), which describes the orientation of the associated grain is then determined. In order to describe the misorientation information associated with a point \( p \) in the grid, consider all points \( q \) in the grid whose Euclidean distance from \( p \) is at most three pixels. Then the misorientation \( m(p) \) is defined as the maximal angle between \( \hat{n}_p \) and \( \hat{n}_q \), where \( q \) ranges over the above-described neighboring grid points. The misorientation field \( m \) is a function on the square base domain \( \Omega \) and takes values between 0 and 90 degrees. For points in the interior of a grain, which are more than three pixels away from any grain boundary, one has \( m = 0 \). On the other hand, strictly positive values of \( m \) indicate that the corresponding pixel is close to a grain boundary, across which the misorientation of the grain normals is equal to \( m \) degrees.

The misorientation fields for six of our hypothetical microstructures are shown in Figure 5. In these figures, light yellow corresponds to interior grain pixels, i.e., to \( m = 0 \),
and black corresponds to $m = 90$ degrees. Within each row, the underlying microstructures have identical orientation distribution, but the misorientation distribution changes from $S^H$ (left column) to $S^U$ (middle column) and $S^L$ (right column). The microstructures chosen in Figure 5 correspond to the respective response fields shown in Figures 2 and 3. From a purely visual point of view, the different misorientation distribution characteristics can clearly be distinguished in Figure 5.

In order to obtain a quantitative assessment of the grain-boundary misorientations, we now employ the homological method described in Section 2.3 to the misorientation field $m$. For a variety of threshold angles between 0 and 90 degrees, we computed the super-level sets $X^+ = X^+(\theta)$ as defined in Section 2.3, as well as the associated Betti numbers $\beta_0^+$ and $\beta_1^+$. In addition, we determined the number of internal components $\beta_{\text{int}}$ and the number $\beta_{\text{bnd}}$ of components touching the boundary of $\Omega$. All of these quantities depend on the threshold $\theta$, and drawing their graphs in a $\theta$-$\beta^+$-coordinate system gives a set of signatures which quantitatively describes the topological complexity of the
super-level sets at various threshold levels. These signatures for the fifteen hypothetical microstructures are shown in Figure 6. In each graph, the five red curves correspond to the misorientation distributions $S^H$, the blue curves correspond to $S^U$, and the green curves correspond to $S^L$.

In the top row of Figure 6 the Betti numbers $\beta_0^+$ (left figure) and $\beta_1^+$ (right figure) are shown. The signatures clearly distinguish between the three different misorientation distributions, and furthermore provide some insight into the structure of the misorientation networks that are visible in Figure 5. In terms of Betti numbers, a set has the characteristics of a network if the number of components of the structure is extremely small when compared to the number of holes. Thus, all of the fifteen misorientation fields exhibit network-like structures for small thresholds $\theta$. This is of course not surprising, since for small $\theta$ the sets $X^+(\theta)$ should more or less be equal to the collection of all grain boundaries. As the threshold angle $\theta$ increases, the network structures break up — yet differently for the three misorientation distributions. In terms of the first
Betti number, one expects the network break-up to be accompanied by a decrease in
the number of holes. This can be seen in the graphs for $\beta_1^+$. In fact, these graphs show
that the network structure for $S^L$ breaks up at thresholds $\theta \approx 20^\circ$, followed by the
networks for $S^U$ which break up at around $\theta \approx 60^\circ$. In contrast, the network structure
persists up to $\theta \approx 80^\circ$ for $S^H$.

More detailed information regarding the sizes of these networks can be deduced
from the $\beta_0^+$-signatures shown in Figure 6. For all microstructures the number of com-
ponents of $X^+(\theta)$ first increases with increasing $\theta$, and then decreases down to 0 again.
The location of the peaks of these curves gives quantitative information regarding the
underlying length scales of the misorientation fields. For the $S^L$-microstructures, the
number of components never exceeds 100. In contrast, the number of components
for the $S^U$-microstructures almost reaches 300, while the $S^H$-microstructures reach almost 400. Since all hypothetical microstructures cover the same area, we see that the
characteristic length scale grows from $S^H$ to $S^U$ and $S^L$.

In order to assess the effects of the finite-size domain for our computations, the num-
ber of components has been further divided into internal versus boundary components.
For this we also computed the Betti numbers for the sub-level sets $X^- (\theta)$ described in
Section 2.3. The corresponding signatures $\beta^+_\text{int}$ and $\beta^+_\text{bnd}$ are depicted in the bottom row
of Figure 6. These graphs show that the characteristic behavior of $\beta_0^+$ is completely
due to internal components. The number of boundary components stays small for all
values of the threshold $\theta$.

The signatures of Figure 6 demonstrate that the topological characteristics of
the grain-boundary misorientations are well-represented by the three classes $S^L$, $S^U$, and $S^H$. Furthermore, one can see that within each class, there is a common notion of
network size or length scale.

3.2 Topology of the Elastic Energy Density

We now turn our attention to the mechanical response fields described in the introduc-
tion, and begin with the elastic energy density fields shown in Figure 2. As before, we
compute the Betti numbers of the super-level sets $X^+$ as a function of the considered
threshold. In order to minimize the effects of artifacts in the homology computations
due to the pixel-based approximation of the sub- and super-level sets [21], we do not
work with the results of the OOF computations directly. Rather, we apply a center-
weighted convolution filter to the data, similarly to the one described in [22]. Examples
of the resulting smoothing for the maximal principal stress are shown in Figure 4.

The Betti number signatures for the elastic energy density networks are shown in
Figure 7. For these computations, we chose thresholds between 10 and 100 $kJ/m^3$. As in
the previous section, the figures in the top row show the number of components and the
number of holes, respectively, while the figures in the bottom row contain the number
of internal and of boundary components. Also in this case, the topological signatures
Figure 7: Betti numbers as a function of threshold for the elastic energy density. The graphs show the Betti numbers $\beta_0^+$ (top left) and $\beta_1^+$ (top right), as well as $\beta_{\text{int}}^+$ (bottom left) and $\beta_{\text{bnd}}^+$ (bottom right).

clearly distinguish between the different misorientation distributions. Moreover, the topological characterizations show that for small threshold values, the super-level sets have network characteristics. However, the network break-up with increasing threshold value is different from the one observed in the grain-boundary misorientation networks. In the case of the elastic energy density, all misorientation classes lose the network characteristic at roughly the same threshold value $40kJ/m^3$. The signatures appear to be more or less scaled versions of each other, indicating similar topological complexity as a function of threshold. The only difference between the classes $S_L$, $S_U$, and $S_H$ is the height of the $\beta_0^+$-curves — and these again quantitatively reflect the observed differences in the network length scales. Finally, the distinction between internal and boundary components again demonstrates that the topological complexity behavior is completely due to internal components, the number of boundary components is comparatively small.
Figure 8: Betti numbers as a function of threshold for the maximal principal stress. The graphs show the Betti numbers $\beta_0^+$ (top left) and $\beta_1^+$ (top right), as well as $\beta_{\text{int}}^+$ (bottom left) and $\beta_{\text{bnd}}^+$ (bottom right).

### 3.3 Topology of the Maximal Principal Stress Networks

Finally we turn our attention to the maximal principal stress networks shown in Figure 3. As mentioned in the discussion of the elastic energy density fields, we apply the homological characterization to smoothed versions of the stress fields, as shown in Figure 4.

The results of the homological analysis are contained in Figure 8. The images show the Betti numbers as a function of threshold values between 10 and 110 MPa. As in the previous two instances, both the network character and the relative length scales for the misorientation distributions $S^L$, $S^U$, and $S^H$ are well-described by the homology signatures. Similar to the case of the elastic energy density, the loss of the network structure occurs at a similar threshold value for all of the hypothetical microstructures, at around 40 MPa. Furthermore, as before the observed effects are completely due to internal effects.
While the signatures for the elastic energy density and the maximal principal stress are very similar, one important difference can be observed. The absolute numbers of components are significantly larger in the case of the elastic energy density, which translates into smaller characteristic length scales. This can be seen upon comparison of Figures 2 and 3.

4 Summary

We have shown that quantitative characterizations for the thermal-elastic response of calcite-based polycrystals can be obtained by employing methods from algebraic topology, in particular homology theory. Our characterization is based on topological measurements such as the number of components and the number of handles of a complex microstructure. These characterizations allow us to characterize both the grain-boundary misorientations in the polycrystal and the resulting energy density and principal stress fields. It is demonstrated that the topological analysis quantitatively distinguishes between different types of grain-boundary misorientations, as well as between the resulting differences in the response fields.

References


