A Brief Overview of Texture and Anisotropy

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Abstract. A brief overview of the state of texture and anisotropy is provided with the motive of inspiring younger readers to engage in this topic. The International Conference on Texture of Materials ICOTOM has been active since 1969 up through the recent 19th meeting in Japan in 2021. The series initially focused on the problem of reconstructing three-dimensional orientation distributions from diffraction data which typically provided two-dimensional projections in the form of pole figures following the pioneering work of Bunge [1] and Roe [2]. In recent years, the advent of automated orientation mapping in the scanning electron microscope [3] and 3D mapping via synchrotron x-rays [4][5] has provided vastly more detailed data on texture and, crucially, has connected texture more closely with microstructure. Alongside this has been the development of simulation tools to predict texture formation and the anisotropic properties of polycrystalline materials. This has mostly been a accomplished via a mix of mesoscale models, e.g. [6], and more detailed methods that include microstructure. The latter are predominantly based on the finite element method complemented by the spectral method [7].

1. Introduction
From the earliest days of x-ray diffraction, researchers realized that the patterns from polycrystalline samples being captured on film were sometimes anisotropic in an obvious fashion, e.g., the work of Wever on changes in preferred orientation from rolling aluminum sheet [8]. Eventually interference counters replaced film [9], no doubt helped by the strong interest in radioactivity at the time. Within a few years, Geiger counters were in regular use for transmission measurements of pole figures, e.g., Decker et al. [10]. Although the variation in absorbance as a function of transmission through a sample can be estimated, Schulz’s invention of the back reflection method diminished the challenges of quantitative analysis of pole figure data [11]. Shortly thereafter, Hu et al. showed how to combine transmission and reflection data to obtain complete pole figures [12]. Bunk et al. worked out an apparatus for translating large samples under the x-ray beam for coarse-grained samples [13]. For what became the standard approach of pole figures measured in reflection, the problem of defocussing and the almost inevitable roll-off in intensity towards the edge required careful calibration of each instrument, which is documented in standard texts [14]. Interpretation of pole figure data, however, was contentious because, except for a few instances where a very few orientations were identifiable, most textures were too complex for quantitative analysis. The key development in texture analysis came in the 1960s with the convergent development of mathematical and numerical analysis of orientation distributions by Bunge [1] and Roe [2]. The latter, however, developed his analysis for polymers at a time when the research community associated that class of materials had less interest than
in metals, e.g., [15]. Roe moved onto other problems whereas Bunge devoted his whole career to the subject and is commemorated with an award in his name issued at each meeting of the International Conference on Textures of Materials (ICOTOM). Both Bunge and Roe realized that the spherical harmonic functions used in physics could be adapted for use in analyzing pole figure data. More specifically, it is possible to write down linear equations between the coefficients derived from fitting the (spherical) pole figure data and those for the underlying three-dimensional orientation distribution. This approach is often referred to as the “series expansion method” because of the mathematics used. The relationship between pole figure data and texture is also often referred to as the fundamental equation of texture because inverting it to compute the orientation distribution function or ODF enabled fully quantitative description of texture.

2. Ghost Problem
With the theoretical foundation developed by Bunge and the availability of sufficient computer power it became possible to compute the orientation distribution function from several pole figures, the number depending on crystal symmetry. Since a pole figure is the projection of the ODF along a crystallographic direction, a series expansion of both in terms of spherical harmonics leads to a relation between the coefficients in both series expansions, so that the ODF coefficients can be calculated from several incomplete pole figures. As remarked above, this was a real quantum leap in texture research since now a new level of texture analysis and interpretation was reached, and in the 1970s texture research was dominated by the measurement of important texture types and a computation of their respective ODF. Soon it was realized, however, that in the computed ODF orientation appeared which obviously did not exist in the pole figure, particularly for very pronounced textures. The reason was soon discovered. The so called ‘ghost orientations’ owed to the symmetry of X-ray reflection, which did not discriminate between a direction \((hkl)\) and \((\bar{h}\bar{k}\bar{l})\). Therefore, only the even coefficient of the ODF series expansion could be determined, whereas the odd coefficients remained undetermined and therefore caused artificial values in the ODF. Texture research in the 1980s was essentially dedicated to this problem. Lücke and coworkers computed a ‘ghost map’ for the prominent texture types in fcc metals or decomposed the ODF in a set of ideal orientations with respective scatter to compute the volume fraction of the main components. Bunge tried to break the symmetry by forcing the ODF intensity positive in the entire orientation space (typically the Euler space) or by setting the ODF value to zero where virtually no intensity was expected. Also, other approaches were proposed for instance by Williams, Imhof, Matthias Vinel (WIMV) [16] or by the application of specific criteria like maximum entropy algorithms (Schaeben) [17]. In the end it turned out that the so-called “true ODF” remained undetermined within a certain albeit small range. Any ODF from that range would render the same pole figures. This problem was essentially solved by the development of fast, large scale single grain orientation measurements by orientation imaging microscopy with EBSD, see Section 5.

3. Simulation of Texture Development and Anisotropy
Within a few years of the solution of the problem of generating orientation distributions from pole figure data so that texture could be understood in 3D, efforts began to predict texture development under plastic deformation according the physics of dislocation motion, i.e., computing the contribution of each slip system as \(d\mathbf{r} \cdot \mathbf{b} \otimes \mathbf{n}\). Taylor had already made such a prediction for tensile deformation of fcc metals [18] but the advent of computers made this routine. Bishop & Hill provided theory that reduced the problem to a search through 28 discrete stress states activating multiple slip (in each grain) [19] although further work was needed to arrive at a compatible set of slip rates. Through the efforts of Kallend & Davies [20] as well as (less well known) Leffers [21], it became apparent that the Taylor model, i.e.,
boundary condition of uniform strain in each grain produced better agreement with experiment than assuming uniform stress (and, by implication, using Schmid factors to predict slip activity). The imperfect agreement obtained prompted much discussion about the boundary conditions and the “relaxed constraints” approach of Honneff & Mecking [22] provided one of the earliest indications of the influence of grain shape on plastic deformation. Eshelby theory [23] came to be applied to the interaction between a given grain and its surroundings which culminated in the widely used viscoplastic self-consistent algorithm of Lebensohn and Tomé [6]. Many workers have incorporated so-called “crystal plasticity” into finite element codes, e.g., Dawson and co-workers [24] which has enabled the effects of the inevitable gradients in strain and stress to be taken into account in simulations. Spectral methods have also been developed for modeling elasto-viscoplastic polycrystals and have certain advantages [7]. Nevertheless, our ability to predict texture development with continuum models remains imperfect which suggests that simulating the behavior of large populations of dislocations may ultimately be required; this approach has already had some success at simulating strain hardening [25].

Understanding the anisotropic properties of materials is closely related to quantitative descriptions of texture and calculation of texture development. Nye’s classic text on the properties of crystals [26], followed by Newnham’s expansion [27] to a wider range of properties provide a theoretical basis and many properties of polycrystals can be estimated as a volume average of the single crystal behavior. Even for elastic response, however, one must choose between different boundary conditions. Just as mentioned above for texture modeling, the simplest lower (Reuss) and upper (Voigt) bounds on the elastic stiffness assume either iso-stress or iso-strain; many use the Hill average of these two [28]. Depending on the choice, the fitted coefficients for the ODF of a material lead to a very efficient calculation of any type of elastic modulus in any direction [29]. Plastic anisotropy is more complex than for elasticity but uses the same approach as described above: instead of repeating increments of strain in the same direction to accumulate total (plastic) strain, the directionality of, e.g., strength is calculated by imposing different strain increments on the same texture. Early work was reported by Kallend & Davies, for example [30] and many details are available in textbooks such as Kocks, Tomé and Wenk [14]. The most common way to visualize the results is to plot yield surfaces, i.e., the variation in yield stress as a function of direction in relation to a reference frame embedded in the material. Although the volume invariance in plastic deformation effectively eliminates the hydrostatic component of stress (and strain), one still has five components from which to draw pairs for plots. The reader should beware of relying on only plotting pairs of, say, principal components or the pi-plane. The practical consequences of plastic anisotropy appear in metal working processes such as sheet forming where embedding plastic anisotropy in a finite element code enables quantitative evaluation of the influence of texture [31]. It is also important to remember that strain anisotropy may be larger in magnitude than stress anisotropy, which is apparent in the variation in the “r-value” or Lankford coefficient that is closely related to the capability of sheet metals to undergo deep drawing [32].

4. Texture in Geological Materials

In contrast to texture research in metallurgy, where the measurement and prediction of anisotropy of processed material was of primary concern, texture research in geology served mainly to reveal and understand the geological history of minerals. When reading geological literature, it is important to note that the term texture typically relates to the morphology of a sample rather than to its crystallographic texture, which is referred to in geology as preferred orientation. Research on geological materials is substantially more complicated than in metals due to the fact that most minerals have a lower crystal symmetry than metallic materials, which dominantly have a cubic or in fewer cases a hexagonal crystal structure, whereas minerals often show only triclinic symmetry. This required the measurement of many more pole figures and
computation of high order series expansion in order to obtain full information on the orientation distribution. On the other hand, geological materials have typically a much larger grain size, which makes the measurement with conventional X-ray texture goniometers virtually impossible. Therefore, crystallographic textures in geological materials are typically measured by neutron diffraction in transmission mode where a larger number of grains is encountered by a neutron beam on its way through the volume. Such measurements cannot be performed in a private laboratory but requires access to large research facilities, and owing to the low interaction of neutrons with crystalline materials the acquisition of pole figures usually takes a long time. Nevertheless, in the course of time texture research in geology has advanced to a most valuable tool for earth sciences, q.v. Wenk’s chapter on geological textures in [14].

5. Electron Back Scatter Diffraction (EBSD)
Most researchers in materials science accept Electron Back Scatter Diffraction (EBSD) as an everyday characterization tool albeit one requiring additional care in sample preparation to remove surface damage. Although advances continue to be made in terms of both hardware and the software to analyze the results, most of the technique is described in the book by Schwartz et al. [3] and an encyclopedia article by Rollett & Barmak [33]. Once it became clear that individual Kikuchi maps could be indexed automatically [34][35], for which we note that the application of the Hough transform proved to be a crucial image processing step [36], then interfacing to the SEM to control the beam implemented automated mapping. Given that commercial EBSD systems are highly reliable when damage-free samples are scanned, it is useful in the limited space to offer some pros and cons from a texture perspective. For typical grain sizes in the range $10^{−18} \text{−} 100 \, \mu m$, choosing a scan size and step size to obtain good resolution of each grain often means that the field of view only includes a few dozen grains. This is not enough to describe the texture of most materials unless the texture is very strong. A rule of thumb is that one needs $\sim 500$ grains to represent most textures and more quantitative guidance was given by Matthies & Wagner [37]. Another caution has to do with the “inverse pole figure color” that is so often used, mostly, one suspects, because the resulting figures are pleasingly colorful: by assigning color to each pixel based on which crystal direction is closest to a chosen sample direction (generally, the surface normal), the 3-parameter nature of orientation is reduced to a 2-parameter description. Accordingly, the reader is encouraged to experiment with other color schemes. EBSD surpasses traditional texture measurement, of course, by revealing local variations in orientation which have revealed important details about orientation gradients, for example [38][39][40]. As discussed in section 7, EBSD opened up the study of grain boundaries and interfaces in general.

6. Controversies in Texture
Despite the use of the Schultz method and the application of point counters the measurement of pole figures in the 1950s remained a tedious and time-consuming procedure, since the counter intensity was usually recorded on a time-linear recorder which required the manual transcription of a linear time-intensity profiles on meter long recorder paper into an intensity distribution in the stereographic projection. This difficulty was essentially removed by the pole figure plotter, where the intensity was associated with a specific color and plotted in a stereographic projection. While the recording of pole figures was substantially simplified by these developments, the analysis and interpretation of the pole figures remained difficult since the pole figures usually consisted of continuous intensity distributions. Despite differences in detail four types of pole figures of rolled sheet were identified in fcc metals, namely the low alloy, high temperature type, the so called ‘copper-type’ texture (Fig. 1) and its associated annealing texture (Fig. 2). The “cube texture” and the high alloy low temperature type, the so called “brass-texture” with the respective “brass recrystallization texture” after annealing of the rolled sheet. Two kinds of analytical descriptions
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Figure 1. Rolling texture of Cu and Cu30Zn (brass30) in terms of their 111 and 200 pole figures.

Figure 2. 111 pole figures of the annealing textures of pure Al (a) and Cu30Zn (b).

of the continuous intensity distributions were proposed, namely the partial fiber (i.e., a rotation about a specific crystallographic axis) approach and the scattered ideal orientation approach. Eventually the latter description became widely accepted but it required extensive TEM work to identify the major ideal orientations, notably the S-orientation (i.e., $(123)[63\overline{4}]$) besides copper
and brass orientation. It is interesting to mention in this context that the ODF representation of rolling textures is nowadays typically described by respective fibers in orientation (Euler) space for both fcc (Fig. 3) and bcc metals (Fig. 4). A major scientific dispute arose about the reason for the two different types of rolling textures, i.e. between brass and copper type texture. The brass texture was attributed to cross slip by one school and deformation twinning by another, until it finally could become evident from TEM work that the low temperature texture was substantially influenced by deformation twinning. The fiercest classical controversy, however, was fought over the development of the recrystallization texture, occasionally touching even the personal level. Dillamore and coworkers associated the recrystallization texture on the basis of transmission electron microscopy and deformation texture simulations according to the Taylor theory (Sect. 3) with a dominant nucleation process during recrystallization (oriented nucleation, ON) [41] whereas Lücke and coworkers promoted the theory of dominant growth of recrystallized grains with a specific orientation relation to the deformed microstructure, specifically in fcc metals and alloys the famous 40°⟨111⟩ rotation (oriented growth, OG) which they derived from growth selection experiments [42]. Only after extensive TEM and EBSD work, refined texture analysis and advanced recrystallization simulation results [43] is it nowadays obvious that both processes, nucleation and growth, and maybe even elastic anisotropy [44] play a role.

Figure 3. ODF of rolled CU in 3D view (a) and 5° sections parallel to φ2 (b).

7. Interfacial Texture and Properties
A major advance, and extension from classical topics, was to consider the crystallographic character of grain boundaries as interface texture and to evaluate it in an analogously statistical fashion to bulk or volumetric texture. This development depended almost entirely on the availability of EBSD, section 5, that could provide large area orientation maps with large numbers of grains, each pair of which has a distinct boundary. The obvious limitation of not knowing the inclination of each individual boundary on a planar cross-section was overcome via a stereological and statistical approach in which sufficient examples of (the zones of traces of) boundaries of each misorientation class were accumulated in a stereogram [45][46]. By normalizing the accumulated intensities and using the local crystal frame as a reference, the distribution of grain boundary normals for each misorientation class is revealed. It quickly became apparent, e.g., that symmetric tilt boundaries did not exhibit any unusually high frequency whereas low energy surfaces predict low energy grain boundaries. Moreover, a strong (anti-)correlation emerged between grain boundary frequency versus energy [47] and the
simulated grain boundary energies of grain boundaries were well correlated with experimentally derived values [48]. Measurement of interfacial energies has long been (mostly) performed by measuring dihedral angles at triple junctions on the assumption that local equilibrium holds. Being able to perform automated serial sectioning with EBSD [49] opened up a wide range of investigation into 3D microstructure [50], including properties of grain boundaries such as energy. The key step in extracting energies from measurements of dihedral angles was to recognize that all the data had to be considered together [51] and that the capillarity vector [52] was the best basis for obtaining reliable results [53]. Although most attention has been given to grain boundaries, surfaces can be characterized in a similar fashion [54], as well as heterophase interfaces [55], and that surface energies can be linked to grain boundary energies.

8. Synchrotron x-rays for Grain Mapping, Diffraction Microscopy

Although the application of synchrotron radiation (x-rays) to materials science in general and texture in particular has a long history, e.g., [56], it is in the past decade that this activity has flowered. A recent book by Poulsen [57] provides a great deal of detail about the various techniques that are now available. Apart from substantial improvements in the resolution of detectors as well as the speed at which data can be read out, the key development was to devise ways in which to identify sets of diffraction spots that originate from the same grain (orientation). This was the major algorithmic and computational challenge because, unlike EBSD, illuminating a polycrystalline sample with x-rays inevitably results in diffraction from multiple grains at any given rotational position of the sample. Nevertheless in its various forms, diffraction microscopy [4] can be used to map 3D polycrystals in a completely non-destructive manner. In one setting with the detector placed far enough away from the sample to identify Bragg rings, known as far-field, each grain is indexed for orientation (∼0.01°), center of mass (∼20µm) and elastic strain (∼10⁻⁴), where the resolution is noted with each quantity. In another setting with the detector very close to the sample, known as near field, Bragg rings cannot be distinguished but the resulting orientation map has a resolution slightly coarser than a micron, albeit without the elastic strain information. Thanks to the non-destructive quality of the technique, it is easy to understand that many different types of microstructural evolution can be performed from mechanical deformation to grain growth. Many examples of the application of diffraction microscopy can be found in the recent review by Bernier et al. [4] and further
development continues, e.g. [58][59].

9. Conclusion and Prognosis

This article provides a brief summary of the development of the subject of texture (fabric in geology) and a selection of its achievements, which have been transformed into practical tools for analysis in many cases. For example, including elastic anisotropy in finite element or spectral calculations is considered routine and adding plastic anisotropy to that is straightforward, albeit with a non-trivial computational cost. Measuring millions of orientations in EBSD in a few hours is considered routine, which while not guaranteeing statistically valid texture measurement, certainly provides large volumes of unambiguously single orientation data. Looking forward, however, one should ask what challenges are apparent at this point. One example is that of the evolution of texture on a local basis within grains. Throughout the literature there are examples of comparisons between both 2D and 3D orientation mapping of successive stages of (plastic) deformation versus simulations which show good statistical agreement but much variation at the local scale across individual grains [60]. One can speculate that the constitutive relations commonly employed that capture the physics-based laws for slip systems do not represent dislocation motion well enough. There are, however, a number of other ideas that have been put forward and all of these deserve to be tested as hypotheses. Another example is that of grain growth which has long been considered to be a straightforward example of curvature-driven coarsening, see, e.g., [61]. Despite the empirical result that polycrystal coarsening obeys (in some limiting sense) a parabolic law, $R^2 \propto \text{time}$, the growth rate of individual grains is clearly more complicated in reality [62] and does not follow the expectations of the theory for growth or shrinkage of 3D grains in a polycrystalline network [63]. Even these brief examples serve to illustrate that texture is a rich field full of puzzles for the young researcher to tackle and solve.

10. References

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