Disclinations and disconnections in minerals and metals

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A different type of defect, the coherency disclination, is added to disclination types. Disconnections that include disclination content are considered. A criterion is suggested to distinguish disconnections with dislocation content from those with disclination content. Electron microscopy reveals unit disconnections in a low albite grain boundary, defects important in grain boundary sliding. Disconnections of varying step heights are displayed and shown to define both deformed and recovered structures.

disconnection | disclination | metal | mineral

Wedge and twist disclinations are line defects characterized by a rotational misfit (Fig. 1). The elastic fields of disclinations were derived by Volterra (1) before they were treated as defects in condensed matter. The first such latter treatment was by Frank (2). After several precursors, mentioned in ref. 3, Frank named them disclinations. The 2 traditional types of disclinations treated by Volterra are the wedge (4) and twist (5) disclinations, which can be perfect or imperfect with a fault plane. We define here another type: the coherency disclination. Differences among these defects are described. The work was motivated by recent discussions about the role of disclinations in the deformation of geological materials (6, 7).

There are 2 broad categories of disclinations, as reviewed by Romanov and Vladimirov (8). The first includes liquid crystals (9, 10), polymers (11), animate organic composites such as sea-shells (5), electrostatic and magnetic domain wall lattices (12), and the Abrikosov lattice in superconductors (13). These lattices are all elastically soft, so that perfect disclinations, characterized by large angles of misfit, can exist in them. These are considered no further here. The second category includes strongly bonded compounds and minerals, as well as metals. These can only sustain small misfit angles, so that all disclinations are imperfect, with an associated defect interface. We follow standard usage and drop the modifier “imperfect,” which is implied.

We first consider types of disclinations, introducing the coherency disclination, as suggested in ref. 14. We then discuss disclination dipoles, the disclination content of disconnections, and address the issue of whether the components of disconnections are more meaningfully described as disclinations or dislocations. Disclinations are then shown to be a practical way to describe equilibrium or near-equilibrium grain boundaries, recovered or annealing twins, and recovered phases formed by a shear transformation. A possible role of disconnections in grain boundary sliding (GBS) is also discussed. Finally, we show that low index terraces and steps (facets), present in twinning systems and for shear-shuffle phase transformations, contain disconnections with coherency disclination content.

Our summary is not intended to be comprehensive. Linear elastic fields of disclinations are treated in refs. 4, 15, and 16. Nonlinear fields, relevant to the motion of perfect disclinations (of particular interest for nanocrystals), are treated in ref. 17. Other than providing the context for connecting the elastic strain fields to those of dislocation arrays, we do not consider these treatments: Our emphasis is on structural properties. Similarly, there are many papers on disclination motion, including those

involved in the deformation of nanocrystals (18–20); these topics are also not considered in detail here.

Types of Disclinations

The elastic fields of 6 types of defects, corresponding to displacements of a surface axially cut in a cylinder, were determined by Volterra (1) more than a century ago. Three of these are dislocations, and 3 are disclinations (see, e.g., ref. 21). Two of these are different versions of a wedge disclination, and one is a twist disclination. The traditional view of a positive wedge dislocation, posited by Volterra and followed in all subsequent treatments, is shown in Fig. 1A. The disclination is formed by displacing the cut surface in a cylinder with a hollow core of radius r_0 . Continuity is restored by inserting (positive, as shown here) or removing (negative) a wedge of material. The defect is characterized by a tangential imposed (or plastic) displacement $u_\theta = r\Delta\theta$ in the isotropic elasticity approximation (anisotropy is briefly discussed later in the paper). In vector form, the imposed displacement $\mathbf{u} = (0, u_\theta, 0)$, which diverges with r , is related to the Frank rotation vector $\boldsymbol{\omega}$ (22) by the following:

$$\mathbf{u} = r(\boldsymbol{\omega} \times \mathbf{i}), \quad [1]$$

and $\boldsymbol{\omega} = \Delta\theta\boldsymbol{\xi}$, with $\mathbf{k}$ a unit vector in the z direction, so $\mathbf{k} = \boldsymbol{\xi}$, a unit sense vector lying along the defect line. In crystals, the strain field of the disclination is equivalent to that of a regular tilt array of edge dislocations at distances from the array greater than the dislocation spacing. The dislocation equivalent is also depicted in Fig. 1A. If the dislocations are further divided into a continuous array composed of dislocations with infinitesimal Burgers vectors [i.e., a Bilby interface (23)], the linear elastic field is identical to that of a disclination (11); differences from a discrete dislocation representation would only be apparent in the non-linear core region over a distance equal to the discrete dislocation spacing. The Burgers vectors are $\mathbf{b} = (0, b_\theta, 0)$.

Significance

A different type of line defect, coherency disclinations that appear whenever a coherent interface terminates, has several types of applications, as do disconnections with disclination content. We anticipate many future applications of the model to twinning, phase transformations, and grain boundary motion, particularly in minerals where slip is usually limited.

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Fig. 1. Three types of disclinations. (A) Projected view of a wedge disclination. Vector $\mathbf{f}$ and opening angle $\Delta\theta$ are shown. Edge dislocation analog, Burgers vector $\mathbf{b}$, and sense vector ξ are depicted. (B) View of a twist disconnection. Vector $\mathbf{f}$, opening angle $\Delta\kappa$, screw dislocation analog, Burgers vector $\mathbf{b}$, and sense vector ξ are depicted. (C) View of a coherency disconnection. Vector $\mathbf{f}$, edge dislocation analog, Burgers vector $\mathbf{b}$, and sense vector ξ depicted.

Alternatively, the disclination can be characterized by the net Burgers vector (*SI Appendix, Appendix A*):

$$\mathbf{f} = n\mathbf{b}. \quad [2]$$

Here, n is the total number of dislocations in the equivalent array. Analogous to the characterization of $\mathbf{b}$ for dislocations, the vector $\mathbf{f}$ can be determined as the closure failure in a Burgers circuit. Both ω and $\mathbf{f}$ are proportional to $\Delta\theta$, so any of these characterize the magnitude of the disclination field. Fig. 1A applies as well to a cut planar surface within a crystal with (r, θ, z) replaced by (x, y, z) .

The twist disclination is shown in Fig. 1B. The imposed displacement $\mathbf{u} = (0, 0, u_z)$, which diverges with r , is given by the following:

$$\mathbf{u} = r(\omega \times \mathbf{i}), \quad [3]$$

with $\omega = \Delta\kappa \mathbf{j}$, and with $\mathbf{j}$ a unit vector in the θ direction. The discrete screw dislocation analog is also depicted in Fig. 1B. The magnitude of the field of the defect is represented by $\Delta\kappa$. In this case, the Burgers vector is $\mathbf{b} = (0, 0, b_z)$.

The coherency disclination is shown in Fig. 1C. The displacements $\mathbf{u} = (u_r, 0, 0)$ are given by the following:

$$\mathbf{u} = \Delta r \mathbf{i} = \mathbf{f}, \quad [4]$$

with $\mathbf{i}$ a unit vector in the r direction. The magnitude of the field is represented by Δr , which diverges with r . The equivalent dislocation array is also shown in Fig. 1C. In this case, the Burgers vector is $\mathbf{b} = (b_r, 0, 0)$. At first order, there is no long-range rotation ω for the coherency disclination, although second-order elastic rotations can be associated with coherency stresses (Poisson and nonlinear effects). The coherency disclination was not considered by Volterra. However, a paper by Das et al. (24) is important in the present context. They describe the formation, climb, and glide of disclination loops, which

implies the existence of mixed twist/coherency disclinations. However, to our knowledge, there has been no consideration of the elastic fields or structures of coherency disclinations.

The parameters for the 3 types of disclination are summarized in Table 1. Traditionally, disclinations have been described exclusively in terms of rotations. However, there are no first-order rotations for the coherency disclinations. All 3 types alternatively could be described in terms of the direction of the vector $\mathbf{f}$, which is unique and present for each type. With consideration of the $\mathbf{f}$ vector, the coherency disclination is seen to naturally fit in with the other types. The strain for all 3 classes of imperfect disclinations scales with f and, for a given f , diverges as r decreases.

(Imperfect) disclinations exist in minerals and metals. The classical example is that of 5-fold twins meeting at a junction line in a $\langle 110 \rangle$ axial whisker in *fcc* metals. Similar junction disclinations have been observed in $\text{YBa}_2\text{Cu}_3\text{O}_7$ (25). Each disclination bounds a fault plane, e.g., a stacking fault, grain boundary, or twin boundary, and hence it is imperfect.

For perfect disclinations in crystals, there are neither fault planes nor $\mathbf{f}$ vectors and the strains scales with $\Delta\kappa$ or $\Delta\theta$. Perfect disclinations could be produced in metals or minerals with large elastic constants only if r_0 were very large (producing a hollow core), or if the disclinations are in a dipole configuration (Fig. 2) with a small length (on the order of several nanometers). For example, one could start with a *fcc* cylinder with a $\langle 111 \rangle$ axis, elastically bend the crystal into a large radius hoop shape and bond the (111) surfaces. A perfect $\Delta\theta = 2\pi$ wedge disclination would result (forming a giant, thin-walled tube, with an inner radius greater than ~ 100 nm to allow possible elastic strains given typical material strengths). Similarly, one could add a twist component by twisting the cylinder tangentially by $\Delta\kappa = 70^\circ 32'$ before bonding, resulting in a perfect twist component. However, in a continuous medium, the strains for such large values of $\Delta\kappa$, $\Delta\theta$, or Δr are so large that the formation of perfect disclinations is impossible.

The structure of chrysotile fibers (a polytype of the mineral serpentine) provide a geologically relevant analogy to the $\Delta\theta = 2\pi$ wedge disclination described above. The fibers form owing to the inherent structural curvature of tetrahedral-octahedral layers. The ideal radius of curvature, r' , is about 9 nm. The radius of curvature of the layers in the fibers increases with fiber radius, r , and elastic strains diverge as $1/r$ at small r . This divergence explains the 5- to 10-nm hollow cores of the fibers (26, 27). Thus, the defects in chrysotile are equivalent to perfect wedge disclinations with $\Delta\theta = 2\pi[1 - (r/r')]$. The outer radius of the fibers appears to be limited by a structural transformation. Transmission electron microscopy (TEM) analyses illustrate combinations of kink bands, a radial (i.e., outward) transition from chrysotile to the “flat” lizardite structure of serpentine, and other defects, associated with larger radius fibers (e.g., ref. 26).

Disclination Dipoles

In most applications, the physically significant defect is a disclination dipole (8, 17–20). In the following figures, we use the dislocation array representation of the disclinations. The representation in Fig. 1, taken directly from Volterra (1) as in many treatments, usefully represent the elastic distortions, mainly comprising the rotational component of the distortion (4, 8, 16).

Table 1. Properties of the 3 types of disclinations

Quantity	Wedge	Twist	Coherency
$\mathbf{u}$	$(0, u_\theta, 0)$	$(0, 0, u_z)$	$(u_r, 0, 0)$
$\mathbf{u}$	$\omega \times \mathbf{i}$	$\omega \times \mathbf{i}$	–
Rotation	$\Delta\theta$	$\Delta\kappa$	0
ω	$\Delta\theta \mathbf{j}$	$\Delta\kappa \mathbf{j}$	0
$\mathbf{B}$	$(0, b_\theta, 0)$	$(0, 0, b_z)$	$(b_r, 0, 0)$
$\mathbf{F}$	$(0, f_\theta, 0)$	$(0, 0, f_z)$	$(f_r, 0, 0)$

Fig. 2. (A) Discontinuous tilt wall. The red arrows represent the repulsive forces between the disclinations. (B) View of dichromatic pattern showing displacements needed to remove incompatibility. (C) f vectors displayed directly. (D) Two semiinfinite disclinations join to form a finite disclination dipole. (E) Two adjunct dipoles join to form larger dipole. Here, the x coordinate points to the right, and y is upward.

The stresses of a dipole are more easily envisioned with the origin at the center of a dipole, Fig. 2A, where a wedge is removed on the right and inserted on the left, partitioning the displacement field. Fig. 2B then represents the displacements of the μ and λ crystals needed to restore compatibility. In a reference lattice, the f vector can be read directly as in Fig. 2C. Essentially, the f vector is partitioned into a pair of vectors $f/2$. The senses of the f vectors follow the convention described in *SI Appendix, Appendix A*. With the centered origin, the behavior at dipole linkages is evident. For example, the superposition of 2 infinite disclinations with opposite $f/2$ vectors, separated by $2L$, creates the dipole shown in Fig. 2D. As another example, if 2 dipoles of length $2L_1$ and $2L_2$ are adjoined as in Fig. 2E, the equal and opposite displacements at the junction annihilate the disclinations and a new dipole with length $2L$ is created. If the $f/2$ vectors were unequal in length, a residual vector would be left at the junction. Fig. 2 demonstrates that the splitting of the f vector is necessary in order that dipoles obey the vector rules of commutation and association. Thus, for continuity, the f vectors must be partitioned, as must the ω vectors.

In embedded (Lagrangian) coordinates, the long-range field of wedge disclination dipoles can be expressed as a simple (engineering) shear strain $\gamma_{\theta\theta}$, as in simple beam bending, or as a tensor strain field with $\epsilon_{\theta\theta} = \epsilon_{rr}$. In laboratory (Eulerian) coordinates, there is also a rigid-body rotation. Fig. 2 illustrates a disclination represented as a discontinuous tilt wall. The tensor stress state associated with such discontinuous tilt walls is given in ref. 21. When that result is converted to the geometry of Fig. 2, the major stress component is as follows:

$$\sigma_{yy} = \sigma_0 \left\{ \frac{y^2}{[(x-L)^2 + y^2]} - \frac{y^2}{[(x+L)^2 + y^2]} + \frac{1}{2} \ln \left[\frac{[(x+L)^2 + y^2]}{[(x-L)^2 + y^2]} \right] \right\} \quad [5]$$

$$\approx \frac{\sigma_0}{2} \ln \frac{(x^2 + y^2)}{L^2} \text{ when } x+L \rightarrow 0$$

$$\approx \frac{\sigma_0}{2} \ln \left(1 + \frac{4xL}{(x^2 + y^2)} \right) \text{ when } (x^2 + y^2) \rightarrow \infty,$$

$$\sigma_0 = \frac{\mu_M b}{2\pi(1-\nu)d} = \frac{\mu_M f}{2\pi(1-\nu)}. \quad [6]$$

Here, μ_M is the shear modulus, ν is Poisson's ratio, and $d = 1/n$ is the spacing of dislocations in the tilt wall. The Burgers vectors

are for grain boundary dislocations, related to perfect lattice vectors b_P by $b = b_P \cos(\theta/2)$. When the finite dislocations are converted to an infinitesimal array, both b and d scale as $1/n$. Therefore, the stresses remain the same except within a distance $\sim d$ from the boundary. Thus, the infinitesimal array, identical to the disclination, and the discontinuous tilt wall have the same linear elastic field, but neither is accurate within a few atomic spacings from the boundary. The disclination misses the atomic discreteness at the boundary, and the linear tilt wall field is inaccurate near the dislocation cores.

Near the core of one of the disclinations, the elastic strain field is proportional to $f/2$, and diverges as $x \rightarrow -L$. This divergence explains the absence of perfect disclinations in hard materials and, similarly, as $r \rightarrow 0$, the hollow core of the chrysotile fibers (25). For large L , the field at one end of a dipole approaches that of a single disclination. The long-range elastic field of the dipole resembles that of a superdislocation pair with Burgers vectors $f/2$ at $x = -L$ and $f/2$ at $x = L$, augmented by the logarithmic term. The far field is simply that of a superdislocation with Burgers vector nb and core radius L , reflecting the smearing of the dislocations over the dipole length. In the infinitesimal limit, b and d both approach zero, but the ratio b/d remains constant. The field in Eq. 5 is then that of a wedge disclination. Complete elastic fields, given in refs. 4 and 16, are considered no further here, since our emphasis is on structural aspects.

The thermodynamic force F is equal and opposite as shown in Fig. 2A. It is equivalent to the Peach-Koehler force on a dislocation at the tip, or equivalently, to the J integral (21). The force is also proportional to f .

The stress field of Eq. 5 is antisymmetric about the origin and vanishes there. The field near the dipole is plotted in *SI Appendix, Fig. S2*, which demonstrates the physical reality of the partitioning. The scale of the distortions is shown for several disclinations in ref. 28. For all 3 types of disclination, or for mixtures among them, geometric parameters of dipole length $2L$, fault plane normal k ; and line direction ξ ; and displacement parameters f and ω , or θ, κ , and Δr are all important characteristics of the disclination dipoles. All analyzed disclination fields are for straight disclination lines, or the equivalent arrays of straight dislocations as in Figs. 1 and 2. In general, the disclinations could be curved (24). Curved wedge disclinations are equivalent to curved edge dislocation arrays. However, curved disclinations of the other types are more complex. They could be equivalent to arrays of mixed dislocations, in which case the rotation angle would vary along the line. Alternatively, if the rotation angle is conserved for the curved disclinations, they can only be composed of Somigliana dislocations, for which b varies in orientation along the line (see ref. 21).

Disclinations as Components of Disconnections

Important applications entail disclinations that are components of disconnections, defined in the topological model (TM) (25, 29, 30). Fig. 3 illustrates the formation of a disconnection by joining a matrix μ and product λ crystal, each containing a surface step. The resulting disconnection has a step with height h separating 2 adjacent terrace interfaces (e.g., a coherent interface or a twin boundary). The step height h is defined as follows:

$$h = mh_0, \quad [7]$$

where h_0 is the interplanar spacing normal to the interface for a unit disconnection and m is an integer. For small h , the defect can be considered to have dominantly dislocation character, while at large h , the defect has dominantly wedge disclination character. The defects are further characterized by the translation vectors (t) in the 2 crystals, such that

$$b \text{ or } f = t(\lambda) - t(\mu). \quad [8]$$

Hence, a disconnection is characterized by the step height h and either the Burgers vector b of any dislocation content or the vector f of any disclination content (8).

Applications of disconnections to twinning are reviewed in ref. 31, and those for grain boundary structure and deformation are reviewed in ref. 32. Most studies of disclinations of the category considered here are for metals or simple compounds. Some added effects for disclinations in complex minerals are presented in ref. 33. Because only a few references treat minerals, we emphasize them in the applications.

Dislocations or Disconnections or Disclinations?

The fact that a disconnection can have either dominantly dislocation character or disclination character means that there is an issue as to which description is more appropriate. All dislocations, disclinations, and disconnections have linear elastic fields that are present only outside a core region that is nonlinear. The major contribution is from any b or f content, although there can be a weak dilatational field (21). This is a weak second-order term for metals at ambient pressure, but it can make an important contribution to the activation enthalpy for disconnection motion in geological materials, especially in the lower mantle, where pressures are 20 to 100 GPa—and even greater in the solid metallic interior. Inside the disconnection core the field becomes

highly nonlinear. Thus, a logical criterion is the following precept:

The defect character of a disconnection is described by the form of the linear elastic field outside the core.

[9]

Typically, a disconnection has dominantly dislocation character when h is less than $\sim 2h_0$, and dominantly disclination character when h is greater than $\sim 3h_0$.

Almost half a century ago, Li (34) noted that the elastic field of a dislocation is equivalent to that of a disclination dipole (see also refs. 8 and 17–20). With the above precept, a unit defect of the sort mentioned by Li is best envisioned as a dislocation. This is the reason that the disclination description for unit disconnections is not followed in dislocation theory. In contrast, a disconnection with a large step height is best described as having a Li-type disclination content, as is the case for $m > 3$. Similarly, a low-angle grain boundary is best envisioned as a discontinuous dislocation wall, while as shown below, a high-angle grain boundary is best described as a disclination.

Classes of Application of Disclinations

Terraces as Coherency Disclinations. The concept of coherency disclinations provides another practical way to define the character of planar defects. Low-index terraces exist as stacking faults, twin boundaries, coherent interphase boundaries, and coherent regions between defects in low angle boundaries. The faults can be described by continuous arrays of infinitesimal dislocations comprising a Bilby interface (35, 36) analogous to the array illustrated in Fig. 1C. If terminated, these planar terraces correspond to coherency disclination dipoles. Hence, the faults correspond to disclination dipoles and their fields must be compensated by terminating defects. Coherency disclinations may be the most prevalent type of disclination.

High-Angle Grain Boundary and Incoherent Interface Disclinations.

The distortion between the crystals bounding high-angle grain boundaries can be described as rotations, with possible misfit strains present. Thus, terminated faults of this class can be described as disclination dipoles of any or all of the 3 types.

Junction Line Disclinations. If multiple boundaries meet at a junction line, i.e., a triple grain boundary junction, the condition that the junction is stress free is that the sum of the ω (or f for coherency disclinations) vectors is zero, modulo 2π , for the i dipoles meeting at the line, provided that all sense vectors ξ

Fig. 3. (A) Joining 2 crystals containing short surface steps creates a twinning disconnection with Burgers vector b and step height h . Two terrace interfaces are created on either side of the defect (dashed lines). If h is large, a disclination with vector f is created. (B) Definition of Burgers vector b or Frank vector f , and step height h . (C) Unit disconnection with dislocation content. (D) Disconnection with disclination content.

point away from or toward the line, and that the ω and f vectors are defined as in *SI Appendix, Appendix A*:

$$\sum \omega_i = 0. \quad [10]$$

This is a direct analog to the conservation of Burgers vectors for dislocations meeting at a node. For distinction, we define junctions satisfying Eq. 10 as null junctions, while those with net residual disclination are stressed junctions. Alternatively, for twist disclinations, the sums of each of the characteristic angles, must be zero, modulo 2π .

Fig. 4A is the classical 5-fold twin junction found in *fcc* crystals (37). In addition to the rotations of the twin boundaries, each a 70.32° wedge disclination, there remains a net angular misfit of 7.35° , so the center is not a null junction. Instead there are 5 superposed 1.47° wedge disclinations, with long-range strains. Fig. 4A is a simulation of such a 5-fold set in Cu, with a free-surface boundary condition. The 1.47° wedge disclinations add local elastic strain as indicated by differing colors. There are also weak effects associated with the twin boundaries and the free surface. The leading nonlinear term is equivalent to that formed when a misfitting cylinder is inserted into a cylindrical hole, producing a strain field $u_r \propto -1/r$ and a stress field $\sigma_{rr} = -\sigma_{\theta\theta} \propto 1/r^2$. The free surface boundary condition results in a superposed hydrostatic compression that increases the magnitude of $\sigma_{\theta\theta}$ and decreases that of σ_{rr} . The major term $\sigma_{\theta\theta}$ is shown in Fig. 4A. The weak contrast at the surfaces represents the terminus of disclinations there.

A 3-fold junction line is presented in Fig. 4B, based on ref. 38. This junction line shows 3 crystals in a body-centered tetragonal crystal, rotated about [010]. The f vectors at the junction line satisfy the condition of Eq. 10. Hence, unlike Fig. 4A, the 3 120° disclinations leave no significant incompatibility and no added disclinations are needed. Thus, the junction lines in Fig. 4B are null junctions of twin boundaries, with no first-order strain fields.

Disclination Dipoles within a Crystal. As indicated in Fig. 1, the glide planes for twist and coherency disclinations are potentially glissile because the fault plane is the glide plane. Hence image force attraction to the surface makes the formation within an otherwise perfect crystal difficult. Wedge disclinations are sessile in the dipole plane but can break up by the glide emission of unit dislocations. They are stable against such dissociation only up to a length $2L$ of the order of 1 or 2 nm (39). Thus, direct formation of disclination dipoles seems difficult. Wedge disclinations with nanometer lengths have been observed in highly deformed

nanocrystalline Fe (40), where large rotations and stress concentrations are present.

Applications

Disclinations in Nominally Stress-Free Equilibrium Structures. At stress-free equilibrium, all grain boundaries can be approximated to first order as disclination dipoles. There are some deviations from disclination description, although a true equilibrium can be attained in 2 dimensions (Eq. 10). In 3 dimensions, arrangements of boundaries in a tetrakaidecahedral geometry are not precisely space filling, so some local curvature near junction lines or nodes where several junction lines meet must be present, even in the isotropic elastic approximation. Curvature causes deviation from the disclination dipole structure and possible local stresses. With elastic anisotropy, the line energies of component dislocations in a tilt wall depend on the orientation of both junction lines and the fault plane. These lead to torques at the junction line, again causing local fault plane curvature and possibly faceting. Finally, there are local nonlinear interactions at junction lines as demonstrated in an atomistic study of junction lines in an *fcc* crystal (41). All of these lead to local stresses near the line, so that the disclination model applies only outside some effective radius from the junction of the order of 1 or a few nanometers in length. Inside this radius, all of the above effects can be present, providing strain fields additional to those of the disclinations. Outside this radius in equilibrium grain boundary structures, disclination dipoles, wedge and twist only, exist, so there are no elastic strains other than in the vicinity of the junctions. They are significant only in establishing the magnitude of rotation associated with the fault plane.

Classical Power Law Creep. Creep involving dislocation climb within grains has been described in a series of advances culminating in power law creep models (42–44), entailing climb and point defect diffusion, as reviewed by Nabarro (45) and Kassner and Pérez-Prado (46). These models lead to strain rates proportional to σ^q . For models relating to dislocation glide/climb within grains, $q = 3$ to 5. A number of other models ensued as reviewed in ref. 45. These models lead to strain rates proportional to σ^q , with $q = 3$ to 5. Many studies on minerals (e.g., refs. 47–50) and ceramic materials (51) fit stress power laws with $q = 3$ to 5, consistent with the classical models. Hence, while there are still reservations about the models (45), the power law description remains empirically robust. All of these models entail dislocations in pileup or other nonuniform type arrangements. Hence, disclinations have no role in this class of creep, other than in describing the structure of the boundary and its effects as a barrier, source, and sink for dislocations.

Fig. 4. (A) Imperfect disclination. Simulation of a 5-fold twin in *fcc* Cu, viewed along [110]. Differing colors indicate the magnitude of the hoop stress, $\sigma_{\theta\theta}$. (B) Perfect disclination. A 3-fold junction line (after ref. 38).

Fig. 5. (A) Three disclination dipoles with equal rotation angles θ forming a pure step. (B) Disclination quadrupole with same θ . (C) Addition of B to A advances disconnection (dashed lines represent annihilation). (D) Addition of disclination with angle θ^* to the pure step (A) produces disclination content (E) with angle θ' . (F) Resulting disconnection with disclination content. (G) HRTEM of a pure step in Cu. CTB and ITB indicate coherent and incoherent twin boundary.

Diffusional Creep with Grain Boundaries as Sources and Sinks.

Models of this type have strain rates proportional to σ^q/g_s^p , where g_s is the grain size. These models are of 2 types, the first entailing point defect diffusion with grain boundaries as sources and sinks. The effect of stress on vacancy chemical potential at grain boundary sources and sinks provides the driving force for point defect diffusion. In Nabarro–Herring creep (52), the rate-limiting diffusion occurs within the crystals with sources and sinks at grain boundaries. This mechanism leads to creep with exponents $q = 1$ and $p = 2$. In Coble creep (53), diffusion occurs along the grain boundaries and the exponents are $q = 1$ and $p = 3$. In both models, the grain boundaries differ markedly from disclination dipoles. The flux of vacancies into or out of boundaries, accompanied by dislocation climb, must be uniform to ensure the similitude of the grain shape. Point defect fluxes set up climb pileups of the grain boundary dislocations with a net Burgers vector normal to the boundary. At steady state, the pileup stress gradients create the precise constant chemical potential gradients that produce the constant flux. Generally, more than one set of Burgers vectors can contribute to the net vector. The length of the pileup is the grain dimension. Creep data for olivine at low-stress, high-temperature conditions (47) exhibit $q = 1$ and $p = 3$ behavior, indicating that the mechanism is Coble creep. For these diffusion models, the boundary arrangement is one of dislocation pileups, so disclination content has no effect on creep. Processes other than dislocation climb occur, including grain boundary sliding, but they are not rate controlling.

Grain Boundary Sliding. This process is reviewed in refs. 32 and 51. In this case, GBS leads to glide pileups over a length proportional to the grain size. The stress at the pileup tips is relieved by climb via vacancy (interstitial) diffusion and/or by emissary dislocations. Analyses of creep for olivine (e.g., ref. 49), ice (ref. 50), and forsterite (ref. 54) lead to power law creep with $q = 2$ to 3, and $p = 1$ to 2, indicating that the mechanism is GBS. Implicit in the classical models (51) is that sliding is produced by gliding grain boundary dislocations. Recent results indicate that the mechanism entails the glide of disconnections in the grain boundary. Unit disconnection motion is observed in several computer simulations and experiments (32, 55–58), including the detailed formation and motion of disconnection by a kink pair mechanism (57). Cordier et al. (6) suggested that disclination motion was a mechanism for GBS. Their work shows local misorientations across grain boundaries consistent with stressed and unstressed disclinations, but the micrometer scale of their observations implies that these are disconnections that have undergone partial

or complete recovery. Moreover, the observations that sliding is accompanied by grain boundary migration normal to the interface (55) are only consistent with a disconnection mechanism. Pileups of these disconnections give deviations from the original plane only near the interface. The elastic field of a disconnection pileup (59) then deviates from a planar pileup only near the tip. This means that the mathematical analysis is not significantly changed. A solution for the associated diffusion model has also been presented (60). Near the boundary with Coble creep, lattice dislocation motion appears to be rate limiting for GBS in some material (47–49). A recovery mechanism consistent with such rate control is presented in *Disconnections with Dislocation Content*.

Grain boundary shear without migration is possible at very high temperatures. This behavior has been demonstrated in a computer simulation (32) that shows the shift from a disconnection to a grain boundary dislocation model with increasing temperature. The major difference between the disconnection model and the dislocation model is that grain boundary disconnections

Fig. 6. (A) HRTEM of labradorite (63), showing a high-angle grain boundary. (B) Unit disconnections on the grain boundary. (C) Set of unit disconnections decorated with amorphous material created by electron beam damage. Reprinted by permission of ref. 63, Springer Nature: *Physics and Chemistry of Minerals*, copyright 2019.

Fig. 7. (A) Inverse glide pileups relaxing the pileup of coherency disconnections at a grain boundary junction. Only dislocation components are shown by the colored symbols; the *Inset* with black defects shows a schematic blowup of the disconnection pileup structure. (B) Inverse climb pileups relaxing the pileup of coherency disconnections at a grain boundary junction.

must have Burgers vector components both within and normal to the boundary (25, 30, 31).

Disconnections with Disclination Content. The importance of disclinations in grain boundaries is emphasized in refs. 6 and 20, where boundaries are constructed from wedge disclination dipoles. All wedge disconnections have some disclination content, as illustrated in Fig. 5. The pure step in Fig. 5A contains 3 wedge disclination dipoles. The rotation $\Delta\theta$ of one crystal relative to the other is the same for all 3 segments, so there is no rotational incompatibility, and no associated elastic strains. The corners are null junctions. The disconnection has step character but zero dislocation or disclination character; it is a pure step. The high-resolution TEM (HRTEM) in Fig. 5G shows a pure step in Cu. Motion from the configuration of Fig. 5A to that of Fig. 5C entails the addition of the disclination quadrupole of Fig. 5B (61).

In all disconnections, the step portion alone produces a pure rotation without long-range strain as in Fig. 5A. If the disconnection contains the added wedge disconnection as in Fig. 5D, its long-range field would superpose on that of the step, creating a disconnection with disclination content, Fig. 5E, with both a step component and a disclination component. For a unit disconnection, the long-range field is that of a dislocation, and the disconnection would have step and dislocation components. These characteristics are formally separate and are displayed (25, 30, 31) or determined (29) naturally in the TM. The TM usage of “disconnection” is general and includes all examples of such defects (29).

The rotational incompatibility at a pure step influences the mobility of the step. The linking of couple stresses and the rotation (15, 60) contribute to the thermodynamic driving force, a term that is second order in stress. Another second-order term arises in the anisotropic elastic case. Specifically, there is a change in strain energy arising from the change in the elastic constant matrix arising from the rotation. Some added nonlinear corner effects are treated in ref. 62. An example of pure step motion is discussed below for the twinning case in agreement with the concepts in ref. 61. For unit disconnections, the Peach–Koehler force, linear in stress, is much larger than the second-order term and dominates the defect mobility. Also, for steps larger than a few nanometers, uniform motion of the step becomes impossible. The larger steps move by nucleation and propagation of disconnection pairs on the step surface as observed in many simulations (e.g., ref. 31). For disconnections with unit disclinations accumulated into a step, the step height coefficient is limited to $m \cong 4 - 8$ (39). Thus, direct motion of disconnections with content of either dipole or quadrupole unit disclinations is limited to this range.

Disconnections with Dislocation Content. Sun et al. (58) modeled unit glide disconnections in a simulation and called them generalized disclinations. Their terminology is ambiguous because it

does not distinguish between stress-free steps with null junctions, and disconnections with elastic strain fields. Furthermore, the wording in ref. 58 does not convey the nature of the elastic strain fields, specifically, that of a dislocation for unit defects and that of disclinations for defects with larger steps. Hence, we propose precept [9] in general. Moreover, they stated incorrectly that the TM does not include the rotational incompatibility at a disconnection. As demonstrated in Fig. 5, the TM precisely includes the rotational displacements, associated with pure step motion, in terms of a disclination quadrupole (61). Sun et al. properly note that this rotation is acted on by a couple stresses to contribute to the change in free energy accompanying step motion. However, they do not mention the second-order term connected with the change in the elastic constant matrix produced by the rotation. In contrast, the dislocation content of a unit disconnection (or disclination content for larger step heights), provides a dominant, first-order, Peach–Koehler contribution to the thermodynamic driving force (21). Finally, the TM specifically includes atom shuffles (30, 33), not mentioned in ref. 58, which contribute to the activation energy for disconnection motion.

Fig. 6A illustrates unit disconnections on a high-angle grain boundary in deformed labradorite (62). As shown in Fig. 6B, the lattices on 2 sides of this boundary have a small mismatch, which is accommodated by periodic grain boundary disconnections. Fig. 6C shows a set of unit disconnections along the grain boundary. The disconnections have been decorated by an amorphous phase resulting from radiation damage in the electron beam. Disconnections with unit step heights are displayed. This observation shows that unit disconnections are present on the boundary, consistent with the concept that GBS occurs by the motion of such unit disconnections.

During deformation, there are junctions or other pinning points where disconnection pileups occur with associated strain fields. The resultant strains can be removed or decreased by several dynamic or static recovery mechanisms. One recovery process entails the emission or attraction of lattice dislocations, shown subsequently for twins. As mentioned in the previous section, in the creep of olivine (48, 49) and ice (50), there are regimes of GBS that appear to be rate-limited by motion of lattice dislocations. Perhaps such emission of lattice dislocations is the relevant mechanism. Fig. 7 illustrates 2 other possible accommodation mechanisms. The step offsets are suppressed for clarity. Fig. 7A displays accommodation by the formation of inverse disconnection pileups on the unstressed inclined boundaries. With a pure-shear applied stress on the horizontal boundary, the inclined boundaries have no resolved shear stress. Hence, inverse glide pileups form. Fig. 7B displays accommodation by diffusional climb, yielding an

Fig. 8. (A) Unit disconnections accumulate to form (B) a wedge disclination dipole. (C) Wedge disclination representation. (D) A slant facet with accumulated dislocation components of the disconnections, forming a disconnection dipole. The Burgers vectors have climb and glide components, b_c and b_g . The disconnection dipole is mixed wedge and glide with vectors f_c and f_g .

inverse climb pileup; a diffusion solution for the model of Fig. 7B in presented in ref. 60. In both cases, grains shear and rotate, and the boundaries can rotate, but the average grain size is unchanged, barring dynamic recrystallization.

Disclinations in Twinning. As mentioned above, coherent twin terraces are coherency disclination dipoles. Similarly, the steps or facets on a twin boundary have disclination character. Fig. 8A shows schematically that unit disconnections can accumulate to form a facet (Fig. 8B). There is a short-range attraction that causes such facets to form up to a height of 6 to 8 interplanar spacings (39). The facet is a disconnection with wedge disclination character (Fig. 8C). There will be a net disclination dipole field because the f vector of the step differs from that of the adjoining terraces. The presence of these disclinations, first noted by Armstrong (64), is generally accepted. The analysis of such a square step as a wedge disclination is presented in ref. 65. The dislocations have fixed spacings, and the tilt wall is constrained not to relax into a double-ended pileup. However, the facet can also be inclined. As shown in Fig. 8D, the disclination then has both coherency and wedge character. There are added possibilities. If the boundary plane is near a coherent plane, it will rotate into that plane to lower the surface energy, even though there are then added disclination elastic fields. Such facets have been observed in hcp metals where the near coincidence boundary is $(0001) \parallel (10\bar{1}0)$. Similar rotations could be induced by anisotropic elastic effects.

The disclination content of the large-step disclinations along twin boundaries can be reduced by the recovery mechanism of lattice dislocation emission (14). This leads to disclinations with reduced f vectors, or, in some cases, pure steps. Fig. 9A illustrates results of an atomistic simulation of Mg, showing a $(10\bar{1}2)$ twin tip with a mixed glide/wedge disclination pair analogous to the sketch in Fig. 8D. As indicated in Fig. 9B, there is a certain step height for which the vector of the disclination is nearly offset by the Burgers vector of the emissary dislocation. The strain energy would be minimum for that step height and in special cases could be zero. For Mg, the minimum energy is for $m = (h/h_0) = 7$. Fig. 9C is a compilation of data from a number of studies showing the

frequency of measured step heights versus m . As expected, steps with $m=7$ are most common. The disconnections with other values of m indicate more disclination content, demonstrating variable amounts of recovery. Similar phenomena can be observed for twins in other materials. Fig. 9D shows such relaxed facets near a relaxed $(10\bar{1}1)$ twin tip.

There is one example of a deformation twin in *fcc* forming with a strain-free, blunt tip, i.e., without disclination content (66). The suggested model is one of a special type of nucleation of successive disconnections with alternating Burgers vectors $A\delta$, $B\delta$, and $C\delta$. Hence there is zero net Burgers vector. This was verified in a dynamic HRTEM study of Cu that revealed $m=3$ disconnections with zero Burgers vector (67). This is a structure of a type suggested in ref. 58.

Summary

Coherency disclinations are introduced and are shown to appear whenever a coherent interface (terrace) terminates. They also can appear at slanted facets on a boundary, combined with a wedge and/or a twist disclination. We have proposed a criterion for separating disconnections with disclination character from those with dislocation character. The disclinations are described in the topological model. This model allows one to predict interface orientation relationships, to determine the optimum combinations of b , f , and h for the disconnection, and to distinguish between strained and recovered interfaces.

The linear elastic field is identical for a disclination dipole and a uniformly spaced dislocation array. Many solutions for curved dislocation loops are available (21). These could be used as Green's functions in the kernel of integrals to yield disclination solutions for curved wedge disclinations. Further work is needed for curved disclinations of the twist and coherency types.

Disconnections are shown unequivocally to be the defects responsible for GBS that encompasses both shear and translation of the boundary. The structure of the disconnections is described in detail in the topological model, which initially focused on phase transformations (25, 30). Applications to twinning are reviewed in ref. 31, and those for grain boundary structure and translation are reviewed in ref. 32.

Fig. 9. (A) A simulated $(10\bar{1}2)$ twin in Mg with disclinations revealed by the strain contrast at the tips. (B) HRTEM showing relaxation of the strain by partial emission in the twin. (C) Distribution frequency of step heights of facets in a recovered $(10\bar{1}2)$ twin boundary in Mg. (D) HRTEM image showing relaxation via partial emission near a relaxed $(10\bar{1}1)$ twin tip in Mg. CTB indicates coherent twin interfaces; SF indicates stacking fault; BP is a facet bonding basal plane in matrix and prismatic plane in twin; BP_y indicates a facet bonding basal plane in matrix and pyramidal plane in twin.

Most studies of disconnections are for metals or simple compounds. Some added effects for minerals with complex unit cells are presented in ref. 33. Because there have been fewer treatments for minerals, we have emphasized the latter in the applications presented here. The TM should be useful in other studies of minerals.

Data Availability. All data and protocols are contained within the manuscript and *SI Appendix*.

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