Order parameter of simple metallic glasses

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We consider the problem of the order parameter of simple metallic glasses. On the basis of the correspondence between the geometric approach and general elasticity theory, we show that the structure of a metallic glass can be characterized by a set of tensor fields describing a medium with continuously distributed linear defects (disclinations). Phase transitions are characterized by a change in the structure of the disclination density tensor ϑ_{ij} that either preserve the overall structure of the deformation tensor e_{ij} or alter it.

One characteristic feature of the structure of simple metallic glasses is the icosahedral ordering of nearest neighbors.[1] The incompatibility of the local icosahedral symmetry and global Euclidean geometry is compensated by a gauge field whose sources can be identified with disclinations. In contemporary theories of glasses,[2–4] disclinations result from a transition from a three-dimensional sphere S^3, where ideal icosahedral packing is possible for a radius $R\simeq 1.6a$ (a is the radius of the rigid spheres forming the local icosahedral ordering),[2] to a Euclidean space. However, these disclinations were not treated as disclinations in general elasticity theory, notwithstanding the fact that the imbedding of S^3 in R^3 must be accompanied by cuts in the medium, a shift of the borders of the cuts, and addition or removal of matter, i.e., by processes that create *Somilian* dislocations (special cases are the usual edge and screw dislocations and disclinations).

In the present paper, we treat a metallic glass as a continuum with continuously distributed linear topological defects. We then assume that the ideal, i.e., defect-free unstressed, state of the medium is realized in a physically unobservable non-Euclidean space (specifically in S^3). In the linear theory, this assumption also removes the well-known divergence of the energy density of an isolated disclination. In the general elasticity theory, such a medium is described by a set of tensor fields.[5] These fields admit a description in geometric terms, defining the so-called "internal" geometry.[6] We ascertain the overall correspondence of this description based on the following considerations. The correspondence of the procedure for measuring distances yields a relationship between the metric tensor g_{ij} and the deformation tensor e_{ij}

$$g_{ij}=2e_{ij}+\delta_{ij}. \tag{1}$$

Here δ_{ij} is the Kronecker symbol. The procedure for constructing a Burgers contour around a dislocation is analogous to the emergence of geometric meaning in the Cartan torsion tensor $T_{ijk}=2\Gamma_{[ij]k}$ where $\Gamma_{ijk}=g_{nk}\Gamma^n_{ij}$ is the affine connection, and indices in square (round) brackets mean that one must take the antisymmetric (symmetric) part. We can thus relate the torsion to the dislocation density tensor,

$$\Gamma_{[ij]k}=-\tfrac{1}{2}\varepsilon_{ijn}\alpha_{nk}, \quad \alpha_{ij}=-\varepsilon_{ikl}\Gamma_{klj}, \tag{2}$$

where ε_{ikl} is the completely antisymmetric pseudotensor and $\varepsilon_{123}=1$. Similar considerations relate the Einstein tensor R_{ij} to the disclination density tensor ϑ_{ij},

$$R_{ij}=-\vartheta_{ij}. \tag{3}$$

Here

$$R_{ij}=\tfrac{1}{4}\varepsilon_{jmn}\varepsilon_{ikl}R_{mnkl}, \tag{4}$$

and the curvature tensor R_{mnkl} is defined in the standard way

$$R_{ijkl}=2(\partial_i\Gamma_{jkl}-g_{mn}\Gamma_{iln}\Gamma_{jkm})_{[ij]}, \tag{5}$$

with $\partial_i\equiv\partial/\partial x_i$. The coordinates x_i are considered to be the coordinates of a point in a local orthonormalized basis in the original (Eulerian) reference system (see below).

In the most general form, the connection takes the form

$$\Gamma_{ijk}=g_{ijk}+t_{ijk}, \tag{6}$$

where

$$g_{ijk}=\tfrac{1}{2}(\partial_i g_{jk}+\partial_j g_{ik}-\partial_k g_{ij}),$$

$$t_{ijk}=\Gamma_{[ij]k}+\Gamma_{[ki]j}-\Gamma_{[jk]i}.$$

Equations (1) and (2) enable us to express Γ_{ijk} in terms of the fields e_{ij} and α_{ij}. In the general theory of defects, the tensor ϑ_{ij} can be expressed both as a curl and as the so-called curvature–torsion tensor κ_{ij} (Ref. 5),

$$\vartheta_{ij}=-\varepsilon_{ikl}\partial_k\kappa_{lj}, \tag{7}$$

which can be expressed in terms of the connection:

$$\kappa_{ij}=\tfrac{1}{2}\varepsilon_{jkl}\Gamma_{ikl}, \quad \Gamma_{i[jk]}=\varepsilon_{njk}\kappa_{in}. \tag{8}$$

We show that the correspondences introduced in this way yield the correct basic field equations for e_{ij}, α_{ij}, ϑ_{ij}, and κ_{ij}. From Eqs. (2) and (8), we have

$$\alpha_{ij}=-\varepsilon_{ikl}\partial_k e_{lj}+\kappa_{ji}-\delta_{ij}\kappa_{kk}. \tag{9}$$

From this relation we immediately obtain the continuity equation for the dislocations:

$$\partial_l\alpha_{lk}+\varepsilon_{pqk}\vartheta_{pq}=0. \tag{10}$$

The continuity equation for the disclinations follows at once from Eq. (7):

$$\partial_i\vartheta_{ij}=0. \tag{11}$$

The symmetric part of Eq. (5) yields, in the linear field approximation,

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$$(\varepsilon_{jkl}\partial_k\alpha_{il}+\vartheta_{ij})_{(ij)}=-\mathrm{Ink}(e_{ij}), \tag{12}$$

where $\mathrm{Ink}(e_{ij})\equiv\varepsilon_{imk}\varepsilon_{jnl}\partial_m\partial_n e_{kl}=\eta_{ij}=\eta_{ji}$ defines the incompatibility tensor well known in elasticity theory. The antisymmetric part of Eq. (5), on the other hand, again yields Eq. (10).

Equations (9)–(12) are the same as those obtained in the general elasticity theory. Therefore, Eqs. (1)–(3), (7), and (8) describe, in geometrical language, dislocations as defects that do not contribute to the Frank vector Ω_i, and disclinations as defects that do not give a constant contribution to the Burgers vector B_i:

$$-\int \kappa_{ij}\,dL_i=\int \vartheta_{ij}\,dS_i=\Omega_j, \tag{13}$$

$$-\int (e_{ij}-\varepsilon_{jmn}\kappa_{im}x_n)dL_i=\int (\alpha_{ij}-\varepsilon_{jqr}\vartheta_{iq}x_r)dS_i=B_j. \tag{14}$$

Here, the integration in the first integrals is over a closed contour, and that in the second integrals over the surface that caps that contour.

The ground state of the glass should be obtainable by minimizing the free energy, expressed as a function of the fields e_{ij}, α_{ij}, ϑ_{ij}, and κ_{ij}, taking (7) and (9) into account. The construction of the total free energy is a separate problem not considered in the present paper. The ground state can be obtained from the following geometric considerations. We assume that the ground state is realized in a space that is tangent at some point in the space of the ideal state. The internal geometry of the ground state then yields the correspondence between distance differentials in the ground state (metric g_{ij}) and the ideal state (metric $g_{ij}^{(i)}$), as well as the relationship between the local bases (connections Γ_{ijk}) of the tangent spaces constructed at different points of the ideal state space. Starting with this correspondence, it is reasonable to assume that the ground state of a glass is realized when the characteristics of the internal geometry are the same as those of the ideal state geometry in the local orthonormal Eulerian coordinate system constructed at the chosen point (chosen for the construction of the tangent space of the observed state) of the ideal state space. To realize the latter in S^3, we have in the first approximation to the deviation from Euclidean behavior, which corresponds to the linear approximation in the fields and $|x|<R$,

$$g_{ij}=g_{ij}^{(i)}\simeq\delta_{ij}+\frac{x_ix_j}{R^2}. \tag{15}$$

Since the connection $\Gamma^k_{[ij]}=0$ in S^3, and hence there are no dislocations in the ground state of the glass ($\alpha_{ij}=0$), we obtain

$$\vartheta_{ij}=\frac{\delta_{ij}}{R^2}, \tag{16}$$

which, if we note that in a medium with icosahedral short-range order, the modulus of the Frank vector of a single disclination $\omega=2\pi/5$, yields an estimate of the mean distance between disclinations:

$$l\simeq\sqrt{\frac{2\pi}{5}}R\simeq 0.9d, \tag{17}$$

where d is the mean interatomic distance. Hence, it follows that the disclinations are the basic structural elements of the glass, and the disclination density tensor can be considered to be a "microscopic" parameter, i.e., can be determined in an elementary cell. We note also that condition (15) makes the energy of elastic deformations of the glass, which is proportional to the square of the elastic deformation tensor $u_{ij}=(g_{ij}-g_{ij}^{(i)})/2$, equal to zero, as required for the ground state, and the realization of the ideal state in S^3 solves the problem of the elastic energy of a disclination.

A metallic glass can thus be described by the deformation tensor e_{ij}, which is inhomogeneous on scales $\simeq R$, and which determines the isotropic incompatibility tensor η_{ij} and, accordingly, the isotropic disclination density tensor ϑ_{ij}. The existence of linear defects in the ground state makes it impossible to establish a relationship between the global Cartesian system of coordinates of the final observed state (Lagrangian system) and the local coordinate system of the initial state (local Eulerian system), so that a description of the glass structure in the Lagrangian system is only possible in the language of tensor fields. The existence of linear defects is manifested at the local atomic level. In particular, the existence of disclinations shows up in the deviation of the coordination number Z from $Z=12$. Frank and Kasper have shown[7] that in media with icosahedral short-range order, only coordination numbers $Z=12$, 14, 15, and 16 are possible.

The isotropic nature of the tensor ϑ_{ij} shows that a metallic glass can be characterized by a disordered grid of disclinations subject to the one requirement that the Frank vector be conserved at points where the disclination lines intersect. Hence, it is clear that formally, transitions are possible to states in which disclination lines are ordered in some way or other. If the disclinations form a structure with translational symmetry, one obtains the well known Frank–Kasper phases.[7,8] When dodecahedral ordering (with dominant coordination numbers $Z=12$ and 16) of the disclinations is energetically favorable, one obtains a typical quasicrystal structure. Such transitions are characterized by nonvanishing components of the tensor $\theta_{ij}=\vartheta_{ij}-(1/3)\mathrm{Tr}(\vartheta_{ij})\delta_{ij}$, with the general structure of the e_{ij} tensor being retained. The glass–liquid transition should be characterized by a change in the structure of the e_{ij} tensor.

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[1] G. Vencataraman and D. Sahoo, Contemp. Phys. **26**, 579 (1985).
[2] D. Nelson, Phys. Rev. **B28**, 5515 (1983).
[3] J. P. Sethna, Phys. Rev. **B31**, 6278 (1985).
[4] J. F. Sadoc and N. Rivier, Phil. Mag. **B55**, 537 (1987).
[5] R. de Wit, *Fundamental Aspects of Dislocations*, Mir, Moscow (1977).
[6] E. Kroner, Arch. Ration. Mech. and Analysis **4**, 18 (1960).
[7] F. C. Frank and J. S. Kasper, Acta Cryst. **11**, 184 (1958).
[8] F. C. Frank and J. S. Kasper, Acta Cryst. **12**, 483 (1959).

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