Geometry and mechanics of two-dimensional defects in amorphous materials

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We study the geometry of defects in amorphous materials and their elastic interactions. Defects are defined and characterized by deviations of the material's intrinsic metric from a Euclidian metric. This characterization makes possible the identification of localized defects in amorphous materials, the formulation of a corresponding elastic problem, and its solution in various cases of physical interest. We present a multipole expansion that covers a large family of localized 2D defects. The dipole term, which represents a dislocation, is studied analytically and experimentally. Quadrupoles and higher multipoles correspond to fundamental strain-carrying entities. The interactions between those entities, as well as their interaction with external stress fields, are fundamental to the inelastic behavior of solids. We develop analytical tools to study those interactions. The model, methods, and results presented in this work are all relevant to the study of systems that involve a distribution of localized sources of strain. Examples are plasticity in amorphous materials and mechanical interactions between cells on a flexible substrate.

amorphous solid | elasticity | reference metric | plasticity | defects

The characterization of defects in amorphous solids is a fundamental problem in material science. In crystalline solids defects are localized structural deviations of matter from its ordered state. The modeling of those defects in the framework of continuum mechanics is via constraints on the configurations of the body (1). When trying to develop plasticity theories for amorphous materials, in which no structural order exists, one faces the problem of how to define defects as intrinsic geometric objects (2–4).

The first attempt to classify defects in a continuum description is due to Volterra (5). In this description, defects are sources of geometric incompatibility that results in elastic stresses. Volterra described elementary states of frustration in elastic materials, using cut–shift–weld protocols. Volterra’s constructions provide a list of pathways that result in geometrically frustrated states. However, these constructions cannot be regarded as definitions of defects, because very different procedures can result in the same material geometry.

The idea to describe distributions of defects using smooth geometric fields began with Kondo (6) and Bilby et al. (7) (more recent works are in refs. 8–10). Inspired by properties of defects in crystalline materials, they suggested to describe defects in continuum by geometric fields such as curvature and torsion tensors. This formalism describes the intrinsic geometry associated with defects, but it was not integrated into the theory of elasticity. Moreover, different types of defects involve different geometric fields, which makes such an approach complicated.

A possibly different approach for the description of defects is motivated by ref. 11 in the context of flexible membranes with a hexagonal crystalline order. Studying the stress state of a disc with a single disclination (a “5” or “7” defect in hexagonal lattice) or dislocation (a “5–7” pair), it was shown that these intrinsic structural defects lead to a source term in the elastic stress equation. Thin discs buckle into 3D configurations, “screening” the stress sources by the Gaussian curvature of the buckled surface. This observation suggests that the perturbation to the crystalline order associated with topological defects affects the mechanical state by generating localized intrinsic Gaussian curvature. It is natural to ask, then, whether similar localized distributions of intrinsic Gaussian curvature can also be found in amorphous materials that undergo irreversible deformations and, if so, what the proper field would be to describe it.

A large volume of work has recently been dedicated to the description of irreversibly deformed amorphous solids, using the framework of incompatible elasticity (12). In this description an elastic body is modeled as a 3D Riemannian manifold, equipped with a reference metric $g$, which represents local equilibrium geometry and mechanical state by generating localized intrinsic Gaussian curvature. It is natural to ask, then, whether similar localized distributions of intrinsic Gaussian curvature can also be found in amorphous materials that undergo irreversible deformations and, if so, what the proper field would be to describe it.

Significance

Modeling defects, or localized strain carriers, are a central challenge in the formulation of elasto-plastic theory of amorphous solids. Whereas in crystalline solids defects are identified as local deviations from the crystal order, it is not clear how, or even if, equivalent intrinsic entities can be defined in amorphous solids. This work presents a new way of defining and describing localized intrinsic geometrical defects in amorphous solids and for computing the stresses within defected bodies. The methods and results that are presented here can be integrated into phenomenological theories of plasticity and can be applied to biomechanical problems that involve strain localization.

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Here \( \text{dVol}_2 \) is the volume element, and \( W \) is a nonnegative energy density that vanishes if and only if \( g(x) = \bar{g}(x) \). Incompatibility manifests in that \( g \) cannot equal \( \bar{g} \) everywhere simultaneously. In this formulation there is a complete separation between the description of the intrinsic geometry of the material (determining \( \bar{g} \)) and the description of the elastic problem (finding the energy minimizing \( g \)). The reference metric is an objective measure that is independent, for example, of the actual configuration or the elastic energy functional.

Incompatible elasticity was recently used in the analysis of thin sheets endowed with an imposed global deformation field, which induces smooth reference Gaussian curvature fields (14–20) (a discontinuous reference metric was considered in refs. 21 and 22). Smooth reference metrics can describe a wide range of geometrically frustrated material; however, they are incapable of describing geometric singularities, such as in localized defects (23). In this work we perform two main steps: First, we identify a set of reference metrics associated with 2D defects in a 3D amorphous material. These defects are expressed by a multipole expansion of the reference Gaussian curvature field. We show that the first three multipoles in the hierarchy correspond to known defects in crystalline materials. We compare our analytical results to experiments with amorphous materials containing an isolated curvature dipole. In the second part of the paper the advantages of the formalism are demonstrated by solving the elastic problem of interacting curvature quadrupoles. We provide analytical expressions for interaction energies of curvature quadrupoles with external stress and with each other. The energy landscape that results from these expressions indicates an increasing tendency to stress localization, depending on the parameters of the system.

Defects generate internal stresses resulting from geometric frustration. It is well known that a crystalline body that contains a defect is residually stressed—it has no stress-free configuration. However, every part of it that does not contain the defect is a perfect crystal. Therefore, once separated from the body, it does have a stress-free configuration. Similarly, we model a defect-free amorphous material by a reference metric that can be embedded in Euclidean space without strain, i.e., isometrically. A body containing a line defect, which in the case of a 2D geometry implies that the defect is concentrated at a point, is therefore modeled by a reference metric that is locally Euclidean everywhere, except at that point (which will be taken as the origin). Local flatness means that every point has a neighborhood that can be embedded in Euclidean space isometrically. Incompatibility manifests in that the entire manifold cannot be isometrically embedded in Euclidean space. The characteristic of such metrics is that the reference Gaussian curvature vanishes everywhere except for the origin, where it is singular.

We are thus looking for 2D metrics that are locally Euclidean. Note that we are focusing our attention on the reference metric of the material. The solution of the resulting elastic problem is addressed further below.

It is known that every 2D metric is locally conformally flat (24), which means that it can be expressed as the product of a Euclidean metric and a positive scalar function. Adopting polar coordinates \((r, \theta)\), a conformally flat reference metric takes the form

\[
\bar{g} = e^{2\varphi(r, \theta)} \begin{pmatrix} 1 & 0 \\ 0 & r^2 \end{pmatrix}. \tag{1}
\]

The function \( e^{2\varphi(r, \theta)} \) can be interpreted as a local expansion factor. Also, we call \( \varphi(r, \theta) \) the conformal factor.

Using the Brioullin equation (13), the corresponding reference Gaussian curvature is

\[
\mathcal{K} = -e^{-2\varphi(r, \theta)} \Delta \varphi(r, \theta), \tag{2}
\]

where \( \Delta \) is the Euclidean Laplacian. It follows that the reference metric is locally Euclidean if \( \varphi \) is harmonic,

\[
\Delta \varphi(r, \theta) = 0. \tag{3}
\]

Using a multipole expansion, we obtain a large family of locally Euclidean metrics by setting

\[
\varphi(r, \theta) = \beta + \alpha \ln r + \sum_{n=1}^{\infty} (A_n r^n + B_n r^{-n}) \cos n(\theta - \theta_0), \tag{4}
\]

where \( \alpha, \beta, A_n, B_n, \theta_0 \) are parameters. Setting \( A_n = 0 \) amounts to \((r, \theta)\) being standard polar Euclidean coordinates as \( r \to \infty \). The parameter \( \beta \) is a homogeneous scaling factor that globally induces zero reference Gaussian curvature and hence may be set to zero.

When plugged into Eq. 1, the parameters \( B_n \) and \( \alpha \) determine a large family of reference metrics, each with a different singularity of \( \mathcal{K} \) at the origin. Mechanically, these singularities act as intrinsic localized sources of stress and therefore can be regarded as defects.

We now study the geometric interpretation of each multipole term in this expansion by considering an annular domain, which represents a cross section of a punctured 3D cylinder. The inner radius serves as a cutoff for the curvature singularity. Consider first the case where \( \alpha \) is the only nonzero coefficient, which corresponds to a monopole of Gaussian curvature. It can be shown that such a metric models a disclination with an excess angle of \( 2\pi \alpha \) (SI Text). The same geometry can be obtained via a Volterra construction (5), by removing/inserting a section 2\( \pi \alpha \) out of/into a dissected annulus. When applied to thin sheets, these constructions lead to cone and anticone configurations (11, 25). In a hexagonal crystalline material \( 6\alpha \) must be an integer leading, for example, to the well-known 5 or 7 defects (11).

Consider next the case where \( B_1 \) is the only nonzero coefficient, which corresponds to a dipole of Gaussian curvature; without loss of generality we may take \( \theta_0 = 0 \), which amounts to setting the \( x \) axis parallel to the dipole. The reference metric takes the form

\[
\bar{g}_D = e^{\varphi(r, \theta)} \begin{pmatrix} 1 & 0 \\ 0 & r^2 \end{pmatrix}. \tag{5}
\]

where \( b = 2\alpha B_1 \). A dipole is a far field approximation of a pair of monopoles of opposite charges. In the present context, a metric of the form (5) is generated by a cone–anticone pair. In crystals, cone–anticone pairs (e.g., 5–7 pairs in hexagonal lattices) are edge dislocations. Thus, the metric (5) represents an edge dislocation in amorphous materials.

Dislocations are classically quantified by a Burgers vector, which in crystalline solids measures a discontinuity in the displacement field, where the latter is expressed in crystallographic units (1). Note that the notion of displacement assumes the existence of a reference configuration; i.e., it is not an intrinsic quantity. In contrast, the geometric description of dislocation in crystalline materials relies on a notion of parallelism. One assumes the existence of a parallel frame field, which represents the crystalline axes (2, 6, 7). The Burgers vector is then associated with an asymmetric parallel transport.

In an amorphous material, the only structure is a metric. Then, the only natural notion of parallelism is induced by the Levi–Civita connection (13), which induces a symmetric parallel
transport. It is a priori unclear how to obtain a nontrivial Burgers vector from a parallel transport that is symmetric.

Assume a reference metric of the form \([5]\). Let \(P_p^r\) be the Levi–Civita parallel transport operator from point \(q\) to point \(p\), induced by \([5]\) (details in SI Text). This operator is well defined because the total curvature enclosed by any loop is zero, and hence parallel transport is path independent. We then follow the classical definition of the Burgers vector by integrating infinitesimal displacement vectors along a closed loop \(\gamma(t)\); however, unlike the classical approach, this integration takes place in the reference manifold

\[
d(r,p) = \int \Pi_{t(0)}^r(\dot{\gamma}(t)) \, dt, \tag{6}
\]

where \(p\) is an arbitrary reference point. \(d(r,p)\) is a vector at \(p\) that depends on the loop \(r\). It is proportional to the number of times that the loop surrounds the singularity \((23)\). Moreover, the vector \(d(r,p)\) is independent of the reference point \(p\). Therefore, we define the Burgers vector \(b\) as \(d(r,p)\) for loops \(r\) that surround the singularity once. This generalizes the notion of a Burgers vector for amorphous materials.

A direct calculation shows that for a reference metric of the form \([5]\) and a reference point \(p = (r_0,0)\), the Burgers vector is given by

\[
b = -be^{-b/2\pi c} \hat{y}, \tag{7}
\]

where \(\hat{y}\) is a unit vector along the \(y\) axis. As expected, it is perpendicular to the axis of the metric dipole. Its magnitude is

\[
|b| = \sqrt{(b,b)_{p_0}} = b.
\]

Conformally flat metrics, and in particular the metric \([5]\), can be induced on an originally Euclidean manifold, by differential swelling. Using this idea, we imposed a reference metric of the form \(\tilde{g}_D\) on annulus-shaped discs of a N-isopropylacrylamide (NIPA) gel, using an experimental technique similar to the one described in refs. 15 and 18. The local swelling factor is set by the cross-linking density of the gel, which is determined by the local exposure of the gel to UV irradiation (SI Text). Note that such a differential swelling generates bodies that contain a single edge dislocation, even though the plastic deformation is smooth everywhere (unlike Volterra’s cut-and-weld procedures).

When such annular discs are flattened, mimicking a cross section of a 3D body, they are stressed. The insertion of a radial cut allows the locally flat body to relax into a stress-free flat configuration. Fig. 1A and B displays two such annuli cut along the \(\theta = 0\) and \(\theta = -\pi/2\) directions. In Fig. 1A the new stress-free configuration exhibits a constant discontinuous shift along the \(r\) axis. In Fig. 1B the new stress-free configuration exhibits a constant discontinuous shift perpendicular to the cut. The plastic deformations needed to restore the bodies as they were before the cut coincide with Volterra constructions of an edge dislocation. This proves that differential swelling can yield a stress field identical to that of a dislocation. Fig. 1C and D displays analytical calculations of isometric immersions of cut discs with metrics of the form \([5]\) for \(b = 5\) mm (details in SI Text). The agreement with experiments is excellent.

Similar to disclinations and dislocations in crystals, the curvature monopole and dipole are “topological defects.” They cannot be removed, or even altered, by local deformations or by the removal of a region around the defect. The mathematical description of topological defects in Riemannian manifolds involves the notion of a monodromy. The monodromy associated with curvature monopoles and dipoles is nontrivial. In contrast, the monodromy associated with curvature quadrupoles and higher-order multipoles is trivial, meaning that by removing the defect locus all stresses can be relaxed \((23)\).

The lowest multipole that can be generated by localized plastic deformations is the quadrupole. It can be identified with strain carriers in phenomenological theories of plasticity \((26–29)\) or with Eshelby inclusions \((30–32)\). Such localized sources of stress appear in a biological context as well, when cells that are deposited on a flexible substrate contract uniaxially. The strains/stresses generated by the cells are known to affect their relative motion and generate collective organization patterns (for a review on this subject see ref. 33 and references therein).

A body that contains a single quadrupole is described by the reference metric \([1]\) in which the only nonzero coefficient in the multipole expansion \([4]\) is \(B_2\).

\[
\varphi_Q(r,\theta) = \frac{Q \cos 2(\theta - \alpha)}{4\pi r^2}, \tag{9}
\]

where \(Q = 4\pi^2 B_2\) and \(\alpha = \theta_2\).

To understand the geometrical interpretation of defects carrying a quadrupole charge, consider an annulus whose initial reference metric with conformal factor \(\varphi = 0\). Change now its reference metric into one with conformal factor \(\varphi = \varphi_Q\) given by \([9]\). Both reference metrics are globally flat, and hence they can be embedded isometrically (i.e., stress-free) in the plane. The comparison between the two stress-free configurations reveals the deformation inducing the curvature quadrupole.

Fig. 2A displays the change in the stress-free configuration for \(\alpha = 0\). The solid lines represent the stress-free configuration for \(\varphi = 0\), whereas the color-filled shape represents the stress-free configuration for \(\varphi = \varphi_Q\). In this case the local deformation that induces the metric is a compression. Fig. 2B displays the change in the stress-free configuration for \(\alpha = \pi/4\). In this case the local deformation that induces the metric is a shear (details in SI Text).
So far we have shown that the reference metric field can describe localized sources of stress in amorphous materials, which share many similarities with defects in crystalline materials. Curvature monopoles and curvature dipoles are equivalent to disclinations and dislocations, respectively. Curvature quadrupoles are equivalent to Stone–Wales defects, and can be generated via localized deformations. The description of defects using a reference metric does not depend on the constitutive laws of the underlying material and does not involve any linearization. In addition, because it is defined in the reference manifold, it does not depend on the actual configuration of the body. This property is important when dealing with problems that contain many defects: Such bodies can be described by a reference metric (Eq. 1), with

$$φ(x) = \sum_i φ_i(x - x_i),$$

where $φ_i(x - x_i)$ is the conformal factor of a single defect, located at $x_i$. This superposition property is exact and is crucial for modeling “many body problems” (Fig. 2C and D). Finally, the resultant (nonlinear) elastic problem can be solved analytically. Given a reference metric, one obtains a partial differential equation for an incompatible stress function (ISF). The ISF is a generalization of the classical Airy stress function.

With these tools in hand, we turn to analyze a mechanism related to strain localization in sheared amorphous solids.

It was recently suggested (31, 32) that the formation of shear bands during the failure of amorphous solids is initiated by the appearance of lines of correlated Eshelby-like singularities. These localized plastic deformations are induced by an external load, but their positions and orientations are driven by their mutual interactions as well as by their interaction with the external load. Thus, to elucidate the formation of shear bands it is necessary to understand these interactions, which is a notoriously hard problem. Analytical solutions for the arrangement of multiple localized plastic deformations were obtained in ref. 31 for the case of few, weakly interacting Eshelby inclusions (such an approximation is required due to the nonadditivity of linear elastic theory with respect to Eshelby inclusions).

Motivated by ref. 31, we proceed to study the mechanical state of an externally loaded amorphous solid that contains a given distribution of localized defects. Specifically, we study the mutual interaction of two curvature quadrupoles in an external stress field. The superposition property of our formalism and its nonlinearity allow a formulation without the approximations made in ref. 31. In particular, we can capture the transition from weak to strong coupling between the quadrupoles. The quadrupoles are located at $(0,0)$ and $R(\cos \Theta, \sin \Theta)$. Their orientations and charges are $α_1, Q_1$, and $α_2, Q_2$, respectively.

Using the ISF method mentioned above, and assuming that the two quadrupoles are separated by a distance, $r \gg \sqrt{Q}$, we obtain the interaction energy of two quadrupoles,

$$U_{QQ} = \frac{YQ_1Q_2}{16\pi R^2} \cos(2(α_1 + α_2 - 2\Theta)), \quad [11]$$

where $Y$ is the Young modulus. Physically, we expect the interaction energy to be large when $R$ is below a core size, $R_c$, and thus we assume $U_{QQ}$ to be given by [11] for $R \geq R_c$ and infinite otherwise.

Fig. 2. (A and B) An analytical calculation of the planar embedding of annuli endowed with reference metrics with conformal factor $[9]$. The case (A) $α = 0$ represents a compression-like deformation, whereas the case (B) $α = \pi/4$ represents a shear-like deformation. (C) An analytic solution of the displacement field induced by a linear array of seven quadrupoles oriented with $\pi/4$ with respect to the external shear direction. (D) A magnification of the region between two adjacent quadrupoles.
The interaction of a quadrupole with an external stress field is computed in a similar way. Taking for example an asymptotic shear stress field, $\sigma^y \rightarrow \sigma^\infty$ as $|y| \rightarrow \infty$, we obtain

$$U_{\text{int}} = -\frac{1}{2} Q \sigma^\infty \sin 2\alpha$$

(detailed calculations in SI Text).

Consider then a body subjected to an asymptotic shear stress field. Suppose the body contains two quadrupoles of orientations $\alpha_1, \alpha_2$ and a fixed magnitude $Q$, located at points $x_1, x_2$, such that $x_2 - x_1 = R(\cos \Theta, \sin \Theta)$. The total interaction energy for $R \geq R_c$ is

$$U_{\text{total}} = \frac{1}{2} Q \sigma^\infty \left( -\sin 2\alpha_1 - \sin 2\alpha_2 + B \frac{R^2}{R^2} \cos(2\alpha_1 + 2\alpha_2 - 4\Theta) \right),$$

where

$$B = \frac{QY}{8\pi R_c^2 \sigma^\infty}$$

is a dimensionless parameter.

Minimizing this energy over $\alpha_1, \alpha_2, R$ and $\Theta$, the state of minimal energy is

$$\alpha_1 = \alpha_2 = \frac{\pi}{2}, \quad R = R_c, \quad \text{and} \quad \Theta = 0.$$

Thus, a state of minimum energy is obtained when the quadrupoles are close to each other, the line that connects them is parallel to the direction of the shear, and their orientations are at an angle of $\pi/4$ relative to the direction of the shear. This prediction is consistent with ref. 31 and extends it as it is valid also for strong quadrupole–quadrupole interactions.

In the above analysis the distance between the quadrupoles is a variable determined by energetic considerations. In other models, however, both the positions and the magnitudes of the localized plastic deformations are predetermined. In these models the distance $R_c$ in the definition of $B$ should be replaced by the actual distance between the quadrupoles.

The fact that the energy minima of the weakly and strongly interacting quadrupoles coincide does not imply that materials behave similarly in these two limits. The difference between the two cases is significant in the presence of noise. Then, the full energy landscape is important and not just the location of the minima. For a strong shear field, i.e., for $B \ll 1$, the total energy is dominated by the interaction with the external field, which implies that $\alpha_1, \alpha_2$ will not deviate much from their optimal value. For a weak shear field, i.e., for $B \gg 1$, the total energy is dominated by the mutual interaction of the quadrupoles, and hence $\Theta$ will not deviate much from $\alpha_1 + \alpha_2 - \pi/2$. For fixed $\Theta$, $\alpha_1, \alpha_2$ may fluctuate as long as their sum remains constant.

Fig. 3 shows the interaction energy landscape as function of $\alpha_1$ and $\alpha_2$ for $R = R_c$ and $\Theta = 0$. Fig. 3A corresponds to $B \gg 1$. The energy landscape displays a unique global minimum at $\alpha_1 = \alpha_2 = \pi/4$. Fig. 3B corresponds to $B \ll 1$. In this case there is a degeneracy with a global minimum along the line $\alpha_1 = \pi/2 - \alpha_2$. Fig. 3C corresponds to an intermediate regime. The deviations from the unique global minimum are shallower along the line $\alpha_1 = \pi/2 - \alpha_2$, and these are expected to dominate noisy statistics in realistic materials.

In summary, we presented a geometric approach to 2D defects in 3D amorphous elastic bodies. In this approach, the defective body is described by a single geometric field—the reference metric. The latter is an intrinsic property, independent of the body’s configuration.

We identified a family of defects associated with multipoles of the reference Gaussian curvature and demonstrated the correspondence between the various multipoles and known defects in crystals. The monopole term corresponds to a disclination, and the dipole term corresponds to an edge dislocation. Both terms are associated with a topological property of the reference manifold—the monodromy. It was demonstrated experimentally that a single dipole defect with a given Burgers vector can be generated in an amorphous gel by controlling the reference metric. Curvature quadrupoles are of special interest in the context of inelastic deformations in amorphous solids and in the context of the mechanical interaction between living contracting cells (33). They can be generated via localized deformations and are qualitatively similar to strain carriers in phenomenological theories of plasticity (26–30). Applying the method of incompatible stress function (35), we obtain the interaction energy of multiple quadrupoles in an external stress field. We identify a dimensionless parameter $B$ that governs the energy landscape of the interaction energy. We show that for intermediate values of $B$ the energy landscape exhibits “soft” deformation modes. These modes are expected to be reflected in the statistics of the orientation and location of defects in amorphous solids under
external stresses. In the present analysis, the magnitude $Q$ of a quadrupole was taken as a fixed parameter. In addition, the reference metric before the formation of the quadrupoles was assumed Euclidean. In reality, $Q$ is determined by the energetics of a nucleation process, and it is formed on top of an approximately Euclidean, noisy reference metric. Our analysis can be extended to include the nucleation of defects by the addition of a term of nucleation energy. Moreover, the amorphous structure of the material can be described by a random conformal factor with proper statistical measures. We expect the geometric approach to defective amorphous solids to be generally relevant to the description of plasticity, in which quadrupoles, as well as higher multipoles, are the fundamental strain-carrying objects.

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