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## Plasticity in amorphous solids is mediated by topological defects in the displacement field

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The microscopic mechanism by which amorphous solids yield plastically under an externally applied stress or deformation has remained elusive in spite of enormous research activity in recent years. Most approaches have attempted to identify atomic-scale structural "defects" or spatiotemporal correlations in the undeformed glass that may trigger plastic instability. In contrast, here we show that the topological defects which correlate with plastic instability can be identified, not in the static structure of the glass, but rather in the nonaffine displacement field under deformation. These dislocation-like topological defects (DTDs) can be quantitatively characterized in terms of Burgers circuits (and the resulting Burgers vectors) which are constructed on the microscopic nonaffine displacement field. We demonstrate that (i) DTDs are the manifestation of incompatibility of deformation in glasses as a result of violation of Cauchy-Born rules (nonaffinity); (ii) the resulting average Burgers vector displays peaks in correspondence of major plastic events, including a spectacular non-local peak at the yielding transition, which results from self-organization into shear bands due to the attractive interaction between anti-parallel DTDs; (iii) application of Schmid's law to the DTDs leads to prediction of shear bands at 45 degrees for uniaxial deformations, as widely observed in experiments and simulations.

Identifying the mechanism of plastic deformation in amorphous solids, such as glasses, is one of the major unsolved problems in condensed matter physics. In crystals, plastic flow is mediated by dislocations. These are topological defects corresponding to one missing crystalline plane in the lattice (edge dislocations) or to a lattice plane shifted by one layer (screw dislocations). While the mechanism of dislocation-mediated plastic deformation in crystals was already figured out in seminal work by Taylor [1], Polanyi [2], and Orowan [3] in 1934, a comparable mechanistic understanding of plastic deformation in glasses is still missing.

Numerical simulation studies and earlier theories of plastic activity in glasses have established the existence of so-called Shear Transformation Zones (STZs) [4]. These arise in regions where atomic motions are strongly nonaffine, i.e. with additional (nonaffine) displacements on top of those (affine) dictated by the macroscopic strain, that are required from mechanical equilibrium [5, 6]. However, STZs have remained poorly characterized in terms of their structure and topology, until pioneering work by Procaccia and co-workers [7] suggested that STZs can be identified with Eshelby-like quadrupolar events in the displacement field that self-organize into 45degrees shear bands to minimize the elastic energy [7] (see also [8]). Although this mechanism of self-organization of quadrupoles can explain observations of sinusoidal density fluctuations in shear bands of metallic glasses [9, 10], the quadrupoles are not the only shape of plastic instabilities, and in certain systems are rarely observed or not observed at all [11, 12].

In this paper, we provide the more general answer to the problem of identifying the mechanism of plastic instability in amorphous solids, and its topological nature. We start by showing that the (nonaffine) displacement field of glasses presents well defined topological singularities connected with the breakdown of the compatible deformation condition, that we demonstrate here for the first time for glasses. These topological structures are similar to dislocations (and/or vortices in superfluids), with the important difference that dislocations in crystals appear in the undeformed lattice, whereas here they appear in the displacement field under deformation. This is linked to the intrinsic out-of-equilibrium nature of glasses and it is also a fundamental difference with respect to earlier works that aimed at describing dislocations in the static structure of undeformed glass [13–16].

We show that these dislocation-like topological defects (DTDs) are the carriers of plasticity, since they lead to an average Burgers vector that strongly correlates with plastic events, and displays a strong global peak at the yielding point. This yielding peak is highly

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correlated throughout the material as expected for a sample-spanning slip system. Based on this evidence, a consistent theoretical description of plasticity in amorphous solids can be formulated, with predictions in excellent agreement with observations.

The mechanical deformation in a material can be characterized by the displacement (vector) field  $u_i$  [17, 18], which defines the deviations of the material points from their original positions  $(x_i)$  in the undeformed frame:

$$x_i' = x_i + u_i \,. \tag{1}$$

The *i* index here indicates the different spatial directions i = (x, y, z). The displacement vector can be decomposed into its affine and nonaffine contributions [19]

$$u_i = u_i^{\mathcal{A}} + u_i^{\mathcal{N}\mathcal{A}} = \Lambda_i^k x_k + u_i^{\mathcal{N}\mathcal{A}}$$
(2)

where  $\Lambda^{k}{}_{i}$  is a matrix of constants. Non-zero nonaffine displacements  $u_{i}^{\text{NA}}$  arise in glasses and noncentrosymmetric crystals in order to preserve mechanical equilibrium in the affine position dictated by the applied strain field [5, 6, 20]. In ordered crystals, the strain tensor  $\epsilon_{ij} \equiv \partial_{(i}u_{j)}$  obeys the so-called *compatibility constraint* [21, 22]:

$$\nabla \times \nabla \times \epsilon = 0, \qquad (3)$$

which is equivalent to saying that  $du_i$  is a closed differential form.

More in general, considering the total displacement field, one can define a Burgers vector [23] as the line integral of the vector field  $du_i$  on a closed loop  $\mathcal{L}$ ,

$$b_i \equiv -\oint_{\mathcal{L}} du_i = -\oint_{\mathcal{L}} \frac{du_i}{dx^k} dx^k \,. \tag{4}$$

As shown below, the Burgers vector vanishes for affine displacements and it is finite for nonaffine ones:

$$b_i^{\mathcal{A}} = 0, \qquad b_i^{\mathcal{N}\mathcal{A}} \neq 0. \tag{5}$$

A non-vanishing Burgers vector indicates the presence of topological defects inside the loop  $\mathcal{L}$ . In particular, it is associated to a non-trivial winding number around the line defect. The presence of a finite Burgers vector is equivalent to the explicit breaking of an emergent topological symmetry expressed in terms of the conservation of a two-form current  $J_I^{\mu\nu}$  [24, 25]:

$$\partial_{\mu}J_{I}^{\mu\nu} \neq 0, \quad \text{with} \quad J_{I}^{\mu\nu} \equiv \epsilon^{\mu\nu\rho}\partial_{\rho}u_{I}, \quad (6)$$

which plays the exact same role of the Bianchi identity in the classical covariant Maxwell formulation of electromagnetism (EM) [26, 27]. In other words, the presence of defects and a finite Burgers vector is in 1-to-1 correspondence to the existence of magnetic monopoles in EM [28].

Other typical examples are those of dislocations in crystals and vortices in superfluids [23, 29–32]. The role of

these generalized global symmetries has been recently recognized to be crucial to classify topological phases of matter á la Landau [33–35]. For more details regarding the connection between generalized global symmetries and nonaffine displacements see the companion paper [25].



Figure 1. **Top:** A snapshot of the interpolated 2D displacement field  $u_i$  for a single replica at  $\gamma = 0.08$ . The colors indicate the amplitude of the displacement field  $|\vec{u}|$ . The red curve is the closed Burgers loop with R = 10 on which the Burgers vector is computed using Eq.(4). **Bottom:** A zoom around a strongly nonaffine region with vortex-like shape.

There [25], we showed more formally that the nonaffine dynamics typical of liquids and amorphous systems necessarily implies the presence of finite Burgers vectors and topological defects. Here, we make one step forward and we demonstrate these concepts on glass deformation data taken from numerical simulations of a coarsegrained (flexible-chain) polymer glass well below the glass transition used in previous work [36], undergoing athermal quasistatic (AQS) shear deformation.

In Fig. 1 we show a typical snapshot of the displacement field at strain  $\gamma = 0.08$ , with a system-spanning Burgers circuit. Several regions with strongly nonaffine configurations exhibiting vortex-like shape are found. At those points, the displacement field is not single valued and the integral of the Burgers vector around those region is non-zero.

The displacement field was measured from the MD simulation and subsequently subjected to an interpolation procedure in order to obtain a smooth field for further formal calculations (for details see the Supplementary Material [37] which includes Refs. [38–40]). Evaluating the Burgers integral according to Eq.(4)gives a non-zero Burgers vector  $b_i$ . As shown in [37], the same calculation on a purely affine displacement field, gives  $b_i = 0$ . Then in Eq.(6), this implies that the displacement field is single-valued and  $\partial_{\mu} J_{I}^{\mu\nu} \neq 0$ . This also implies the violation of the compatibility condition [41] already in the small deformation (elastic) regime of glasses, which was speculated to occur when the deformation is nonaffine [42], and that we demonstrate here for the first time for glasses. This finding also indicates that not only the reference metric space is curved [16], but also that the affine connections (Christoffel symbols) are not symmetric in their lower indices and the Einstein-Cartan torsion tensor is non-zero [43]. Importantly, while the above facts have been established in crystal plasticity for large plastic deformations [41], we demonstrate here microscopically that they apply to glasses even in the elastic infinitesimal deformation regime, providing a direct link between geometry and plasticity.

In order to make the analysis of the data robust, 10 replicas were created and each was analyzed with stressstrain and Burgers vector analysis of the DTDs. The results are shown in Fig. 2. As already anticipated, the norm of the Burgers vector  $|b_i|$  averaged over the different replica displays a dominant and sharp peak at the location of the yielding point, around  $\gamma \approx 0.1$ . As shown explicitly in the Supplemental material [37], (I) the norm of the Burgers vector computed on the single replica is able to locate not only the yielding point but also the secondary plastic events manifest in the stress-strain curve as sudden stress fall-off. Strikingly, we observe clear peaks of  $|b_i|$  in correspondence of these mechanical instabilities signalled by nearly-zero or slightly negative eigenvalues of the Hessian matrix [44, 45]. And, (II) the norm of the Burgers vector is independent of the topology of the closed Burgers loop, This is a manifestation of the topological nature of this object, which "counts" the nonaffine displacements inside the close loop, and demonstrates that these DTDs are genuine topological invariants.

In Fig. 3 we present a different analysis of the same data, where now we vary the linear size of the Burgers circuit used to measure the norm  $|b_i|$  as a function of strain. This analysis reveals much of the spatial extent of the various plastic events. It is seen that, upon increasing the linear size of the Burgers circuit  $\mathcal{L}$  or its radius R,

the peak of  $|b_i|$  corresponding to the yield point  $\gamma = 0.1$ , grows enormously, much more than the peaks of the plastic events at  $\gamma = 0.05 - 0.06$  and  $\gamma = 0.08$ , and even more than the post-yielding peaks at  $\gamma = 0.15$ . This fact indicates the formation of a *slip system* spanning the whole material right at yielding, consistent with the formation of shear bands in Fig.4. A systematic plot of the Burgers peak amplitudes as a function of loop radius R for plastic events at varying  $\gamma$  is shown in [37].

Based on the above observations, it is possible to formulate a mechanism of strain-softening and plastic yield in glasses mediated by DTDs and their mutual interaction. After having verified Eq. (4) on the basis of the MD simulations, and assuming polar coordinates  $(z, \theta)$ , the displacement field around a DTDs follows immediately as  $u_i = b_i \theta/2\pi$ , with the corresponding local elastic strain field being singular,  $\epsilon_{\theta z} = \epsilon_{z\theta} = b/4\pi r$  [46], where  $b \equiv |b_i|$  is the modulus of the Burgers vector.



Figure 2. The magnified stress-strain curve (purple circles) and the norm of the Burgers vector  $|b_i|$  (orange) averaged over 10 independent replica. The vertical dashed line indicates the location of the main peak. The gray shaded area emphasizes the position of the yielding point.

By simple geometry [25], one can show that  $|b_i| \propto |u_i^{NA}|$ . In turn, from theory, numerical simulations and experiments [19, 47–49], it is known that  $|u_i^{NA}| \propto \gamma$ , where  $|u_i^{NA}|$  is an average over the sample. This implies that, due to the nature of nonaffine displacements to grow with  $\gamma$ ,  $|b_i|$  has, on average, a tendency to grow with the applied strain  $\gamma$  as well. This is not exactly what emerges from the single replica shown in the Supplemental information [37], where the behaviour of  $|b_i|$ vs  $\gamma$  is rather noisy and intermittent, and occurs mainly through bursts (peaks) in correspondence of major plastic events, and it is these bursts that grow as  $\gamma$  increases. Although a precise mechanism for DTDs multiplication and growth upon increasing the strain is yet to be identified, it becomes statistically more likely that DTDs begin to interact with each other in the plastic events where  $|b_i|$  becomes large. In particular, there is an increased likelihood that two DTDs come together with anti-parallel Burgers vectors  $\mathbf{b}_1$  and  $\mathbf{b}_2$ . It can be shown, using the Peach-Köhler force, that this gives rise to an attractive interaction force given by [18]:

$$f = -\frac{G b_1 b_2}{2\pi r},\tag{7}$$

where  $b_1$  and  $b_2$  are the moduli of the Burgers vectors of the two interacting DTDs and G is the shear modulus. This force is clearly large around the main plastic events where |b| is large.



Figure 3. **Top:** The norm of the Burgers vector  $|b_i|$  as a function of the closed loop radius R for a single replica. In purple the corresponding stress-strain curve. **Bottom:** The same plot with the norm of the Burgers vector for R = 10.

Hence, it is possible to have a mechanism whereby the rate of encounter and "coagulation" between two DTDs with anti-parallel Burgers vector becomes large. DTDs therefore attract each other, with an effective attraction force given by Eq.(7), and tend to coagulate into larger aggregates in correspondence of plastic events. This shear-induced aggregation process eventually leads to the formation of slip systems (i.e. shear bands), as the strain increases.

By leveraging these concepts, it is also possible to predict the orientation of the slip systems. Let  $\sigma = F/A_0$ be the tensile stress acting on the sample, for example a uniaxial stress, with F the applied tensile force and  $A_0$  the sample cross-section area. Denoting with  $\phi$  the angle between the normal to the slip plane and the direction of the tensile force F, and with  $\lambda$  the angle between the slip direction and the direction of F, the slip plane area is thus given by  $A_s = A_0/\cos\phi$ . Hence the tensile force resolved in the slip direction,  $F\cos\lambda$ , gives rise to a resolved shear stress given by the well-known Schmid's law [50, 51]:

$$\sigma_{RSS} = \sigma \cos \phi \cos \lambda. \tag{8}$$

In general, the three directions are not coplanar, hence  $\phi + \lambda \neq 90^{\circ}$ , while  $\phi + \lambda = 90^{\circ}$  is the minimum possible value [50, 51]. DTDs will, in general, aggregate into slip bands that are oriented randomly. For a given  $\sigma$ , slip systems will therefore be initiated by facilitated motion of DTDs that self-organize in a slip plane which experiences the largest resolved shear stress  $\sigma_{RSS}$ , similar to what happens with avalanches that initiate in a spatial direction where the resolved stress is largest and thus can overwhelm frictional resisting forces. The largest resolved stress clearly corresponds to the maximum value of  $\cos\phi\cos\lambda$ . Under the constraint  $\min(\phi + \lambda) = 90^{\circ}$ , this happens for  $\phi = \lambda = 45^{\circ}$ . Hence, for a uniaxial deformation or for a simple shear deformation, shear bands due to aggregation of DTDs will form at an angle of  $45^{\circ}$ with respect to the tensile axis as observed in our MD simulations, Fig.4, as well as other simulations and experiments [7, 9, 10].



Figure 4. The evolution of the displacements vector  $\vec{u}$  by increasing the external strain  $\gamma$ . The background color shows the Burgers vector norm and the arrow its direction and local amplitudes. The dashed white lines guide the eye towards the  $45^{\circ}$  shear band forming.

In summary, we have shown that nonaffine displacements in the deformation of amorphous materials lead all the way to the formation of topological singularities (DTDs) in the displacement field, which can be quantitatively characterized by Burgers vectors. We have demonstrated that DTDs are responsible for plastic events on the example of athermal quasistatic shear of model polymer glasses quenched at low temperature. The spatially averaged norm of the Burgers vectors displays peaks corresponding to the plastic events, and an extremely evident non-local (system-spanning) peak at the yield point. Treating DTDs in analogy to dislocations may allow one to formulate a self-consistent mechanism of slip band formation due to the attractive force between anti-parallel DTDs and due to their growing population upon increasing the strain. The preferential alignment of coagulated DTDs (shear bands) along the  $45^{\circ}$  degrees direction with respect to the tensile axis is predicted by the Schmid's law, in agreement with all experiments and numerical simulations. This work provides the quantitative identification of the long-sought "defects" which mediate fluidity and plasticity in amorphous solids [52]. Different from crystals, and from earlier work on glasses [13], the dislocation-like topological defects are not to be found in the static structure but, crucially, in the displacement field under deformation. Furthermore, they originate directly from nonaffine displacements [5, 6, 19]. Since the nonaffine displacements in turn originate from the locally low degree of centrosymmetry in the *static* structure of amorphous systems, which is a quantifiable [53, 54], this

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finding opens up the way for identifying the structural signatures of plasticity in glasses [55–57], but now in terms of atomistically well-defined quantities. Furthermore, it can provide a metric to better distinguish ductile from brittle first-order like failure [55, 58].

Finally, this work provides a quantitative identification of topological effects in amorphous systems [59] leading to a new geometrical description of plasticity and deformations in glasses. This has potential to open new directions in the chase for "order" in disordered systems.

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