11-8-2019

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Repository Citation

Liu, C., Song, X., Li, Q., Ma, Y., Chen, C. (2019). Smooth Flow in Diamond: Atomistic Ductility and Electronic Conductivity. *APS Physical Review Letters*, 123(19), 1-6. American Physical Society.
<http://dx.doi.org/10.1103/PhysRevLett.123.195504>

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Smooth Flow in Diamond: Atomistic Ductility and Electronic Conductivity

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(Received 1 July 2019; published 6 November 2019)

Diamond is the quintessential superhard material widely known for its stiff and brittle nature and large electronic band gap. In stark contrast to these established benchmarks, our first-principles studies unveil surprising intrinsic structural ductility and electronic conductivity in diamond under coexisting large shear and compressive strains. These complex loading conditions impede brittle fracture modes and promote atomistic ductility, triggering rare smooth plastic flow in the normally rigid diamond crystal. This extraordinary structural change induces a concomitant band gap closure, enabling smooth charge flow in deformation created conducting channels. These startling soft-and-conducting modes reveal unprecedented fundamental characteristics of diamond, with profound implications for elucidating and predicting diamond's anomalous behaviors at extreme conditions.

DOI: [10.1103/PhysRevLett.123.195504](https://doi.org/10.1103/PhysRevLett.123.195504)

Diamond is best known for its extremely stiff and brittle nature described by steep stress responses and abrupt cleavages under strain; also notable is its large electronic band gap spanning a wide optical spectrum. While extrinsic factors like defects may influence material performance, intrinsic stress responses and electronic properties of the pristine crystal set fundamental benchmarks that are essential to defining material behaviors and deciphering atomistic mechanisms. Such benchmarks can be well described by stress-strain relations and electronic band structures from first-principles calculations that provide key knowledge for elucidating mechanical and electronic properties [1,2]. Recent studies have generated rich insights for understanding uniaxially strained diamond and other strong solids [3–14] and unexpected strengthening effects in multiaxially strained iron [15] and covalent compounds [16–18]. However, material behaviors under complex strains remain largely unexplored, raising exciting prospects for breakthrough discoveries.

In this Letter, we report that shear strains under proper compression constraints cause a surprising structural softening, triggering an uncharacteristic ductile smooth flow in the usually very rigid diamond crystal. Analysis of associated bonding changes reveals that compression constraints prevent cleavage-type graphitization that commonly occurs in severely strained diamond and, instead, produces local bonding rearrangements via anomalously large angular variations that open new pathways for exceptional creeplike shear flow deformations. Remarkably, this structural flow process creates distinct charge-flow channels for electronic conduction, producing metallic diamond in an extended

strain range. These robust structural, mechanical and electronic behaviors under constrained shear strains are in stark contrast to traditional benchmarks of diamond, showcasing unprecedented soft-and-conducting modes that redefine this quintessential superhard and insulating solid. The present findings offer key insights for elucidating and predicting novel behaviors of diamond in a variety of extreme loading environments, e.g., in strained anvils, under indentation or wear conditions, or in planetary interiors.

First-principles calculations are well suited for capturing prominent phenomena and key mechanisms underlying diamond's stiff and brittle nature, since these intrinsic behaviors are dictated by local bonding characters at length scales suitable for such accurate computations. For example, calculated tensile stresses along major crystallographic directions elucidate the mechanism for the dominant brittle cleavage on the (111) planes [3], and computations of shear stresses identify the (111)[11-2] easy shear slip directions and the surprisingly anisotropic (111)[-1-12] shear stress response [4]. These and other studies [10–12] all find steep rises of stresses and load-bearing bond lengths in diamond in response to increasing strains, leading to abrupt brittle structural failures via graphitization. Here, we adopt established procedures [16,17] to compute and evaluate stress responses of diamond under complex, previously unexplored strains in extreme loading environments [19], and we operate with the true (Cauchy) stresses.

Under [111] tensile strains, the main load-bearing bonds in diamond align in the direction of strain, making bond elongation the dominant deformation mode with minimal angular changes, and such restricted deformation produces

FIG. 1. (a) Stress response of diamond under (11-2)[111] pure shear (PS), σ^{PS} , and constrained shear (CS), σ^{CS} . A normal-to-shear stress ratio of 2.475 is maintained during CS, corresponding to biaxial stress fields under Vickers indentation. Data in open symbols indicate dynamic instability revealed by imaginary phonon modes (see Fig. S1 [19] for details). Maximal strains sustained by stably deformed diamond crystal under the PS and CS loadings are labeled as ϵ_m^{PS} and ϵ_m^{CS} , respectively, and marked by the two vertical dashed lines passing through all the panels. (b) Variation of the bond angle α_{143} between atom pairs 1-4 and 4-3 [see panel (e)] in deformed diamond crystal under the PS and CS strains. (c),(d) Variation of three key bond lengths, d_{14} , d_{24} , and d_{34} , in deformed diamond crystal under the PS and CS strains. (e) Structural snapshots at zero, maximal PS and CS strains, along with valence charge density showing changes in bonding strengths [3] (see Fig. S2 [19] for more details).

the lowest peak tensile stress that defines the well-known (111) easy cleavage planes in diamond [3]. This observation motivated us to probe shear deformations with the slip direction aligned with the [111] bonds. We have systematically examined stress-strain relations with the [111] slip in multiple shear planes under various loading conditions. Below, we present results under (11-2)[111] shear as a prototypical case and, later, will show that all the main findings remain robust under a wide range and variety of loading conditions.

We first assess diamond's stress response to (11-2)[111] pure shear (PS) strains, corresponding to nonzero shear stress in the specified direction and zero for all other five stress tensor components, and the obtained stress-strain relation is shown in Fig. 1(a), exhibiting behaviors typical for strong covalent solids. The responding stress rises to a

sharp-tipped peak where the main load-bearing 1-4 bonds in the [11-2] direction break [Fig. 1(c)], with nearly complete charge depletion at the maximal PS strain ϵ_m^{PS} [Fig. 1(e), middle] immediately preceding a catastrophic structural failure via graphitization [4,11,12]. Dynamic structural instability signified by the appearance of imaginary phonon modes develops as stress approaches the peak value, slightly shortening the deformation range, which has been observed in highly strained diamond, and the overall stress and structural responses under (11-2)[111] PS strains are similar to typical diamond behaviors under extensively studied (111)[1-2] PS and constrained shear (CS) strains [10–12,17].

In sharp contrast to the PS case, extraordinary structural deformation modes appear when diamond is subjected to CS strains with simultaneous presence of shear stress and compressive stress normal to the shear plane. Such biaxial stress environments are often encountered during wear and indentation processes and have produced novel strength enhancements in strong covalent solids [16–18,27,28]. Here, we examine structural responses under previously unexplored (11-2)[111] CS strains, maintaining a normal-to-shear stress ratio of 2.475, corresponding to the biaxial stress field in Vickers indentation [29,30], which is commonly employed to probe material hardness and deformation. We will show below, however, that our findings are robust and insensitive to this specific constraint. Under the CS strains, the stress response σ^{CS} [Fig. 1(a)] initially rises at a much slower rate compared to the PS case, and then stays essentially flat over a wide range of shear strain until dynamic instability sets in. Such creeplike deformation occurs in some metals and, more generally, in materials at elevated temperatures close to melting, but this kind of smooth structural flow without any temperature effect is unprecedented in strong covalent solids and is especially surprising in normally stiff and brittle diamond.

Analysis of structural data reveals a novel deformation mechanism in diamond under CS strains. The angle between the bonds connecting atoms pairs 1-4 and 4-3 increases from 109.5 degrees to 137.0 degrees at the largest dynamically stable strain [Fig. 1(b)], much smaller than 121.0 degrees under PS strains. This angular deformation mechanism is driven by the normal compression constraint, which hinders the elongation of the 1-4 bonds, thus, preventing the graphitization that occurs under the PS strains. This unusual mechanism has profound impacts on structural responses. First, it acts to accommodate rising strains through angular changes, thus, allowing a significantly reduced overall bond elongation under CS compared to PS [Figs. 1(c) and 1(d)], leading to a much reduced rate of stress increase with rising strains. Consequently, different bond lengths converge under CS to create a more sustainable deformation in diamond crystal, in contrast to the diverging bond-length changes under PS with an early structural failure due to the breaking of the singularly

FIG. 2. (a) Electronic band gap E_g of deformed diamond along the PS and CS paths in Fig. 1(a) from first-principles calculations. Also shown are integrated density of states (IDOS) of electronic states within 0.3 eV on both sides of the Fermi energy under CS strains, as a measure of diamond's ability for electronic conductivity. Stress-strain curves from Fig. 1(a) are shown in the background to offer a visible reference. (b),(c) Electronic density of states from Heyd-Scuseria-Ernzerhof hybrid functional calculations [19] at select PS and CS strains, highlighting band gap reduction under PS and full closure and metallization under CS. (d),(e) Electronic band structures revealing directional electron and hole conduction at CS strains of 0.22 and 0.28. Inset in (d) shows Brillouin zone with high-symmetry points.

stretched 1-4 bonds [Fig. 1(c)]. Second, the angular deformation also transfers the main load-bearing function from 1-4 bonds under PS strains to a more even distribution among three sets of bonds under the CS strains [Fig. 1(d)], further reducing the rate and extent of bond-length increases, resulting in a much slower stress rise. Third, increasing strains induce considerable but partial charge depletion on the main load-bearing 4-3 bonds aligned in the [111] shear slip direction [Fig. 1(e), bottom], weakening, yet still sustaining these bonds, which explains the extended flattening of the CS stress-strain curve despite the continuing bond elongations at large strains [Fig. 1(d)].

The anomalous structural deformation of diamond has profound impacts on its electronic properties. In Fig. 2(a), we present the calculated band gap of deformed diamond that decreases with rising strains under both PS and CS

loadings, which is opposite to the effect of uniform compression that enhances the band gap, while stress anisotropy causes certain gap suppression [31]. Here, under the PS strains, the band gap remains open up to the maximal strain ϵ_m^{PS} . In stark contrast, CS strains drive a band gap closure early on during the deformation process, leading to diamond's metallization at surprisingly modest compressive stress of 146.5 GPa and shear stress 59.2 GPa. At increasing CS strains, an integrated density of states (IDOS) near the Fermi energy grows monotonically [Fig. 2(a)], reflecting CS strain enhanced metallic nature of deformed diamond, and the total electronic density of states at select strains under PS and CS strains are shown in Figs. 2(b) and 2(c). We have also tracked the evolution of the electronic band structure under increasing CS strains, and identified directional charge transport channels inside deformed diamond crystal. Results in Fig. 2(d) show that, under CS strains, the conduction-band bottom first crosses the Fermi level along the line connecting the Γ (0,0,0) and Z (0,0,0.5) points in the Brillouin zone, indicating that CS deformation created electronic conduction flows in the [001] direction along the normal compression shortened bonds. Meanwhile, hole pockets develop around the zone center. At increasing strains, as shown in Fig. 2(e) for CS strain 0.28, the electron pockets grow in size and position closer to the Z point, and the hole pockets move toward the M (0.5,0.5,0) and X (0,0.5,0) points that lie in the lateral plane. These highly directional channels suggest anisotropic electron and hole conductivity in CS strain deformed diamond.

To assess the robustness of the extraordinary structural and electronic smooth flow phenomena in CS strained diamond, we have explored a wide range of loading conditions. We adjusted the normal-to-shear stress ratio, and calculated results [Fig. 3(a)] reveal the same creeplike deformation behaviors accompanied by electronic band gap closures when the ratio is set to 2.00 and 3.00, suggesting the smooth flow in diamond is viable under a wide range of biaxial loading conditions. We also examined CS shear modes other than (11-2)[111]. Results [Fig. 3(b)] show similar smooth flow behaviors under (10-1)[111], (12-3)[111], and (22-3)[334] CS shear strains, indicating that the characteristic structural and electronic response under biaxial CS strains exist under not only multiple [111], but also similarly aligned (e.g., [334]) shear slip modes. Finally, we evaluated shear deformation of diamond under a constant large normal stress, corresponding to extreme wear loadings. Results [Fig. 3(c)] again reveal similar smooth flow behaviors. In all the cases studied, band gap closure occurs early on during the CS deformation process, creating a wide range of shear deformed diamond in metallic state (see Fig. S4 [19] for details). These assessments demonstrate that CS-driven atomistic ductility and electronic conductivity is a robust phenomenon in diamond under a diverse type and range of loading

FIG. 3. Robustness of smooth structural and charge flow in diamond under CS loadings. Stress data in open symbols indicate dynamic instability revealed by imaginary phonon modes (see Fig. S3 [19] for details). (a) Creeplike smooth-flow stress responses of diamond under (11-2)[111] CS strains with a normal-to-shear stress ratio of 2.00 and 3.00, and the associated electronic band gap closure and rising IDOS, similar to those shown in Fig. 2(a). (b) Similar smooth-flow stress, band gap and IDOS behaviors under (12-3)[111], (10-1)[111], and (22-3)[334] Vickers CS strains. (c) Similar smooth-flow stress, band gap and IDOS behaviors under (11-2)[111] CS strains at fixed normal stress (180 and 190 GPa).

conditions. The essential role of the normal stress is to prevent the graphitization process usually occurring under simple tensile or shear strains. Exact normal-to-shear stress ratios or specific forms of the normal stress are not crucial, as long as graphitization is suppressed to allow CS deformation to proceed.

Our results challenge the long established paradigm on bonding and mechanical characters of diamond, and introduce unprecedented structural deformation modes and stress and charge responses under a distinct and broad class of constrained shear loading conditions. A prominent scenario concerns loaded diamond anvil cell (DAC), in which structural instability usually initiates in a small region above anvil tip where the highest stresses with large compressive and shear components appear [32,33]; coexisting extreme compressive and shear stresses also exist in the anvil culet region [34]. Smooth structural and

electronic flow could conceivably occur in these small regions, while the majority of the less strained DAC remains gapped and transparent. Such a scenario would greatly impact DAC behavior and operation, as metallization of DAC tip and culet regions would impede optical probes, and creeplike plastic flow would compromise DAC stability. Hitherto, there has been no report on experimental observation of smooth plastic flow or undoped metallic state in diamond. However, detecting the predicted soft-and-conducting modes in diamond are well within current experimental capabilities for rational experimental investigations, especially in nanoscale specimens that are nearly defect free and exhibit strains and stresses approaching theoretical limits [35,36]. Moreover, stress-strain curves and ultimate stresses and strains for diamond under complex loading are part of the nonlinear elasticity rule which is necessary for simulation and understanding of the processes in DAC, and their effect is crucial [1,2]. Another notable case is that of Robert C. DeVries which observed unusual plastic deformation of diamond under extreme wear with coexisting large compressive and shear stresses, assisted by moderate temperatures, and coined the term “work-hardening of diamond” without elucidating the underlying mechanism [37]. Our findings indicate that such wear conditions may promote smooth plastic flow to facilitate plastic shear deformation. These cases show that well controlled indentation and wear may open effective avenues for exploring novel structural flow phenomena and associated electronic properties in a variety of diamond specimens once brittle fracture modes are hindered by proper constraining compressive stress. It is noted that similar plateaus in the stress-strain curves [3–5] and metallization [5] have been seen in other covalent crystals due to elastic lattice instability caused by zero elastic moduli in the loading direction before phonon instability sets in.

The present findings offer powerful insights and guidance for experimental exploration of the predicted novel behaviors in diamond, and may also prompt reexaminations of previously encountered but unexplained phenomena. The distinct mechanisms for diamond’s unusual structural and electronic evolutions add new ingredients into modeling and simulating structural responses and elucidating resulting mechanical and electronic properties of diamond under diverse constrained shear strains by connecting to measurement details [35,36,38–40]. The newly identified constrained shear deformation proceeds through anomalously large bond-angle variations, and this distinct mechanism is in sharp contrast to previously known brittle fracture modes dominated by bond elongation with much smaller angular change or defect mediated processes via bonding variations in the vicinity of defect sites, which are all restricted to much smaller strain ranges. These robust material phenomena and favorable probing conditions make the smooth flow phenomena accessible to experimental

verification and characterization and raise exciting prospects of discovering such exceptional behaviors in other strong covalent solids. Our discovery defines diamond's new benchmark properties that have broad implications for materials research, and our findings may open new areas of research on complex strain driven phenomena in a large variety of technologically important covalent materials like silicon, germanium, and silicon carbides, among others.

This research was supported by the National Key Research and Development Program of China under Grant No. 2018YFA0703404, the Natural Science Foundation of China under Grants No. 11622432, No. 11474125, and No. 11534003, and the Program for the JLU Science and Technology Innovative Research Team.

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