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Mechanical insights from functional materials

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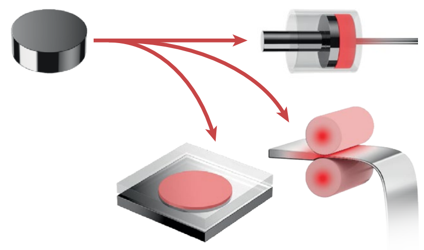
Our knowledge of deformation behaviour in functional materials is pushing the frontiers of mechanics, informing design strategies and enabling scalable manufacturing.

Materials that possess inherent electrical, optical, magnetic, thermal or chemical properties can perform specific functions, while their mechanical properties such as strength, plasticity, stiffness and toughness are considered mainly to ensure structural durability and reliable performance under operational conditions. Interestingly, the pursuit of functionalities in materials has also sparked discoveries of deformation mechanisms or mechanically modulated properties not recognized before. These insights are reshaping how we design, process and integrate materials. In this issue of *Nature Materials*, we present a focus collecting recent research and discussion that bridges functional material design and fabrication with mechanical insights.

Bonding configurations govern the deformation pathways of materials and hence their mechanical properties. Metallic bonds allow atoms to slide past each other with relative ease. Strong covalent or ionic bonds in ceramics often result in brittle fractures under stress. Van der Waals (vdW) materials — prized for their exceptional physical and electrical properties — present a unique bonding landscape: strong in-plane covalent bonds, weak interlayer interactions, variable stacking arrangements and pronounced surface and edge effects in their two-dimensional (2D) architectures. This combination creates a distinctive system for probing deformation pathways across different bonding regimes at the atomic scale.

In this issue, two Articles explore the role of interlayer coupling in the fracture behaviour of 2D materials. In an Article, Zhigong Song and colleagues identify two fracture modes — asynchronous and synchronous — in multilayer hexagonal boron nitride. The asynchronous mode features cracks propagating along different paths in each layer governed by interlayer friction. By contrast, the synchronous mode involves a single crack transversing multiple layers simultaneously, driven by interlayer bond formation and reconstruction at the crack tip, which reduces the fracture resistance and induces brittle failure. Experimental observations show that the initial flaw size dictates the competition between the two modes, a finding corroborated by multiscale mechanics analyses. Second, in an Article, Xiaodong Zheng and colleagues reveal an unexpected twist-toughening mechanism in 2D materials. The fracture toughness of twisted bilayer transition metal dichalcogenides can reach up to 1.9 times that of the untwisted layers. Initially, the cracks of the two layers propagate along different directions. Then, crack edges re-bond and form grain boundaries after interlayer sliding, followed by a secondary fracture. Both works underscore the role of interlayer mechanical interactions and bond formation in governing the fracture behaviour of 2D vdW materials, as commented in the accompanying News & Views article by Kangsik Kim and Zonghoon Lee. These findings illuminate the fundamental and unique fracture mechanisms in vdW materials, laying a basis for their application design. However, capturing the rapid propagation of cracks alongside real-time atomic structural changes calls for continued advancements in characterization and analytical techniques.



Adapted from the Letter by Gao and colleagues, Springer Nature Limited.

The ability to withstand deformation is crucial not only for maintaining the operational reliability of materials, but also for shaping them into application-specific forms. This need is especially pronounced in flexible and wearable devices, which require materials that can bend, fold, stretch or conform to complex surfaces without compromising performance. It poses a challenge for semiconductors, as most are brittle. Although a growing number of ductile semiconductors have been identified in recent years (*Nat. Mater.* **22**, 1161; 2023), achieving plastic forming of bulk semiconductors is desired for compatibility with industrial-scale fabrication processes.

In an Article in this issue, Yuechu Wang and colleagues reveal that $Ag_2Te_{1-x}S_x$ ($0.3 \leq x \leq 0.6$) deforms through a transformation of the Te/S sublattice into a brittle amorphous state even under very small external stress, a phenomenon previously overlooked in these materials. The amorphous phase can be recovered into the crystalline state by simple annealing. These observations help clarify the wide variability in reported mechanical properties. Building on this insight, Wang and colleagues develop an iterative crystalline–amorphous transition strategy, achieving a high extensibility of up to 10,150%, which enables forming processes such as cold rolling, curved wire drawing and pattern forging. Also, in this issue, Zhiqiang Gao and colleagues present an alternative metal-like processing approach for bulk semiconductors in their Letter. They demonstrate that materials such as Cu_2Se, Ag_2Se and $Bi_{90}Sb_{10}$ can be processed by rolling, extrusion and flatbed press (pictured), at temperatures around 400–500 K, achieving extensibility up to 3,000%. The brittle-to-ductile transition is attributed to temperature-dependent collective atomic displacement and thermal vibration. Notably, both works show that the electrical and thermal properties of the semiconductors remain intact following mechanical processing, as emphasized in the accompanying News & Views article by Atsutomo Nakamura and Yan Li. While some microscopic mechanisms warrant further confirmation, these findings offer promise in semiconductor manufacturing and encourage further exploration in the cost-effective plastic processing of more brittle nitride or oxide semiconductors.

While the studies discussed above concentrate on inorganic semiconductors for electronic devices, the impact of mechanical engineering on functional materials reaches far beyond, in diverse fields including energy storage and conversion, biomaterials, optical components and actuators. It connects a material's inherent properties to manufacturability and real-world performance, as the boundaries of mechanics continue to evolve and converge with other disciplines.

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