

observed by Meiklejohn and Bean¹ (cobalt particles in shells of antiferromagnetic cobalt oxide); both are inhomogeneous and the coexistence of a ferromagnetic and an antiferromagnetic phase gives rise to large exchange bias.

This demonstration of tuning the composition of certain Heusler alloys to attain exceptionally high exchange bias fields indicates a route for designing rare-earth-free hard magnets, built of two hard magnetic phases in contrast to exchange spring magnets where a soft

magnetic phase is exchange coupled to a hard magnetic phase. A second step towards exchange-biased hard magnets would be realized if the fraction of non-percolating ferromagnetic phase could be increased, thus achieving much higher magnetization, while possibly maintaining high values of the exchange bias and the coercive field. This would provide high enough remnant magnetization for an applicable permanent magnet. The remaining big challenge is to find the material combination where these

favourable hard magnetic properties are preserved well above room temperature. □

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DISLOCATION NUCLEATION

Diffusive origins

A growing body of evidence suggests that nucleation of a first dislocation in a pristine crystal is associated with a diffusion-controlled process. Understanding this is critical for strain-engineered devices at ultrahigh stresses.

Ju Li

Point defects and dislocations in crystals are known to facilitate diffusive and displacive processes, respectively¹. Unlike point defects, dislocations have no thermal equilibrium concentration, since their formation energy diverges at zero stress: instead, they are created at finite load. A mobile dislocation can glide and increase its length relatively easily, cutting and re-stitching atomic bonds to accomplish displacive shape change of a crystal. Dislocations can also multiply, via, for instance, a Frank–Read source, or when a high-speed dislocation hits a surface and nucleates more dislocations, which

leads to explosive displacive plasticity in small-volume specimens after the first mobile dislocation is nucleated². But a conundrum exists: where does the first dislocation come from? Since point defects have equilibrium concentrations at finite temperature, it is tempting to speculate that their diffusion might play a role in the emergence of a dislocation. Now, writing in *Nature Materials* Lisa Chen and colleagues report³ quantitative uniaxial tensile strength measurements of pristine Pd nanowires with uniform cross-sections. They characterize the statistics of the first measurable inelastic event,

which they attribute to the nucleation of a mobile dislocation from the surface of the nanowires. An analysis of stress-ramp data spanning 77 K to 475 K reveals that an unidentified, stress-aided surface diffusion mechanism may be essential in dislocation formation. Schuh and co-workers had previously reached a similar conclusion based on temperature-dependent nanoindentation experiments on single-crystal Pt (refs 4,5). Thus, a diffusion-based theory seems to be gaining traction in rationalizing the nucleation of an initial dislocation at room temperature in a pristine crystal.

Such understanding is important because the relatively new areas of ‘ultrastrength’ materials⁶ and elastic strain engineering⁷ depend critically on the time–temperature–sample size envelope to be able to confidently apply large deviatoric stresses (exceeding 10% of the ideal strength) to metals, semiconductors and ceramics without stress relaxation. Elastic strain engineering allows functional properties (for example, bandgap, carrier mobility, superconductivity, ferroic transitions, catalytic activity) to be tuned by ultrahigh tensorial stress in materials. Nucleation of the first mobile dislocation, however, would relax the stress and degrade — or even destroy — strain-engineered device components⁷ (Fig. 1).

Dislocation nucleation that has been pre-conditioned by surface diffusion may have a number of features. First, under ultrahigh stresses it might be possible for

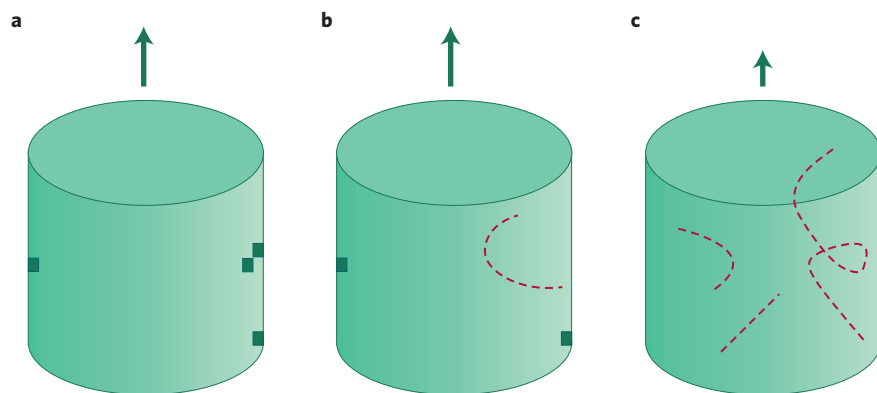


Figure 1 | Schematic representation of dislocation development. **a, b**, Application of a deviatoric stress promotes surface diffusion at specific sites (marked by green boxes; **a**), possibly leading to surface-associated nucleation of an initial mobile dislocation in **b** (red dashed line). **c**, Rapid dislocation breeding/multiplication is then likely to occur, after which elastic strain engineered functional properties will degrade and disappear, caused by stress relaxation. Size of arrow indicates stress level across the width of the specimen.

sub-10-nm surface morphologies (terraces, steps, and so on) to evolve at timescales ranging from microseconds to months at room temperature⁸. This could be due to the altered characteristics (nonlinear and anisotropic⁶) of diffusion from those described by standard diffusional creep theory. Second, even when diffusional flow does not make a large contribution to stress relaxation directly at room temperature, it may alter the surface atomic configurations that can, in turn, significantly lower the athermal stress threshold for subsequent dislocation nucleation. This was indicated by a recent diffusive molecular dynamics study⁹. Third, the dislocation nucleation process is a thermally activated, purely displacive event, with an activation volume ($\sim 5-15b^3$, where b is the Burgers vector) characterizing the ‘displacive uncertainty’ in strength that arises solely from atomic momenta (phonon) fluctuations at a fixed atomic configuration¹⁰. However, uncertainty in the athermal stress threshold, which depends sensitively on the precise surface configuration, and is affected by prior surface diffusion (heretofore named ‘diffusive uncertainty’), is likely to overwhelm the displacive uncertainty. The statistical signatures of the first dislocation nucleation measured by Chen *et al.* (activation volume $\sim 0.13b^3$, with a nucleation rate prefactor

nineteen orders of magnitude lower than the estimate from Debye vibrational frequency³) could therefore be indicators of cascading uncertainties in the diffusive preconditioning, rather than just the displacive nucleation process itself.

Furthermore, even though Chen *et al.* tried to prepare identical pristine Pd nanowires, the actual atomic configurations cannot be identical between different experimental samples, unlike in atomistic simulations, where one can prepare a configurational ensemble with truly identical starting atomic positions, and only different initial atomic velocities¹⁰. The starting surface condition therefore adds another source of uncertainty, which depends on the processing history, on top of the more ‘intrinsic’ diffusive and displacive uncertainties that arise during the load-ramp mechanical test. The three factors discussed above control the probability distribution of the first-nucleation stress. In practical elastic strain engineering⁷, one has to keep track of all three sources of uncertainties.

Dislocations are critical for plastic deformation. In elastic strain engineering however, one would like to suppress them completely. Using state-of-the-art, lab-on-a-chip tests, Chen *et al.* reveal that the first measurable inelastic event might be of a hybrid diffusive–displacive nature. In

the very low temperature limit, diffusion may be completely frozen out, giving rise to purely displacive dislocation nucleation. However, both the results of Chen *et al.*³ and Schuh and colleagues^{4,5} suggest that attention should be directed towards diffusive–displacive transitions in room-temperature load-ramp tests that occur at multiple timescales with cascading uncertainties. New simulation techniques^{9,11} and theories may help to pinpoint the exact origin of the first mobile dislocation. \square

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X-RAY MICROSCOPY

Beyond ensemble averages

Imaging the dynamics of local phenomena in materials with resolution down to the individual grain level is poised to transform our understanding of material behaviour.

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Materials that perform advanced functions are often complex due to inhomogeneities at length scales ranging from atomic to macroscopic and due to structural dynamics over timescales from nanoseconds to years. Controlling the physical properties of polycrystalline materials, which are made up of tiny (typically 10 nm to 100 μm) misoriented crystals called grains is particularly challenging due to the impact of local crystal orientation, grain boundary type and the diversity of boundary conditions around each grain. Thus, chemical processes, phase transitions or deformation under load, all nucleate at distinct locations in a material and subsequently evolve

in ways that depend critically on the local microstructure.

Until recently, structural changes in polycrystalline materials were studied primarily by X-ray diffraction measurements of the average properties of ensembles of millions of grains, with virtually no knowledge of their local environment or individual grain behaviour. Now, writing in *Nature Materials*, Jianwei Miao and co-workers report the dynamics of individual silver bromide (AgBr) crystal grains as they evolve during a rapid photoinduced phase transition¹. This work exemplifies emerging tools to characterize local materials structure and dynamics, made possible by powerful X-ray

synchrotron² and transmission electron microscopy methods^{3,4}. Moreover, it points the way towards even more powerful four-dimensional (spatial- and time-resolved) tools in the future, which might characterize both ensemble average and local dynamics for unprecedented tests of materials theory.

Miao and colleagues used time-resolved X-ray nanodiffraction to identify changes in the orientation and lattice spacing of particular atomic planes inside single nanoscale AgBr grains during photoinduced chemical reactions. To understand their experiment, some simple X-ray diagrams are helpful. Strong X-ray or electron scattering from crystals