Molecular dynamics simulations of crystallite interactions in shock-compressed columnar polycrystals

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Introduction

The need for a fundamental understanding of the response of crystals that are deforming extremely rapidly under high stress has driven intense research efforts on both theoretical and experimental fronts. Recent advances in "ultrafast" x-ray imaging techniques have made it possible to track how a material evolves during the course of extreme deformation processes that might take place over the course of only a few nanoseconds. The form of the x-ray image depends to some extent on the manner in which the crystallites of which it is composed interact with each other during the deformation process. We have performed a study of the physics of crystallite interaction in a shock-compressed metal using multi-million atom simulations. Our study reveals that neighbouring crystallites in the wake of the shock can deform in a "cooperative" manner, in which one crystallite expands while the other contracts. We quantify the change in atomic arrangement effected by this cooperative deformation by calculating inter-planar spacings. We further find that cooperative deformation can actually replace ordinary deformation mechanisms at lower pressures, and activate new deformation mechanisms at higher pressures.

Simulation setup

When shock-compressed to sufficiently high pressure, a single crystal will flow somewhat like a liquid to relieve the high stresses imposed upon it. Typical metals are an aggregate of very many crystals, as depicted in **Figure 1**. A grain in a polycrystal must therefore accommodate the deformation imposed by shock-loading in such a way that it remains in contact with its neighbours. In other words, each grain influences the manner in which its neighbours deform. It is this physics that we seek to capture in our simulations.

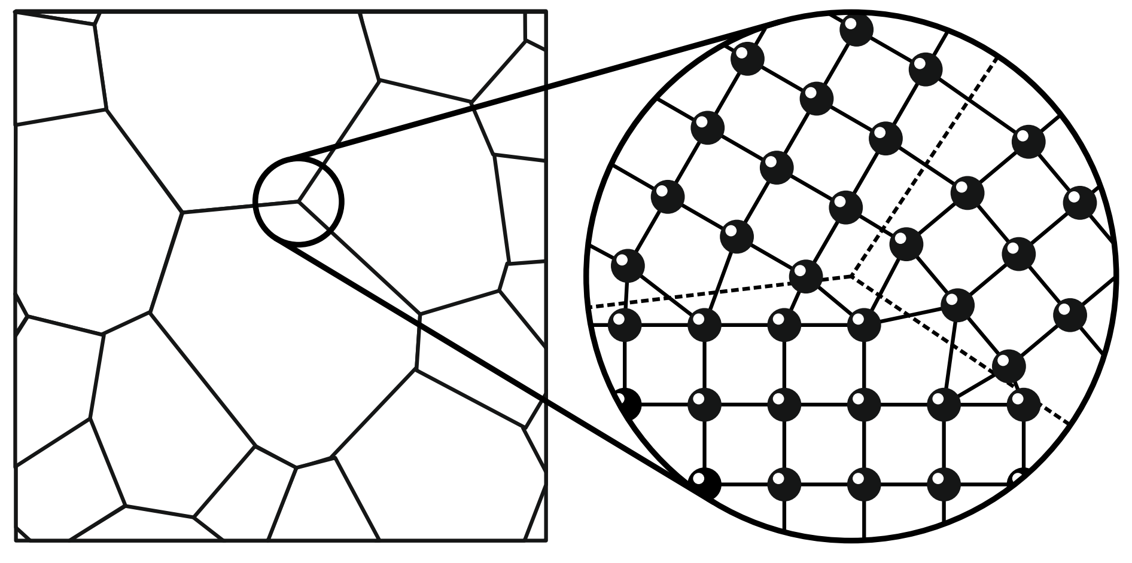

Fig. 1: Schematic depiction of a polycrystal. A polycrystal comprises a great number of single crystallites (or grains) within which all atoms are arranged in a regular lattice.

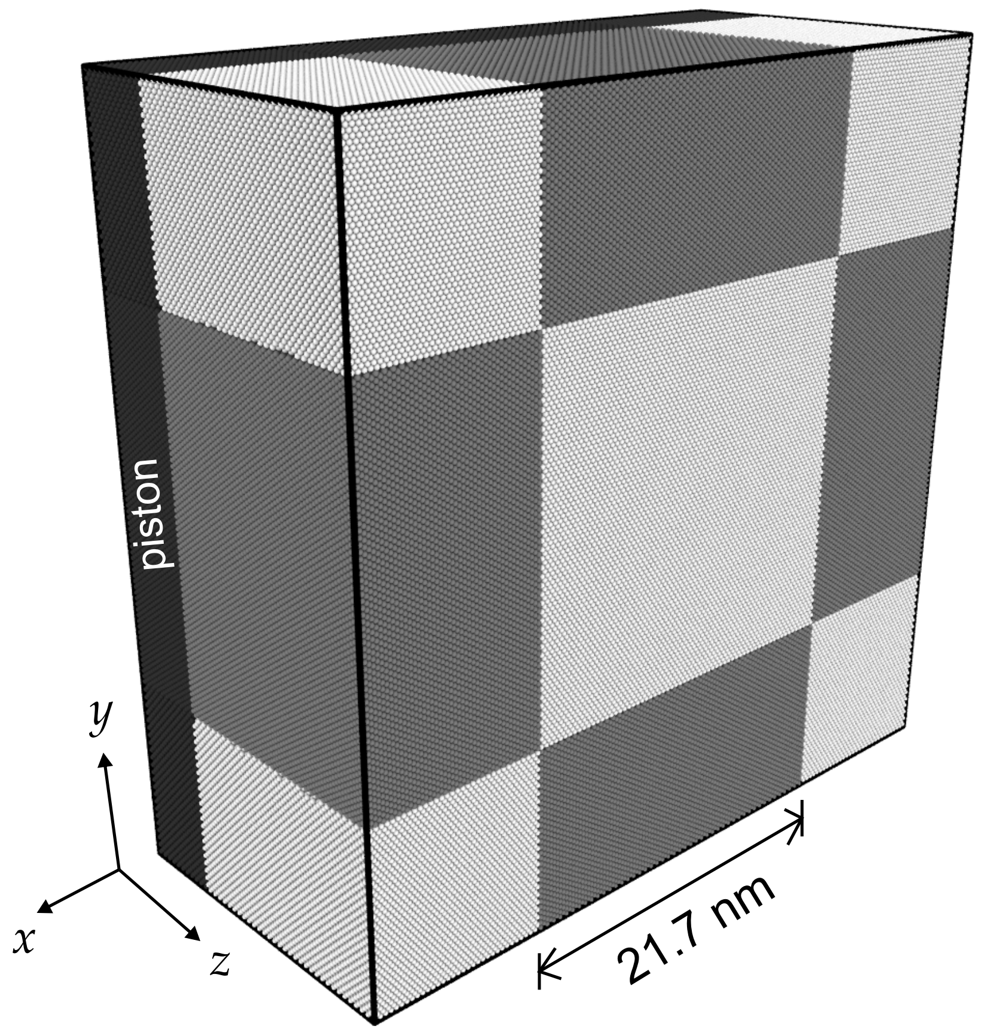

Fig. 2: Front end of the computational cell used in molecular dynamics simulations of a shock-compressed columnar polycrystal. The system was visualised with Ovito [1].

We simulate the response of crystals to shock-compression with **molecular dynamics (MD)**, a computational method in which a material is modelled numerically at the level of its constituent atoms.

The polycrystals comprise four identically-shaped, column-shaped grains with square cross-sections (see **Figure 2**). The orientations of adjacent grains are related by 90 degree rotations around z, the shock direction. Single crystals were constructed with the same orientation as the central grain in the polycrystals, so their response could be directly compared and the effect of one grain on another identified.

Compression of the crystals was realised with a 'piston', a group of atoms that travels at constant speed along the shock direction.

All MD simulations were performed with the LAMMPS code [2], using potentials for tantalum created by Ravelo et. al. [3].

Single-crystal response

When a liquid is compressed **uniaxially** (i.e. along a single direction), its constituent atoms move past one another freely in order to reach the state of least potential energy. This is the **hydrostatic state** in which, on average, the atoms comprising the liquid are equally spaced in all directions, as we show in **Figure 3a**.

The atoms in a solid crystal cannot move freely when compressed, but they can still reach a hydrostatic state via **plastic flow** (see **Figure 3b**). Here, atoms on neighbouring planes slide past one another in a regimented fashion. In tantalum, plastic flow is realised either by **slip** (which leaves behind a perfect lattice) or by **twinning** (which forms a new grain).

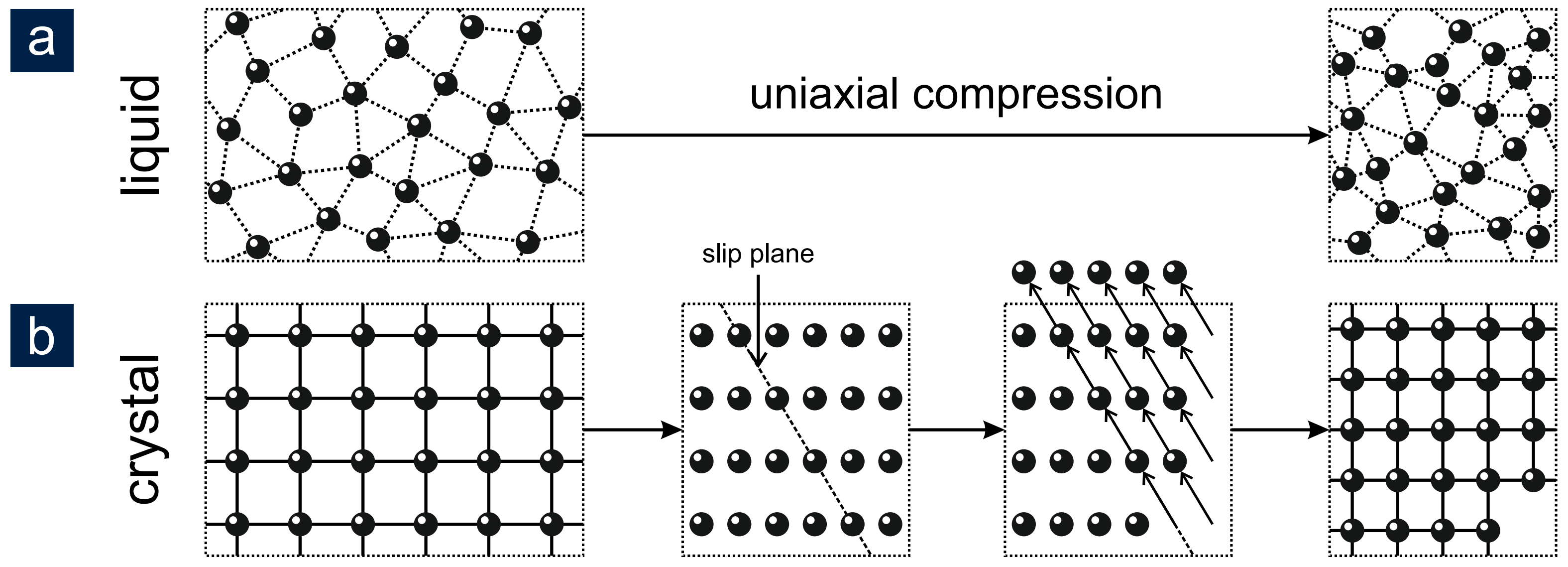

Fig. 3: Schematic depiction of (a) a liquid and (b) a crystal responding to uniaxial compression.

Plastic flow in the single crystal is realised in two stages (see **Figure 4**). The first stage is rapid flow in the xz-plane that allows atoms to move apart in the z-direction and together in the x-direction. The second stage, which takes place relatively slowly, involves motion in the xy-plane, and allows atoms to move together in the y-direction.

The spacing of the atomic planes **not quite** equal in each of the three directions: the elastic strains differ by around 1%. This is a manifestation of the crystal's **strength**.

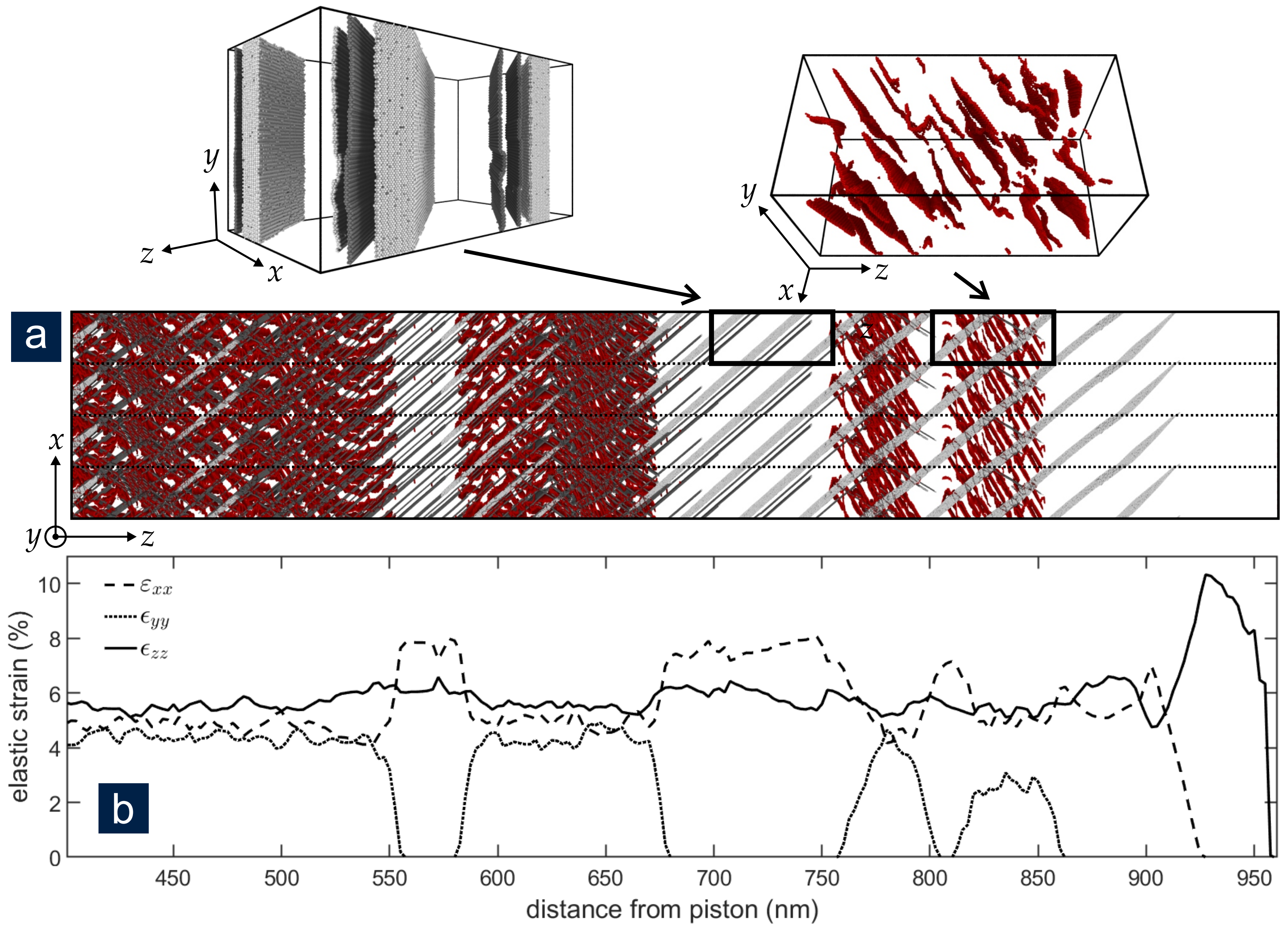

Fig. 4: Response of single crystal shock-loaded along the z-direction to 40 GPa. (a) Atoms located in proximity to slip or twin planes. White and grey atoms experience relative motion in the xz-plane, red in the xy-plane. (b) Elastic strains along the x-, y-, and z-directions as a function of distance along the crystal. The strain quantifies how closely spaced atomic planes are in each direction.

Polycrystal response

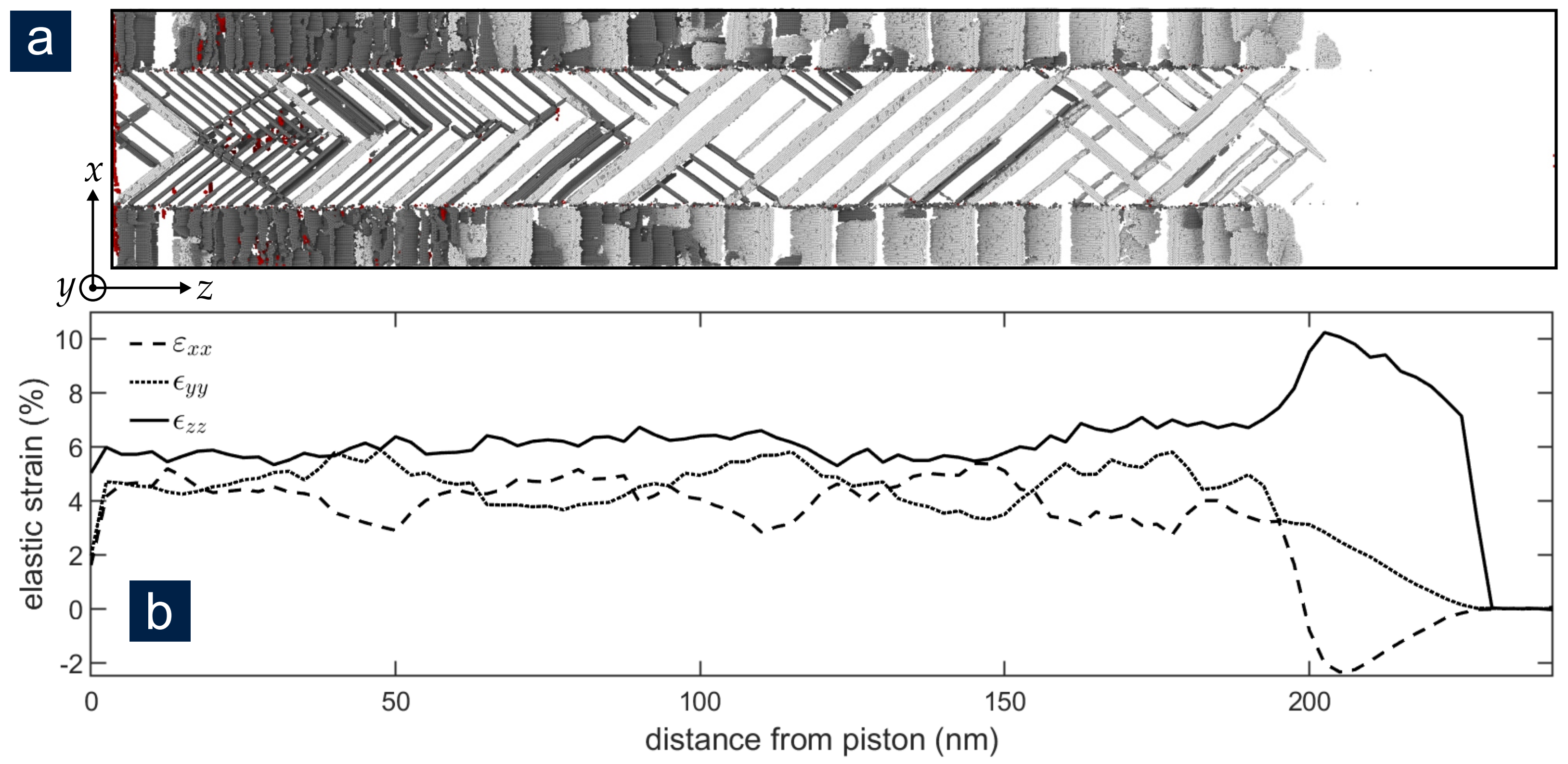

Fig. 5: Response of polycrystal shock-loaded along the z-direction to 40 GPa. (a) Atoms located in proximity to slip or twin planes. White and grey atoms experience relative motion in the xz-plane, red in the xy-plane. (b) Elastic strains along the x-, y-, and z-directions as a function of distance along the crystal. The strain quantifies how closely spaced atomic planes are in each direction.

When the polycrystal is shocked at low pressures (< 60 GPa) the second stage of plastic flow is almost entirely absent. This is because neighbouring grains can cooperatively compress one another along their (local) y-axis, which fulfills the same function as transverse slip in the monocrystal. Thus, intergranular interactions **replace** a plasticity mechanism under low-pressure conditions.

At higher pressures, these interactions actually **activate** a new plasticity mechanism. Each grain compresses its neighbour to such an extent that they 'buckle' and undergo twinning, not in the xz-plane, but in the xy-plane.

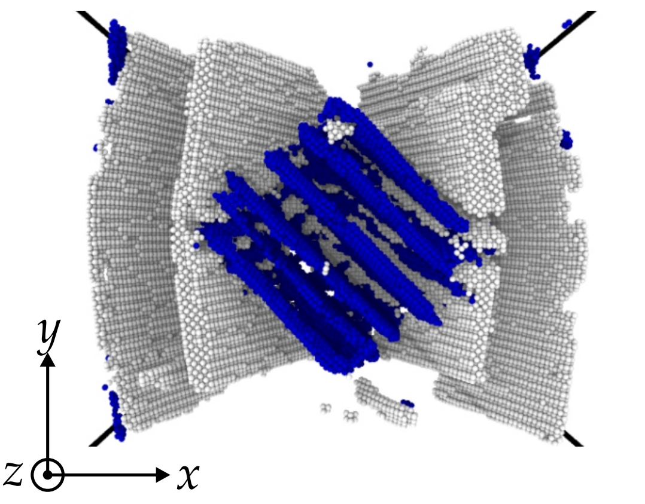

Fig. 6: transverse twinning in a grain in a polycrystal shocked to 60 GPa.

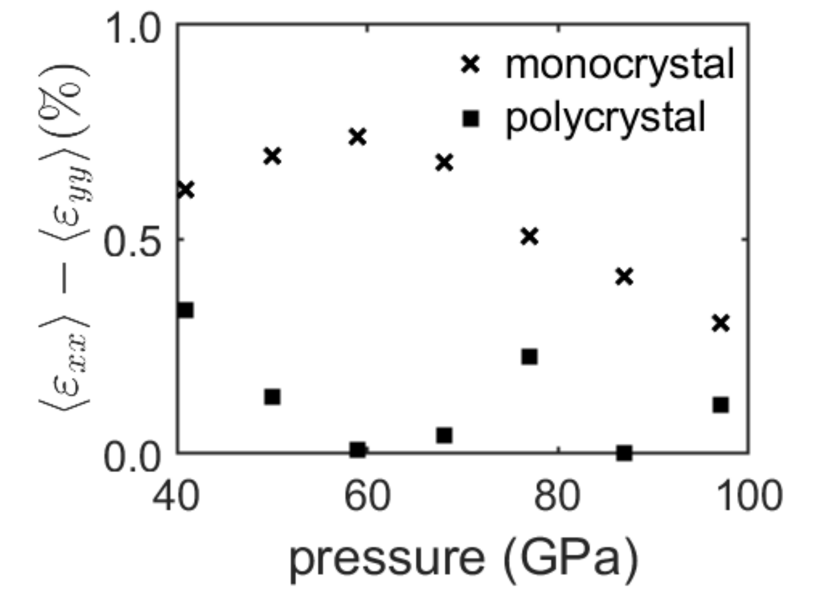

Fig. 7: Difference between the two transverse components of elastic strain as a function of pressure for the monocrystal and the polycrystal.

Since the grains can alter their interatomic spacing in the transverse directions not only by plastic flow but also by cooperative grain interactions, the extent to which the crystal can reach the hydrostatic state is not so limited by strength. We show in **Figure 7** that the difference between the transverse strains in the polycrystal is always lower than that in the single crystal at a given pressure.

Conclusion

We have performed multi-million atom MD simulations of mono- and polycrystalline crystals shock-compressed to between 40 and 100 GPa. Grains in the polycrystal deform by a mixture of conventional plastic flow (slip and twinning) and cooperative deformation with neighbouring grains. At low pressures, this cooperative deformation replaces the transverse slip observed in the monocrystal, while at higher pressures (p > 60 GPa), it activates twinning in the transverse direction. Overall, the cooperative motion allows the polycrystal to reach a more hydrostatic, lower energy state than the single crystal.

References: [1] A. Stukowski, Modelling Simul. Mater. Sci. Eng. **18**, 015012 (2010); [2] S. Plimpton, J. Comput. Phys. **117**, 1 (1995); [3] R. Ravelo, T. C. Germann, O. Guerrero, Q. An, B. L. Holian, Phys. Rev. B **88**, 134101 (2013).