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Probing Mechanical Properties of Nanostructured Materials via Large Scale Molecular Dynamics Simulations

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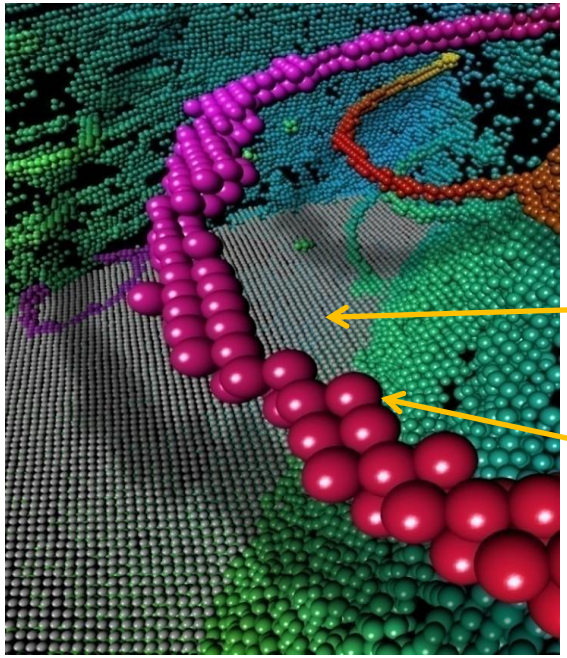
Origin of high strength and high ductility in nanotwinned copper

Dislocation is the microscopic carrier of plastic deformation (line defects shown below), and its activities predominantly control mechanical properties of materials, such as strength, toughness, and work hardening

The **motivation** of this research is to explore the origin of high strength and high ductility in **nanotwinned copper**, which is a new type of hierarchical nanostructured material with a high density of twin boundaries (grey planes below). In-depth investigations based on massive parallel computations will provide the fundamental understanding of deformation mechanisms (strengthening/softening), and guide for designing (structural optimization) and processing of nanoscale materials

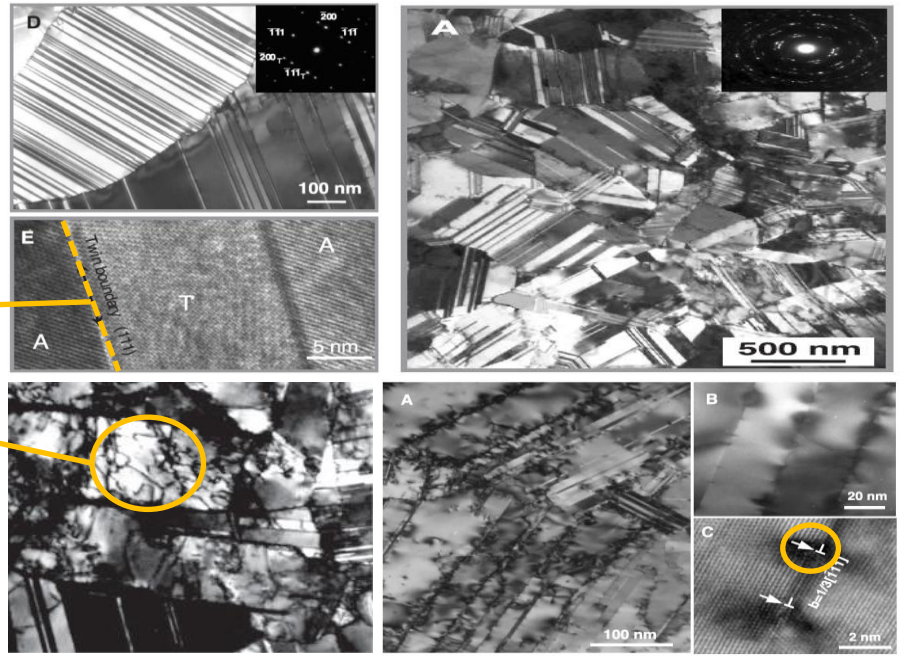
Computer Simulations

Gao et al., *Nature*, 2010

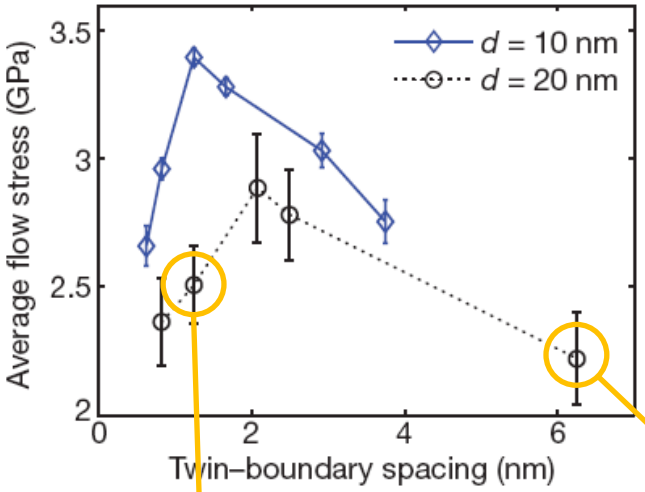


Experiments (TEM Images)

Lu et al., *Science*, 2004 & 2009



Transition of deformation mechanisms

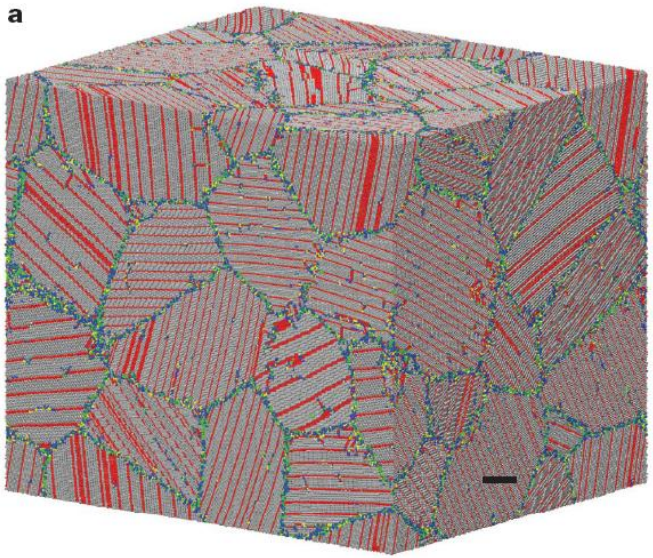


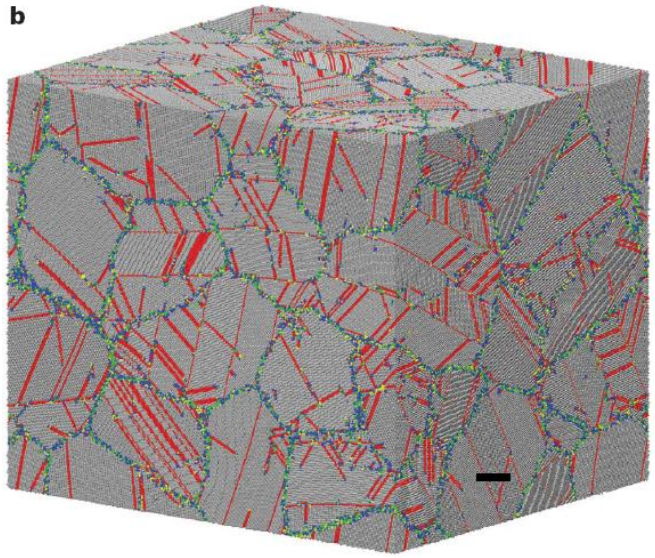
Technique details

Simulated systems contain a total of 140 million atoms, and the total simulation time is 0.75 nanoseconds. These simulations consume 22.8 CPU years on the Kraken Cray XT5. Local crystal order method is used to identify defects (grey: fcc atoms; red: hcp atoms; green: dislocation cores or gain boundaries; blue: vacancies; yellow: fully disordered atoms)

Observations

In **a**, plastic deformation is dominated by partial dislocations gliding parallel to twin planes, whereas in **b**, dislocations cutting across twin planes are the controlling deformation mechanism





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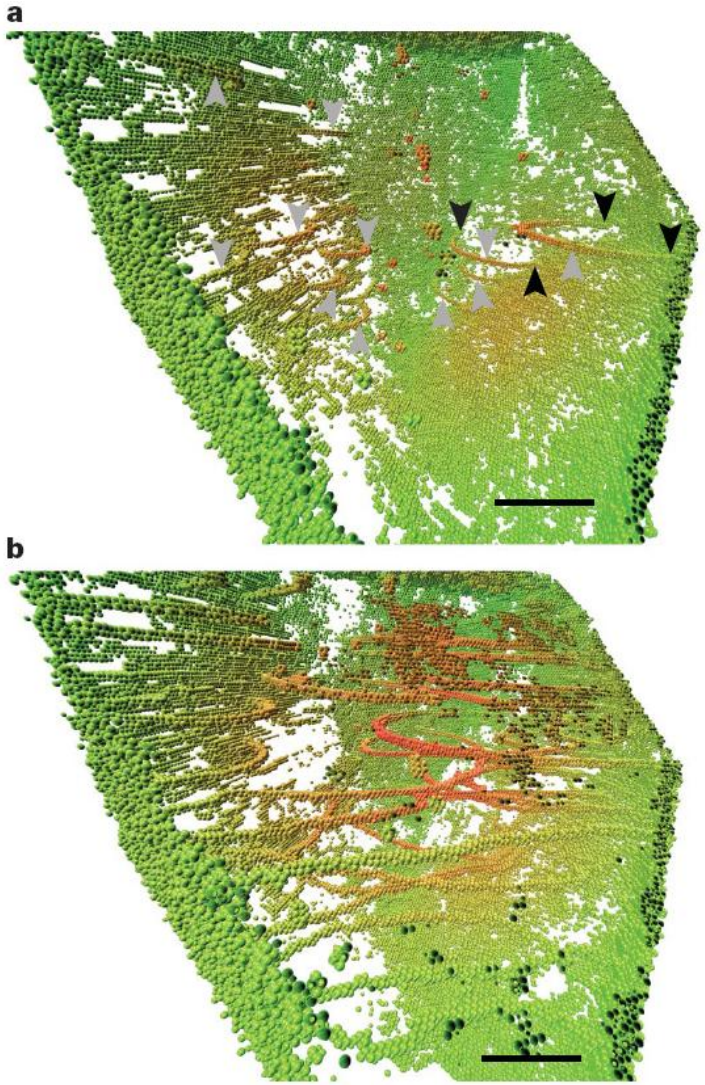
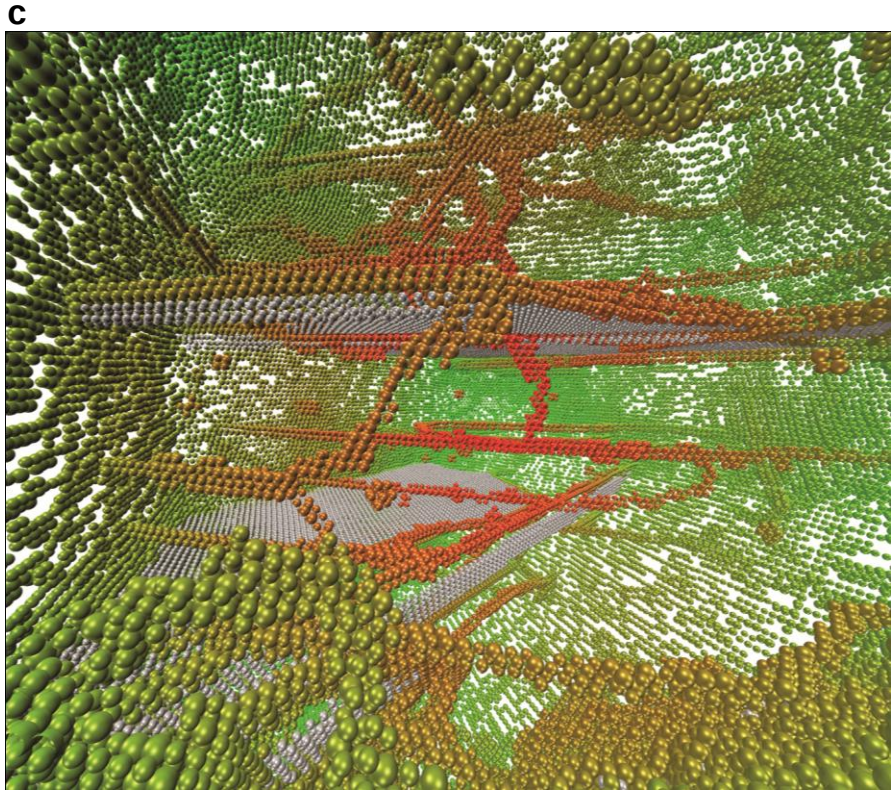
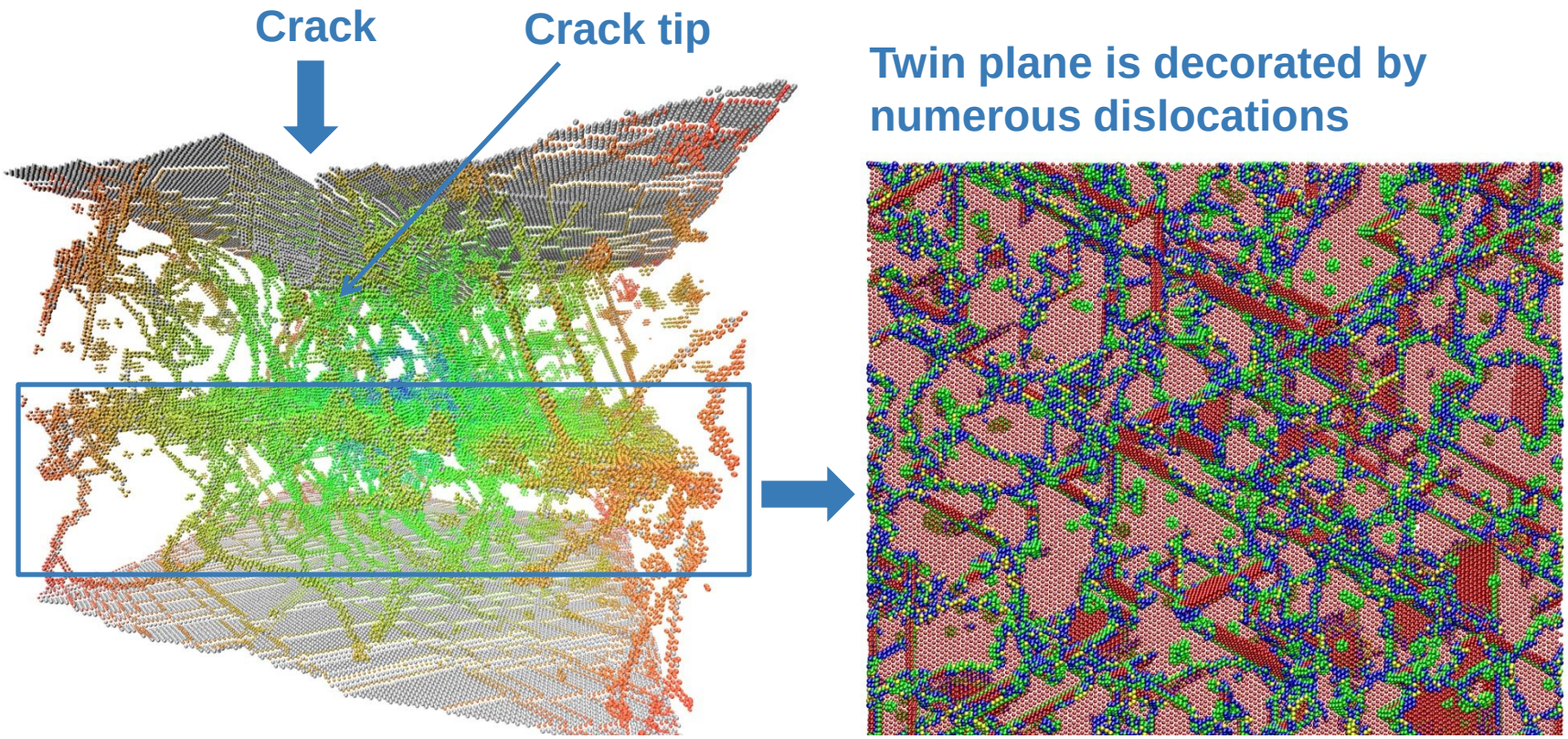
Dislocation structures for different mechanisms





In **a** (small twin thickness), dislocations (grey and black arrows) nucleate from grain boundaries and move parallel to twin boundaries. In **b**, dislocations glide on twin boundaries. In **c** (larger twin thickness), dislocations are entangled. It is noted that dislocation activities are highly organized by existing twin boundaries. These results show that the high strength of nanotwinned copper originates from the hierarchical structures of nanoscale twins being incorporated as subgrain structures

Further research on fracture of nanotwinned copper



An edge crack is placed in front of a twin plane. During deformation, a large number of dislocations emit from the crack tip and impinge on the twin plane. As a result, most dislocations remain in the twin plane, causing it to become a dislocation wall which blocks the further motion of dislocations. This property is critical for nanotwinned copper to retain high ductility without sacrificing strength. The simulations provide a useful guide to create hierarchical materials with both high strength and high ductility

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