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Nanoindentation

Simulation of defect nucleation in a crystal

Nanoindentation is the penetration of a surface to nanometre depths using an indenting device. It can be simulated using the Bragg bubble-raft model[1], in which a close-packed array of soap bubbles corresponds to the equilibrium positions of atoms in a crystalline solid. Here we show that homogeneous defect nucleation occurs within a crystal when its surface roughness is comparable to the radius of the indenter tip, and that the depth of the nucleation site below the surface is proportional to the half-width of the contact. Our results may explain the unusually high local stress required for defect nucleation in nano-indented face-centred cubic crystals.

Nanoindentation of face-centred cubic metals causes a load-versus-displacement response that is separated into regions of elastic deformation and discrete displacement bursts[2–4] (Fig. 1a). The first displacement burst generally occurs when maximum shear stress generated under the indenter is of the order of the theoretical shear strength[2,3]. This high local stress seems to cause homogeneous nucleation of dislocations beneath the surface, producing a displacement burst[3].

To confirm these observations, we used the bubble raft as a model for nanoscale atomic contact, in which the bubble positions represent the equilibrium positions of atoms[1] and allow visualization of deformation, dislocations, adhesion and fracture[5–7]. We prepared the bubble raft as described[1,6,7]. Indentation along the <121> direction of the raft proceeded orthogonally to the <110> closed-packed direction in the {111} plane. We flattened the raft's contact edge by removing extraneous bubbles with a soldering iron.

A completed raft, comprising more than 10^4 bubbles, measures about 250 mm $\times$ 250 mm, and simulates semi-infinite boundary conditions. Each bubble was 1 mm in diameter, representing an atom of diameter 0.3 nm. All other relevant dimensions in the model are converted to atomic dimensions by using this conversion scale.

We indented a single-crystal bubble raft, which was initially defect-free, in the plane of the raft along the <121> direction by using indenters of simulated tip radii 8 and 28 nm. The indenter, which was constructed of aluminium plate, was positioned in the plane of the raft and slightly below the surface of the solution. We applied the load by controlled increase in displacement using a screw-driven mechanism (Fig. 1b). The in-plane shear stress beneath the indenter was maximal at a ratio of depth, z, to contact half-width, a, of 0.78 (Fig. 1c), as predicted by two-dimensional hertzian indentation theory[8].

Figure 1c, d shows dislocation nucleation under atomically flat surfaces for two different indenter radii. In both cases, a dislocation nucleated beneath the indented surface along the loading axis at a depth of 0.78a; this location was determined by direct observation of z and a. The dislocation then split in two: one dislocation glided into the crystal and the other ran to the surface, creating a slip step. Burgers circuits confirmed the dislocations as edge-type, with Burgers vector, **b**, in the <110> direction. Dislocations nucleated at a constant depth of 0.78a; nucleation occurred farther below the surface as the indenter radius increased.

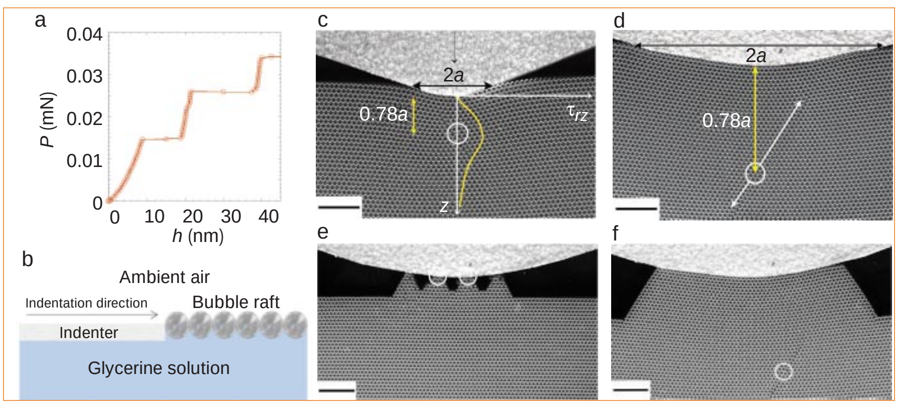

Figure 1 Dislocation nucleation during nanoindentation. **a,** Indentation load, P, plotted against depth, h, in (133) single-crystal aluminium, showing elastic deformation separated by displacement bursts attributed to dislocation nucleation[3]. **b,** Diagram of bubble-raft indentation. **c, d,** Initially defect-free rafts in which dislocation nucleation is induced by loading with indenters of different tip radii but at the same normalized depth, $z = 0.78a$ (white circle), where a is half the width of the contact. This is the position of maximum shear stress, τ_{rz}, shown in **c**. Nucleation (white circle) of a dislocation dipole is seen in **d**: one dislocation proceeds to the surface and the other into the crystal (white arrows). **e,** Indentation of atomic-scale asperities, showing plasticity (white circles) at the surface. **f,** Indentation of surface ledges of width comparable to the indenter radius causes dislocation nucleation within the crystal (white circle). Scale bar, 10 mm (representing 3 nm in our analogy).

Our observations provide a valid assessment of stress distribution down to simulated atomic dimensions. This suggests that our approach could correctly describe elastic stress in actual nanoindentation, which is consistent with the elastic response seen before the first displacement burst during nanoindentation of face-centred cubic metals (Fig. 1a)[2,3].

Indentation of an atomically 'rough' surface initiates plasticity at the contact surface (Fig. 1e). Figure 1f shows nucleation inside the crystal, caused by indentation of a surface ledge of width comparable to the indenter radius. This trend supports the idea that roughness induces plasticity during nanoindentation of metals — that is, surface roughness (in the form of asperities and ledges) is expected to cause dislocation nucleation near the surface of the crystal if the width of the ledge is substantially smaller than the tip radius. If the width of the ledge is greater than the tip radius, available sites for heterogeneous nucleation are sufficiently distant from the point of maximum stress beneath the indenter to sustain dislocation nucleation within the crystal.

For typical nanoindentation with an indenter tip of radius 50 nm, surface asperities larger than 50 nm should show a similar indentation response to that for an atomically flat surface. As crystalline specimens are routinely polished to a roughness of 50 nm or more, this explains why the first displacement burst shown in Fig. 1 corresponds to stresses that approach the theoretical shear strength.

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