

moment can provide information on magnetic structures, and neutron wavelengths are comparable to atomic length scales. Neutron microscopy will find applications—for example, in morphology and crystallization studies—in probing materials from a variety of scientific and industrial fields.

RICHARD LOUIE

### Simulations Indicate Aluminum Has a Higher Ideal Shear Strength than Copper

The theoretical shear stress or ideal shear stress is the stress necessary to deform a perfect crystal without defects. Usually this value is obtained through theoretical first principles-calculations, although in some instances nanoindentation techniques can serve as an experimental measurement of the ideal shear stress. In the case of aluminum and copper, a recent report of calculations based on density functional theory (DFT) showed that copper has a higher ideal shear strength than aluminum. However, Shigenobu Ogata, Ju Li, and Sidney Yip from the Massachusetts Institute of Technology have found the opposite result also from DFT calculations, as they report in the October 25 issue of *Science*.

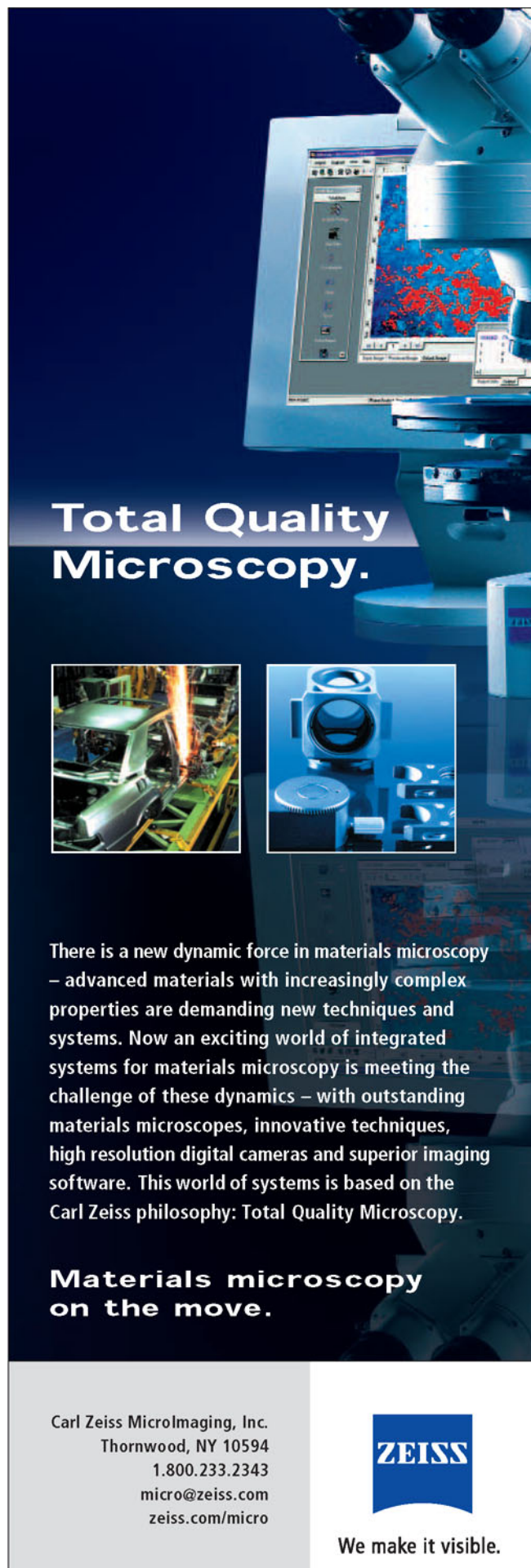
After performing calculations using various DFT methods, results showed that aluminum has the higher ideal shear strength. The scientists followed the same procedure used to obtain the results previously reported, and also used additional methods that further corroborated their results. The researchers based their simulations on a six-atom supercell of three {111} layers to calculate the equilibrium lattice constant and the relaxed and unrelaxed {111}<112> shear moduli. A 24-atom supercell of 12 layers for aluminum (10 for copper) served to calculate the intrinsic and unstable stacking-fault energies. The state of stresses considered for the calculations was pure shear or simple shear, with calculated stress values having an uncertainty of <0.1 GPa.

The investigators attribute this result to the fact that the elastic strain of aluminum at the maximum shear stress is more than 50% larger than that of copper. The ideal pure shear strength of aluminum is 32% larger than that of copper, despite the fact that the latter has a 25% larger pure shear modulus along the {111}<112> system. The investigators also attribute this effect to the differences in ion relaxations in both materials: aluminum has almost no relaxation in the *x* direction, and copper in the *z* direction. Therefore, stress applied in the <110> direction hardens copper and softens aluminum, and stress applied in the <111> direction has the opposite effect. As a consequence, interpretation of results from nanoindentation has to account for analysis of the state of stress, said the researchers. Aluminum atoms also have directional bonding which causes a longer shear deformation, higher intrinsic stacking-fault energy, and higher ideal shear strength, they said.

SIARI S. SOSA

### Neutrons Used for Holographic Imaging of a Pb Crystal

Electron and x-ray holography are well-known techniques for imaging the atomic structure of condensed materials. However, these methods are still limited because electrons interact strongly with matter, allowing only surface imaging as a practical matter, and x-rays experience great variations of sensitivity for different atomic elements. Recently, L. Cser and Gy. Török from the Central Research Institute for Physics, Hungary, and C. Krexner from the University of Vienna, Austria, proposed experimental setups that enable holography imaging using thermal neutrons with wavelengths close to inter-atomic distances. The first approach, called an “inside-source concept,” is based on large incoherent neutron scattering cross sections of nuclei such as hydrogen that could serve as pointlike sources of neutron spherical waves inside the sample. The second, called an “inside-detector concept,” is based on the use of strongly neutron-absorbing isotopes acting as pointlike detectors in the sample.




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