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THE ATOMISTIC ORIGIN OF MATERIALS PROPERTIES BY Z-CONTRAST MICROSCOPY, ELECTRON ENERGY LOSS SPECTROSCOPY AND FIRST-PRINCIPLES THEORY.

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The combination of atomic-resolution Z-contrast scanning transmission electron microscopy, electron energy loss spectroscopy, and first-principles theory represents a powerful set of tools to link the atomic and electronic structure of materials and nanostructures to macroscopic properties. Two examples will be presented, the first concerning the origin of electronic properties, the second mechanical properties. The electronic properties of grain boundaries in perovskite ceramics such as $SrTiO_3$ have long been utilized in varistors and capacitors. However, the microscopic understanding of the effect has remained elusive. We show that grain boundaries are intrinsically non-stoichiometric, which sets up band bending and the electrical barriers. Bi has been known to embrittle Cu for over 100 years, but again the microscopic mechanism has remained elusive. We show that it is not the atomic size that is important, but it is the additional electrons supplied by the Bi which fill antibonding states and reduce the cohesive energy. It changes the properties of Cu, the classic ductile material towards those of its neighbor Zn, the classic brittle metal.