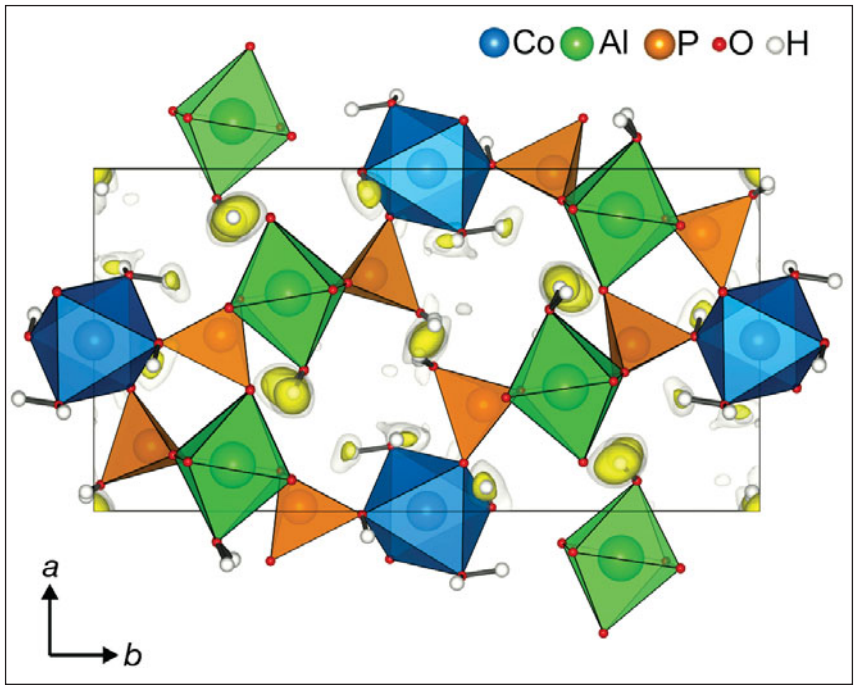
Nano Focus

Electron diffraction enables localization of hydrogen atoms in nanocrystals

It has not been possible thus far to use diffraction methods, such as x-ray diffraction, to localize the precise locations of hydrogen atoms in nano-sized crystals due to their strong atomic vibrations and small scattering cross sections.

An international team of researchers from the Institute of Physics of The Czech Academy of Sciences, Laboratoire de Cristallographie et Sciences des Matériaux (CRISMAT), and Laboratoire Catalyse et Spectrochimie has now developed a method to locate hydrogen atoms within submicrometer crystals. As reported in a recent issue of *Science* (doi:10.1126/science.aak9652), this was achieved using the recently developed method of dynamical refinement of precession electron diffraction tomography data.

"We followed standard crystallographic routine to collect a complete diffraction data set, then localized the heavy atoms (i.e., all non-hydrogen atoms) by *ab initio* methods and further refined using our dynamical refinement method," says Lukáš Palatinus from The Czech Academy of Sciences and lead author. "The key ingredient in this procedure is the dynamical refinement method, which enables us to calculate the diffracted intensities and the difference potential map. This allows the localization of hydrogen atoms, which are found at the maxima in the difference potential map," adds co-author Philippe Boullay of CRISMAT.



Projection of cobalt aluminophosphate crystal structure with superimposed difference potential map. Hydrogen positions are located by finding the local maxima of this potential map. Credit: *Science*.

"The dynamical refinement method developed by Palatinus et al. features an impressive enhancement in accurate determination of crystal structure by electron diffraction technique, with reduced discrepancies in atomic positions and more meaningful reliability factor," says Doug Perovic, an expert in scanning transmission electron microscopy and spectroscopy of nanomaterials structure and chemistry at the University of Toronto, who was not involved in this study. "The ability to localize the lightest atom-hydrogen is a clear demonstration of the capability of this method," he adds.

"We hope our work can attract newcomers in the field to develop, extend, and democratize the use of electron crystallography," Boullay says. In the future, the researchers plan to take their refinement method to the next stage by analyzing and improving remaining imperfections, and extending the scope of analysis to twinned crystals, for example.

Xiwen Gong

Size matters in mechanical behavior of bulk metallic glasses

Metallic glasses are amorphous materials produced by rapidly quenching metallic alloys, "locking" them into a glassy state rather than the crystalline structures into which metals typically form.

The unusual atomic structure of bulk metallic glasses (BMGs) affords ultrahigh yield and tensile strengths, low stiffness, and often a remarkable fracture resistance putting BMGs among the most damage-tolerant materials known. These desirable qualities make metallic glasses an interesting engineering materials system. Indeed, more than 50 years after their discovery, BMGs are now among the most promising candidates for use in consumer electronics frames and casings, cardiovascular stents, and precision surgical instruments.

However, BMGS are yet to gain widespread use due to the large variability in their mechanical performance: the unpredictable fracture and toughness behavior of this class of materials have compromised their potential use for many structural applications. As William L. Johnson, a prominent figure in these efforts, said in 2015 based on his experience in commercializing bulk metallic glasses for golf clubs, "it takes at least 15–20

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