Crystal structure library gets a 'data lift'

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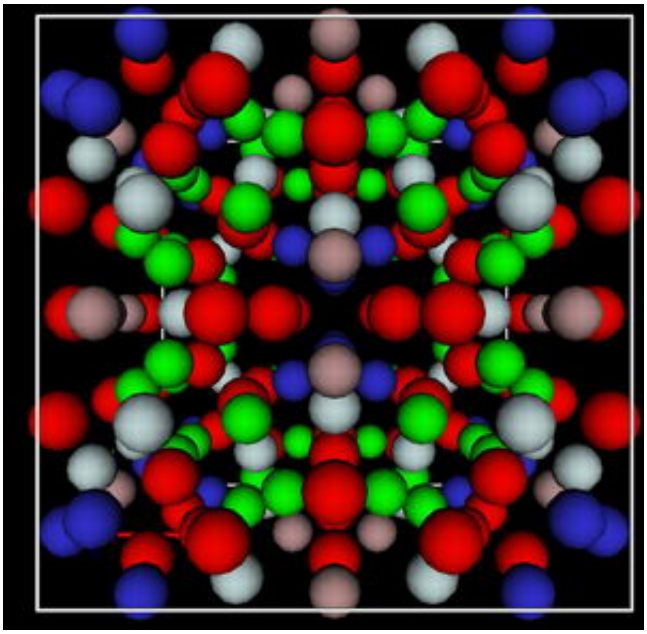

Image credit: NIST

Much of science these days depends on "black (or beige) boxes," scientific instruments that invisibly analyze data and then, voilá, identify the chemistry and/or structure of a sample. While scientists and engineers may be glad that the data crunching is invisible, the quality of the data used is critically important to something that they do care deeply about--getting an accurate answer.

Through two years of meticulous evaluation studies, the National Institute of Standards and Technology (NIST) has helped ensure that

"black boxes" that identify crystal structures will have the best possible data. The NIST Structural Database is a compilation of chemical data and three-dimensional crystal structures for approximately 20,000 materials, primarily metals, alloys and intermetallics. (Intermetallic materials are compounds of two or more metals with mechanical properties often resembling a cross between metals and ceramics.)

While the database has been available previously, this latest upgrade features a re-evaluation of all 20,000 crystal structures to ensure that the highest quality data are included. The upgrade efforts include improved standardization of the data provided for each structure and additional data fields for each entry. The structure data provided can be imported into Virtual Reality Modeling Language (VRML) players that allow researchers to view the structures in three dimensions and to rotate them in space.

The database is typically licensed by software companies and instrument manufacturers. For example, the database may be incorporated into software used to identify chemical compositions and/or crystalline structures using electron diffraction. Diffraction instruments work by aiming a beam of radiation (such as X-rays, electrons, neutrons, etc.) at a sample and then analyzing the resulting scattering patterns produced.

Source: NIST

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