3D printed crystallographic models & open-access crystallography resources

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While 3D printing has already been available for some 20 years, cost and performance improvements have only recently made 3D printing practical for usage by researchers and educators to create handouts of crystallographic models [1-7]. The 3D printing process requires files of the models in the industry-wide accepted Standard Tessellation Language (STL) or WRL syntax. Virtual reality computer programs that include direct conversions from CIF to STL and WRL for molecules, crystal structures, grain boundaries, and crystal morphologies have been written by Werner Kaminsky and are freely available for non-commercial purposes [5,6]. A related program by him produces 3D print files of representation surfaces of anisotropic physical properties of crystals [7]. A French-Mexican collaborative team offers the conversion to 3D print files of such representation surfaces together with their on-line visualizations at the Material Properties Open Database [8].

A selection of 3D printed models representing crystallographic 3D point and space group symmetries as well as black-white layer group symmetries will be presented at the 2016 Symmetry Festival. The STL and WRL files of these models (and many more) can be visualized interactively and downloaded freely from the website of the Open Access Crystallography project at Portland State University.

Thanks to the tireless efforts of Saulius Gražulis (of the Institute of Biotechnology, Vilnius University, Lithuania) and numerous international volunteers over the last decade, the Crystallography Open Database has accumulated more than 360,000 entries and is now the world's premier open-access source for the CIFs of structures of small molecules and small to medium unit cell sized crystals [9]. Other open-access sources of CIFs are the Worldwide Protein Data Bank, the AtomWork Inorganic Materials Database (which is the on-line version of the Linus Pauling File), the American Mineralogist Crystal Structure Database, and the above mentioned Open Access Crystallography project. Crystallographic models of molecules, Bravais lattices, crystal structures, space and point group symmetries, crystal defects (local and extended, e.g. grain boundaries), and crystal morphologies are all examples of what can be encoded in the very well documented and versatile Crystallographic Information Framework (CIF) file format that is utilized by both the above mentioned open-access databases and file conversion programs [5,6].

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