Crystallographic models make geology clear

Paul Pillot
Lycée Simone Veil, Valbonne, France (paul.pillot@ac-nice.fr)

Experimental sciences require the ability to envision a phenomenon at different scales, from the atomic or sub-atomic level up to the astronomical level. Geosciences are no exception. If remote sensing data, outcrops, rock samples and microscopic slides studies are common in our teaching, the crystallographic level is on the contrary one of the least accessed by our students probably due to a lack in suitable pedagogical resources.

Chemical and biological atomic structures are freely available from several public databases (e.g. the Protein Data Bank), and software that display these structures have been in use in labs for many years (e.g. the open source software RasMol released in 1993). Providing students with the tools used by researchers allow them to lead investigations, process data, solve problems in much the same way as scientists do. Thus, embedding the use of molecular visualization software in class has proved to be a successful approach in the study of molecular biology for undergraduate classes by allowing students to peer into the unseen atomic world.

An effort through creating an open repository for crystallographic models has been pushed by the Crystallographic Open Database initiative. On the software side, most of the existing crystallographic packages in use are too specialised for students to focus on content rather than on container. The Jmol open source software has undergone a tremendous growth in its capabilities in the late years, now providing the scientific community with a suitable framework for studying crystal structures.

MinUSc is a free open source web application software, accessible online or available as a stand alone application, that brings together data picked for its educational relevance with the outstanding visualization capabilities from Jmol in a friendly setting to provide students with molecular structures of minerals, they can actually display, manipulate and analyse in a 3D environment.

MinUSc main functions for growing crystals from unit cells, navigating into crystal structures, displaying different representations, and calculating formulae as well as mineral’s density will be presented. Furthermore, beyond the general display of common minerals structures, two different case studies involving the MinUSc software will be presented:
- Gathering evidences for a meteoritic impact from quartz
- Revealing the source of water in calc-alkaline magmatism from minerals.

Finally, taking advantage of being a web application, new developments in the MolUSc software focus at offering the ability to store, retrieve and exchange data between users in the form of interactive slides that could lead to novel ways of opening and sharing class work beyond the class walls.