BOLD NEW GRAPHICS AND MINERALOGY

Paul Schroeder

This is a true story... I am sitting in my office, minding my own business, and a student walks in and says, "Dr. Schroeder, is geology getting better or is it just getting cooler?" I think the student astutely observed that the number of majors recently doubled in geology, and she was curious as to why. I have my own theories about the upswing in geology enrollments, but that's a topic for another day. Her question sparked one in my own mind about mineral science, which was, "What advancements are really taking place?" Those of you who have read my Clay Minerals Society President's Corner in *Elements* will know of my penchant for motorcycling. In the motorcycle industry, new models arrive at the dealer each year. When the manufacturers can't improve on their product, they employ the age-old tactic of "bold new graphics," better known as BNG. The motorbike is exactly the same product underneath, but the buyer sees the BNG, pays the extra cash for a newer one, and never thinks otherwise. I suspect the same ploy is played out for products used in your particular hobby or passion outside of science. Unbeknownst to my student, she helped foster the following thoughts about developments in mineral science over the past decade.

Let's start with computer programs that take crystallographic data and generate dynamic 3-D images of a unit cell. They are absolutely wonderful. Free access to databases such as the Mineralogical Society of America's Crystal Structure Database is the result of Herculean and Athenian efforts of people like Bob Downs and Michelle Hall-Wallace, their colleagues, countless mineralogists whose information populates the database, and peers reviewing the accuracy and quality of the work. Standing in front of my class, I can now search a mineral, download data, project its structure, and have it spinning in front of their eyes, all in under a minute. If they are wearing red/blue 3-D glasses, I can get an extra "Wow man. Is that what the 70s were really all about?" Now ask yourself, is such software just BNG? Let's face it, the crystal structure of α–quartz at 25 °C has not changed dramatically in the past half century, so ball and stick models can equally convey the point. In part, it is BNG if we are not teaching the fundamentals of crystal symmetry operations to our students. There is little substitute for putting an object in a student's hands and having him or her spatially reason the presence of an inversion center.

The heart and soul of graphical software resides in the crystal database. However, much like the GPS in your car, the software is only as good as the database that feeds it. My wife, Linda, and I often disagree about directions while driving. Now, with a GPS on board, we have a third person to argue with. I choose Sean Connery's voice to minimize the disputes with Linda, so when we arrive at our destination we're shaken, not stirred. I hope you see my point, which is that we need to advance Earth and planetary material databases to include more structures like inorganic-organic complexes. Note the term is hyphenated. Even James Bond knows two components can interact in different ways.

Our ability to advance understanding of material structures is directly tied to resolution. History tells us this. As major advances in microscopes and telescopes are made, so is knowledge of object ordering, ranging from subatomic to light-year scales. If an analytical technique, whether *in vivo*, *in vitro*, or *in silico*, can't resolve the ordering of a structure, then we can't advance the science. As we flirt with concepts of nanoscale ordering, the current debate about the structure of 2-line ferrihydrite provides a prime example of how to advance our science. This nanocrystalline material is widespread on Earth and possibly occurs on extraterrestrial bodies. It is used as a catalyst in metallurgical processing, it sorbs toxic elements like Pb, Cs, and As, and it is a putative core component of ferritin, which is an iron-storage protein noted as early as 1963 by mineralogist Ken Towe and others. Almost 50 years later, competing theories for the ferrihydrite structure promoted by two hard-working and knowledgeable groups appear in volume 96 of *American Mineralogist*[1,2]. Most of us are not experts in the nuances of ferrihydrite, but Glenn Waychunas recently pointed out to me that in the realm of nano-ordering it is quite possible to have multiple structural states. At the nanoscale it is not only the structure itself, such as with ferrihydrite, but also what it interacts with. The bulk properties of ferrihydrite-like materials are more markedly influenced by their surface structures than the highly crystalline material we have long been studying. Our traditional "XRD-, EXAFS-, DSC-, TEM-, PDF-, TG-DSC-, IR-, NMR- or whatever-microscopes" haven't resolved the difference yet.

The next challenge is building structure databases to include things like (1) nanocrystalline materials of what has traditionally been called 2-line ferrihydrite, (2) organo-mineral complexes such as methane in the interlayer sites of mixed-layer clay minerals like illite–smectite and their variants of *cis-/trans*-vacant ordering, (3) carbon dioxide on the surface of iron sulfates, such as jarosite (not only under Earth-surface conditions, but on Mars-surface conditions), and, perhaps the most elusive of all, (4) the interface of mineral surfaces (nano- or macrocrystalline) and living membrane surfaces, where protons, electrons, and essential elements get passed along.

Is geology getting better? ...

It gets better in small increments over long periods of time.

So at this point, are you wondering what I said to the student that entered my office? I said to her, "Geology has always been cool." Occasionally bold new graphics come along and enhance what we already know. Is geology getting better? I said to her, "Yes, but not by doubling overnight, like your class enrollment. It gets better in small increments over long periods of time." It is in the excitement of debates, like that of the ferrihydrite nanostructure, where it really gets better. I dare to speak for the entire readership of *Elements* when I say thanks to all the dedicated people who advance this side of science. Let's encourage support for base-level research to increase our resolution to the nano- and picoscale (yes, I know basic research is risky...), because the alternative is potentially just repackaging more of the same, and we know what lies underneath BNG.

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1 Xu W, Hausner DB, Harrington R, Lee PL, Strongin DR, Parise JB (2011) Structural water in ferrihydrite and constraints this provides on possible structure models. American Mineralogist 96: 513-520

2 Manceau A (2011) Critical evaluation of the revised akdalaite model for ferrihydrite. American Mineralogist 96: 521-533

Triple Point raises issues of broad interest to the readers of *Elements* and explores different aspects of our science (teaching, publishing, historical aspects, etc.), our societies, funding, policy, and political issues. Contact Bruce Yardley (B.W.D. Yardley@leeds.ac.uk) if you have an idea for a future topic.