Review: Leung and de Polo, *The crystal structures behind the optical properties of minerals – a case study of using TotBlocks in an undergraduate mineralogy lab*

Comments

1. This is a new and innovative way to use 3D printed materials to support and enhance student learning. Having students build their own crystal models with these 3d printed components is really cool.
2. Application of learning theory to explicitly design and implement this teaching activity is laudable. This includes active learning, constructionalism, spiral learning trajectories, and cooperative learning. This is all really great.
3. Building the 3D structures of the biopyriboles is a great way for students to understand the relationship between crystal chemistry and crystal structure. Note that these approaches have been advocated since the mid 1990s, see two references below.
4. My main criticism is the extension of using these crystal structure models to demonstrate optical properties of minerals. Using the structures works moderately well for demonstrating the relation between crystal structure and physical properties like cleavage. However, the expression of optical properties such as pleochroism and extinction angle requires also that the orientation of principle vibration directions (X,Y,Z) are shown with respect to the crystallographic axes (a,b,c). This is not so difficult using biotite, or even ortho amphiboles and pyroxenes. But, this can be really confusing for the monoclinic varieties. I did not see that students were asked to locate the orientation of the vibration axes in or on the crystal structures. So I don't see how they can effectively determine what pleochroic colors should be attributed (usually denoted as e.g., X=green Y=brown Z= red), and similarly, I'm not sure how the extinction angle can be related to the crystal model without some representation of where the vibration axes are located.
5. For publication, I think the authors need to address the relationship between crystallographic orientation and orientation of vibration directions. These would be similar to the perspective crystal drawings showing crystal form, cleavage, crystal axes, and optical orientations in standard Mineralogy texts and atlases like Deer, Howie and Zussman. The models are really cool. Interpreting cleavage is a nice extension of the understanding of the crystal structures. But I think that extension to optical properties is a step too far without additional optical orientation information.

Review Criteria:

1. Addresses relevant scientific question. The challenge of developing spatial thinking by students is of interest and concern in most geoscience fields. This is particularly challenging when trying to teach Mineralogy and Crystallography.
2. A novel approach is used to create mineral models using 3D printing
3. The methods are clearly stated. Application of learning theory is a strength.
4. Results are clearly presented to show learning gains and limitations.
5. Prior work is cited appropriately. I provided two additional reference that might be included just for historical context.

6. The title accurately reflects the content of the article. Although I do question whether these models can be used to demonstrate optical properties of minerals without adding critical information about the orientation of principle vibration directions with respect to crystallographic axes.
7. The abstract is appropriate
8. The presentation is adequate, but some more description and context of what the students actually experienced in doing these activities would be interesting.
9. Language used is appropriat4e
10. References are appropriate.

Other Comments:

The use of manipulatives has been shown to strongly enhance learning about spatial objects—so this manuscript is well-grounded in established theory and practice. I think that this is a great exercise to demonstrate the fundamental architecture of the family of "biopyriboles" that have the same basic T-O-T layering but with single or double chains ot 2-D sheets. And it is a good way to demonstrate the physical property of cleavage, particularly for the perfect {100} cleavage of biotites. It's a bit of a jump for students to also see the {110} cleavage of pyroxenes and amphiboles, but in the correct orientation looking down [001] (i.e., the "end section view") students should be able to see the cleavage following the weaker bonds between the M sites at ~90 degrees for single chains and ~120-60 degrees for double chains. That's all great stuff. For the clinopyroxene and clinoamphibole examples, question a) what type of cleavage and angles, could use some more direction as only one cleavage direction will be seen looking perpendicular to any of the prismatic faces (parallel to c or [001]) and the two cleavages and their angle will only be observed if you know to look down the c-axis or [001]. It would be a better learning exercise if students were directed to look down different directions on the model and then compare features.

I have a little bit of an issue extending this application to optical properties as these have to be understood in terms of the relationship between the crystallographic axes (a,b,c) and the principal vibration directions (X,Y,Z). For pleochroism in biotite, this is easy to demonstrate as biotite is close to pseudo-hexagonal (monoclinic in detail), so pleochroism can easily be demonstrated parallel to the E-W or N-S cross hairs with e.g., X= brown and Y=Z dark brown. But for amphiboles and pyroxenes, this becomes more complex depending on a) is the crystal system orthorhombic or monoclinic, and b) the pleochroic color depends on which vibration direction you are looking down, and if you're not looking down one of the vibration axes you will get some intermediate color. Similarly, with extinction angle I can see why comprehension of the students did not improve as much. Again, with biotite it's simple to demonstrate parallel extinction with respect to {001} cleavage which is parallel with a vibration direction. This is also easy with the ortho amphiboles and pyroxenes where the vibration directions are parallel with crystallographic directions. But for the clino amphiboles and pyroxenes this is much more complicated for students. To be in the proper orientation to measure extinction angle, you have to be looking down the optic normal (Y) to be able to measure the correct Z to c angle. That requires understanding numerous rotational degrees of freedom to a get the crystallographic axis aligned with a cross hair, and then b) longitudinally rotate the crystal so that the optic normal is parallel with the line of sight. Any other orientation will result in an incorrect extinction angle that can range from 0 degrees (parallel) to the actual extinction angle of ~20 degrees for many clinoamphiboles or ~40 degrees for many clinopyroxenes. So, I guess the shortfall that I see here is not being able to simultaneously show the vibration directions compared to the crystallographic axes in these ToTblock models.

I'm delighted to see the application of learning theory with reference to Kolb and Fry (1975) and constructionism (Harel and Papert, 1991) (I would use constructivist theory as an alternate expression, but a rose is a rose). "Spiral" learning progressions and cooperative learning approaches are also applied in this activity, and this is also supported by learning theory.

I don't think you can answer the question for clinopyroxene part b, which orientation would show inclined extinction without having reference to the vibration directions. And for part ii) I don't think the model as shown can address the question of what orientation is needed to demonstrate clino (inclined) from ortho (parallel) pyroxenes based on extinction angle.

Lines 20-21, In the early Teaching Mineralogy workbook that derived from a NSF-sponsored workshop followed by publication of lab exercises by MSA, two early contributions used this approach using traditional ball and stick models and also building crystal structures with templates using plasticene balls. The use of 3D printing of crystal structure components is a really nice natural evolution of this tradition.

Mogk, D.W., Directed-Discovery of Crystal Structures Using Ball and Stick Models, in Brady, J., Mogk, D. W., and Perkins, D., (editors), 1997, Teaching Mineralogy, a workbook published by the Mineralogical Society of America, 406 pp. available on line at https://serc.carleton.edu/NAGTWorkshops/mineralogy/activities/ballstick.html

Hollacher, K., Building Crystal Structure Ball Models Using Pre-Drilled Templates: Sheet Structures, Tridymite, and Cristobalite, in Brady, J., Mogk, D. W., and Perkins, D., (editors), 1997, Teaching Mineralogy, a workbook published by the Mineralogical Society of America, 406 pp. available online at https://serc.carleton.edu/NAGTWorkshops/mineralogy/activities/buildball.html