**A 21st Century Approach to Crystallography: Modern Tools and Diverse Content**

*-Vincent Sokalski, DOWD Fellowship Proposal*

***The goal of this proposal is to implement advanced computational and lab tools for the course 27-201 – "Structure of Materials." Techniques will include use of advanced crystallography software to develop digital 3D stereo-rendering of structures and use the IDeATe network to print 3D crystal models. As part of this proposal, existing labs will be augmented to honor the work of diverse historical figures who contributed to the development of the field of crystallography.***

Our ability to characterize and describe periodic arrangements of atoms, known as crystals, is foundational to the engineering design of new functional materials. This topic is central to many disciplines including geology, metallurgy, physics, chemistry, materials science, and by extension, a number of other engineering fields. However, the standard teaching approach today does not leverage computational tools and laboratory techniques that would support established blackboard-style methods. Indeed, advanced concepts in crystallography can be especially difficult to visualize in two-dimensions.

The MSE department recently acquired a license to the latest version of CrystalMaker X (http://crystalmaker.com/index.html). This offers students a digital platform to build complex crystal structures and simulate their interaction with x-rays and electrons, which is the primary mechanism by which they are characterized experimentally and is already an integral part of the course. However, this software also comes ready with other features that have not previously been incorporated including ready to export 3D printing scripts that can be taken directly to the CMU IDeATe facilities (or any other lab on campus with 3D printing capability). This has been executed by one student in our department already to build models of quartz crystals. Moreover, the software allows for rendering of graphics to enable 3D depth visualization of crystal structures, which can be used with a standard pair of stereo glasses or by creating a stereo-pair (e.g. the DNA pair in figure 1a).

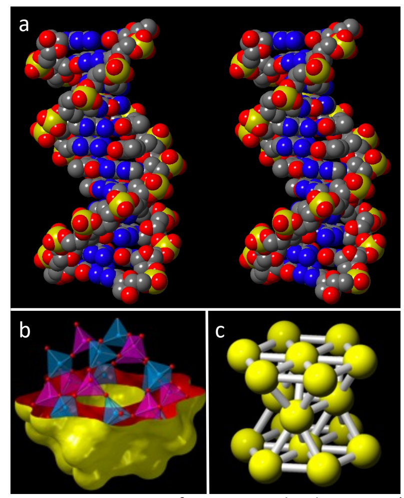

*Figure 1: Output from Crystalmaker X. a) Stereopair for 3D visualization of DNA. B) Example aluminosilicate (sodalite) highlighting free space for water absorption. C) An hexagonal close packed model appropriate for 3D printing.*

These features are valuable from an educational standpoint enhancing our students' ability to visualize structures in 3D, but also serve to spark some excitement about the topic. It will emphasize an important point to students that is often glossed over: *presentation matters*. As part of the required lab component, groups of students will use these new tools to present their own mini lecture on a structure of their choosing.

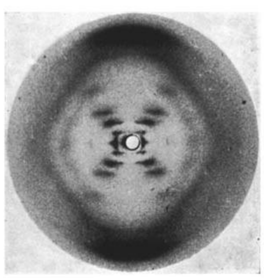
*Figure 2: Famous X-ray diffraction pattern photograph from DNA, which will be replicated optical in the laser pointer lab.*

The second component to this course redesign is the incorporation of curricular content that honors diverse figures – present or historical – that have led to the development of this field. As an example, the 1962 Nobel prize in physiology was awarded for the discovery of the structure of DNA. Throughout history, the critical contributions of English chemist Rosalind Franklin have not been properly acknowledged (although it is heartening to see that her name is becoming more commonly recognized by incoming students). The University of Wisconsin-Madison Institute for Chemical Education[1] provides a kit for re-creating Rosalind Franklin's famous photo 51 experiment[2] with a laser pointer and a transparent pattern instead of x-rays and real DNA. This kit will be used to supplement our existing laser point lab during the 1st week of the course and will help foster discussion about the often-minimized contributions of women in STEM fields.

Lastly, the MSE department continues to collaborate with the curators at the Hillman Hall of Gemstones at the Carnegie Museum of Natural History, where an expansive array of minerals are displayed. The curators are generous in offering a free tour to this class where details on both the minerals themselves and the history of their discovery are highlighted. As part of this proposal, I will work with Travis Olds (a new curator for the exhibit) to highlight examples from around the globe including recognition of the diverse mineralogists and geologists who discovered them.

Based on my prior efforts in strengthening this course combined with experience developing more diverse & inclusive lectures in other teaching, I am confident this proposal will be well-received by students and enhance their educational experience in the College of Engineering.

[1] University of Wisconsin-Madison. Institute for Chemical Education. https://icestore.chem.wisc.edu/product/dna-optical-transform-kit

[2] Franklin, R., Gosling, R. Molecular Configuration in Sodium Thymonucleate. *Nature* **171,** 740–741 (1953). https://doi.org/10.1038/171740a0