

Teaching the Reciprocal Lattice

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When the direct lattice and the reciprocal lattice are introduced together, many students seem eternally confused. In *Foundations of Crystallography with Computer Applications*,¹ the approach is to divide the book into Part I Symmetry (or if you will theory) and Part II Experimental. The symmetry section includes the direct lattice, unit cell, G matrix, point groups, and space groups. The experimental section opens with the reciprocal lattice, i.e., the lattice of the diffraction pattern. The reciprocal lattice is compared and contrasted with the direct lattice. Properties of the reciprocal lattice include \mathbf{G}^* , a^* , b^* , c^* , α^* , β^* , γ^* , V^* , \mathbf{H} , and $\cos\theta^*$. Three examples are given: hexamethylbenzene (triclinic), anhydrous alum (trigonal), and the superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ (orthorhombic). Three applications that use the reciprocal lattice are also given: calculate d -spacings, calculate the angle between crystal faces, and interpreting entries in the Powder Diffraction Files.² Finally, a Python programming exercise produces the reciprocal cell superimposed on the direct lattice with the volumes normalized to one.

Reference

- {1} Julian, M.M. (2014). *Foundations of Crystallography with Computer Applications (2nd ed.)*. CRC Press, doi.org/10.1201/b17342.
Julian, M.M., Slebodnick, C., Julian F.T. *Foundations of Crystallography with Computer Applications (3rd ed.)*. CRC Press, in preparation.
- {2} Gates-Rector, S., & Blanton, T. (2019). *The Powder Diffraction File: A quality materials characterization database*. *Powder Diffraction*, 34(4), 352-360, doi.org/10.1017/S0885715619000812