

A century of mineral structures: How well do we know them?

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ABSTRACT



This decade marks the centenary of the discovery of X-ray diffraction. The development of mineralogy as a scientific discipline in which the properties of minerals are understood in terms of their atomic-scale structures has paralleled the development of diffraction crystallography. As diffraction crystallography revealed more precise details of mineral structures, more subtle questions about mineral properties could be addressed and a deeper understanding of the relationship between the two

could be attained. We review the developments in X-ray single-crystal diffraction crystallography over the last century and show how its power to provide fundamental information about the structures of minerals has evolved with the improvements in data quality and the increased technological capacity to handle the data. We show that modern laboratory X-ray diffraction data are of the quality such that mineralogical results are no longer limited by the data quality, but by the physical validity of the refinement models used to interpret the data.

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