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Simulations of Debye-Scherrer and Gandolfi Patterns Using a Bruker SMART/APEX Diffractometer System.

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Debye-Scherrer (DS) pattern simulations were compared to five NIST reference powder data (674a: TiO₂, ZnO, Cr₂O₃; 640b: Si; 660: LaB₆). In addition, Gandolfi pattern simulations from a platy, low-symmetry mineral (chlorite, triclinic) were compared to a calculated powder pattern from single-crystal data of the same material. Both series of tests were based on a corundum-calibrated (NIST 674a: Al₂O₃ using a 0.2 mm capillary) system using Mo radiation.

Unit-cell parameters based on the DS pattern simulations differed from the NIST reference material by an average of 0.003 Å, indicating that quality unit-cell data can be obtained from a powder on the Bruker system. Intensity data [R=0.139 (TiO₂), 0.087 (ZnO), 0.120 (LaB₆)] were close to the NIST references for samples showing minimal preferred orientation. For the Gandolfi pattern simulations, the unit-cell data were consistent with the single-crystal data. Intensity data will be discussed further, as will details and limitations on data collection and processing.

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