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# PoDFluX: A New Monte Carlo Ray-Tracing Model for Planetary Applications of X-Ray Powder Diffraction and Fluorescence

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A Monte Carlo ray-tracing model for the simulation of x-ray powder diffraction (XRD) and x-ray fluorescence (XRF) is presented. The model is primarily intended as a tool to aid the development of XRD/XRF instruments for in situ mineralogical and chemical analyses of planetary surfaces, but could also be employed for terrestrial applications. In the model, x-rays are produced either by an x-ray tube or a radioactive source. The x-rays interact sequentially with a user-determined series of model elements which can include apertures, micropore collimators, Söller slits and powder samples. Model samples are assumed to be ideal powders of any mineral or mixture of minerals for which the crystal structures are available. X-ray propagation ceases at the CCD detector(s), at which accurate quantum efficiency and energy redistribution effects are calculated. Given the appropriate characteristics, further source and detector types could easily be added. All model elements are treated as infinitely-thin surfaces which may be flat or curved (spherical or cylindrical).
In addition, a secondary model has been developed to explore the parafocusing effect. This model affords insight into the powder XRD technique, whereas PoDFluX simply predicts the result for a given configuration. In combination, the two models form a powerful optimization tool. Results of both models will be presented together with comparisons with experimental data.