



Diffuse Scattering and Defect Structure Simulations: A cook book using the program DISCUS (International Union of Crystallography Texts on Crystallography)

Reinhard B. Neder, Thomas Proffen

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Diffuse Scattering and Defect Structure Simulations: A cook book using the program DISCUS

(International Union of Crystallography Texts on Crystallography) Reinhard B. Neder, Thomas Proffen

In recent years it has become apparent that knowing the average atomic structure of materials is insufficient to understand their properties. Diffuse scattering in addition to the Bragg scattering holds the key to learning about defects in materials, the topic of many recent books. What has been missing is a detailed step-by-step guide how to simulate disordered materials. The DISCUS cook book fills this need covering simple topics such as building a computer crystal

to complex topic such as domain structures, stacking faults or using advanced refinement techniques to adjust parameters on a disordered model. The book contains a CDROM with all files needed to recreate every example given using the program DISCUS. The reader is free to follow the principles behind simulating disordered materials or to get down into the details and run or modify the given examples.

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