12. ADVANCES IN POWDER DIFFRACTION

12.X-1 DIRECT METHODS IN CRYSTAL STRUCTURE DETERMINATIONS FROM POWDER DIFFRACTION DATA.

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The applications of neutron powder diffraction to the determination of crystal structures from powder data have been advanced by the development of algorithms for direct methods. These algorithms have been implemented in software packages such as SHELX and PHASER. The use of neutrons allows for the determination of structures with high resolution, which is essential for neutron diffraction. The high-resolution data obtained in neutron powder diffraction has proven very effective for refining structures of moderate complexity.

12.X-2 HIGH RESOLUTION NEUTRON POWDER DIFFRACTION AND APPLICATIONS TO STRUCTURAL CHEMISTRY.


The use of high-resolution neutron powder diffraction has been applied to a wide range of materials, including zeolites, metal-organic frameworks, and inorganic compounds. The high resolution allows for the determination of structures with high precision, which is particularly useful for materials with complex structures. The use of neutron powder diffraction has been particularly successful in the determination of structures of materials that are not amenable to X-ray diffraction.

12.X-3 STRUCTURAL REFINEMENT FROM PULSED-NEUTRON-SOURCE POWDER DIFFRACTION DATA.


The use of pulsed neutron sources has provided significant improvements in the quality of neutron powder diffraction data, allowing for higher resolution and better peak resolution. The use of pulsed neutron sources has led to the development of high-resolution neutron powder diffraction (HRD) techniques, which are particularly useful for materials with small unit cells and high density.

12.X-4 CHEMICAL APPLICATIONS OF NEUTRON POWDER DIFFRACTION.


The applications of neutron powder diffraction to the study of chemical reactions have been advanced by the development of novel techniques, such as in situ neutron powder diffraction. These techniques allow for the study of chemical reactions under conditions that are not possible with conventional methods, such as high temperature and pressure.

The operation of two time-of-flight neutron diffractometers at the Intense Pulsed Neutron Source has provided significant improvements in the quality of neutron powder diffraction data, allowing for higher resolution and better peak resolution. The use of pulsed neutron sources has led to the development of high-resolution neutron powder diffraction (HRD) techniques, which are particularly useful for materials with small unit cells and high density.