CCMX-ScopeM Advanced Course
2018

X-ray Diffraction in Material Science

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Abstract

The term X-ray diffraction (XRD) describes a family of material characterization methods, which allow investigation of material properties on a large range of length scales. On the atomic scale it is possible to determine atomic coordinates and interatomic vectors with accuracy better than 0.01 Å. Structures to be determined may be as complex as proteins or viruses and details of phase transformation mechanisms can be monitored down to the atomic level. On the nanometer scale one can investigate molecular packings and interactions, the formation of supramolecular architectures and the sizes of nanoparticles. Finally, macroscopic properties such as texture, stress, quantitative composition of multi-phase materials or symmetry of physical properties can be directly measured or concluded from the atomic structure of the material under investigation. Such multi-scale properties can frequently be extracted from one simple experiment. XRD experiments are sample averaging methods, what makes them complementary to local scale sensitive characterization methods such as electron diffraction or any kind of microscopy.

For performing successful experiments there are only modest demands on the sample, but many XRD methods require crystalline material. In most cases sample preparation for X-ray experiments can be done within a few minutes. The typical amount of material required for performing experiments ranges from a few μm^3 to some mm^3. In principle, XRD is non-destructive, what allows investigations of the same sample under changing conditions (e.g. T, p).

The lecture will present the fundamental theory behind XRD and explain the principles of a selection of experimental techniques frequently used in material science. An overview of possibilities and limitations will be given. We will briefly discuss the relation of XRD to electron and neutron diffraction and introduce some additional possibilities when synchrotron radiation is used.

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