
X-ray Diffraction, XRD

Fortgeschrittenenpraktikum I/II

October 8, 2018

Abstract

This experiment will give you the possibility to gain knowledge in X-ray diffraction (XRD) by using a commercial analyser. XRD belongs to a family of non-destructive analytical X-ray techniques which reveal information about the crystal structure, chemical composition, and physical properties of materials and thin films. It is based on observing the diffracted intensity of an X-ray beam hitting a sample surface as a function of incident and scattered angle. In the experiment you will analyse the diffraction patterns of different ionic crystals. To get used to the instrument and the technique variations of the acceleration voltage, the filament current and the exit aperture. By using the characteristic peaks of different ionic crystals the transition energies of the Cu-anode will be examined and compared with the theoretical predictions. By fitting the short wavelength limit of the spectra in dependence of the anode voltage the Planck constant will be determined.

Contents

1	Introduction	3
2	Experimental Goals and Tasks	3
2.1	Detection of X-ray Radiation and Measurement of its Intensity with a Geiger-Müller-Tube.	3
2.2	Bragg-Reflection: Determination of Lattice Constants in Single-Crystals	3
2.3	Verification of the Duane-Hunt Relation and the Determination of the Plancks Constant	3
3	Literature	4

1 Introduction

X-rays are electromagnetic waves. The wavelengths of X-rays range between 0.1 Å and about 100 Å [1 Å=0.1 nm]. As it is usual for other electromagnetic waves, X-rays can also be described as radiation consisting of photons which travel at the speed of light and have energy $h\nu$, where h is Planck's constant (6.626×10^{-34} Js) and ν is the frequency of oscillation of the electromagnetic wave. Here the wave properties will be analysed by recording the angles for coherent and incoherent scattering of X-rays from a atomic crystal lattice. When X-rays are incident on an atom they excite the electron cloud around the atoms. The movement of these charges re-radiates waves with the same frequency (Rayleigh scattering). W.L. Bragg explained the patterns of reflected X-rays occurring for crystalline solids by modelling the crystal as a set of discrete parallel planes separated by a constant parameter d . The incident X-ray radiation produces a Bragg peak if their reflections off the various planes interfered constructively. The interference is constructive when the phase shift is a multiple of 2π ; this condition can be expressed by Bragg's law $n\lambda = 2d \sin \theta$.

2 Experimental Goals and Tasks

Details of the experiments and the setup can be found in the Handbook provided for the experiment. After discussion with the assistant also other experiments can be made, please check the Handbook for some examples!

2.1 Detection of X-ray Radiation and Measurement of its Intensity with a Geiger-Müller-Tube.

- Determination of the counting rate N as a function of the emission current I .
- Determination of the counting rate N as a function of the acceleration voltage U of the tube.
- Estimation of the Geiger tube's dead time.
- Influence of the exit aperture and the Ni filter.

2.2 Bragg-Reflection: Determination of Lattice Constants in Single-Crystals

- Measurement of the diffraction spectrum of a LiF single-crystal.
- Measurement of the diffraction spectrum of a NaCl single-crystal.
- Measurement of the diffraction spectrum of a KBr single-crystal.

2.3 Verification of the Duane-Hunt Relation and the Determination of the Planck's Constant

- Determination of the critical wavelength λ_{min} with reference to the tube high voltage U .

Assistant: Rémy Pawlak, Raum 3.01a, Tel.: -73725, Email: remy.pawlak@unibas.ch

3 Literature

X-ray Diffraction, Crystallography and Symmetry

- Phywe Handbook, X-ray experiments
- L.H. Schwartz and J.B. Cohen, Diffraction from Materials, 2nd Edition, Springer, 1987
- W. Kleber, Einführung in die Kristallographie, Oldenburg, 1998
- C. Kittel: Einführung in die Festkörperphysik, Oldenburg, 14. Auflage, 2006
- C. Giacovazzo, Fundamentals of Crystallography, IUCr, Oxford Science Publications, 2002 (English)
- J. Als-Nielsen, Elements of Modern X-ray Physics, Wiley, 2001 (English)
- L. Azaroff, Elements of X-ray Crystallography, McGraw-Hill, 1968 (English)
- T. Hahn, International Tables for Crystallography, Volume A, D. Reidel Publishing Company, 1987 (English)