

Introductory Lecture CRYSTALLOGRAPHY

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This introductory lecture is devoted to those who are not familiar with crystallography and/or diffraction. The basic concepts presented here will be useful for some other lectures. This lecture will consist in two parts of 1H30 (see outline below), both illustrated by examples and small exercises. The aim of the first part is to acquire a good knowledge of the description of a crystal in real space, based on the symmetries, and in the end to be able to read and understand the description of the 230 space groups given in the International Tables for Crystallography. The aim of the second part is first to become familiar with the concept of reciprocal space, second to learn the basics on diffraction by a crystal: conditions of diffraction, structure factors and consequences of the space group symmetry operations on the diffracted intensities, *i.e.* symmetry of the diffraction pattern and extinction rules. Last, a few examples of diffraction experiments will be shown, in relation with the concepts discussed during the lecture.

Introduction

1st part: CRYSTALLOGRAPHY IN DIRECT SPACE

I.1. Orientation symmetry

- Elementary point symmetries
- How to obtain and name all crystallographic point groups?
- Examples of point groups
- The 32 point groups and 11 Laue classes

I.2. Translation symmetry

- Lattice and motif, Unit cell
- The orientation symmetries of lattices:
 - the 6 conventional cells, 7 crystal systems and 14 Bravais lattices
- Lattice directions and net planes

I.3. Space group symmetry

- Glide planes and screw axes
- The 230 space groups
- The International Tables for Crystallography

2nd part: DIFFRACTION - CRYSTALLOGRAPHY IN RECIPROCAL SPACE

II.1. The reciprocal space

- Definition
- Examples
- First Brillouin zone
- Properties

II.2. X-ray and neutron diffraction by a crystal

- Diffraction condition
- Diffraction by an atom: scattered amplitude
- Diffraction by a crystal: structure factor
- Symmetry and extinction rules

II.3. Experiments

- What to measure and what for?
- Example 1: powder diffraction
- Example 2: single-crystal Laue diffraction
- Example 3: single-crystal four-circle diffraction