Introductory Lecture CRYSTALLOGRAPHY

Béatrice GRENIER, UGA & INAC / MEM / MDN – CEA, Grenoble, France

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: <u>CRYSTALLOGRAPHY IN DIRECT SPACE</u>

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