Chapter 1
Fundamentals of Kinematical X-Ray Scattering Theory

ABSTRACT

The broadening of X-ray line profiles is usually described by the kinematical scattering theory. In this chapter, the basic concepts and equations of the kinematical X-ray scattering are presented in order to better understand the theory of line profile analysis. The correlation between the crystal structure and the diffracted intensity distribution is shown. The scattering angles of the diffracted peak maxima are given by the Ewald construction in the reciprocal space. The correspondence between the reciprocal lattice vectors and the lattice planes is also presented, and the relationship between the scattering angle and the lattice plane spacing is given by Bragg's law.

INTRODUCTION

Wilhelm Conrad Röntgen discovered X-ray radiation in 1895 and recognized that its absorption depends on the mass density of materials. He received Nobel prize for his achievement in 1901. In the beginning of 20th century, the physicists suggested that X-ray is a form of electromagnetic radiation. For the justification of this supposition an interference experiment was necessary to perform on a periodic lattice with a similar period length as the suspected wavelength of X-rays (10^{-10} m).

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Assuming that crystalline materials have periodic lattice structure, Max von Laue calculated the conditions necessary for diffraction by X-rays. In 1912 according to Laue's calculations Friedrich and Knipping place a copper-sulphate single crystal in the path of X-rays and detected interference intensity spots on a film. With this experiment they established the fact that X-rays are electromagnetic in nature and opened the way to the investigation of the crystal structure by X-ray diffraction. Laue was awarded by Nobel prize in 1914. Since then, X-ray diffraction became a basic method of crystal structure determination in materials science.

In the kinematical theory of diffraction it is assumed that (i) the scattering is elastic, i.e. the wavelength of X-ray photons does not change in the scattering event, (ii) the diffraction is coherent, which means that the phase change of the X-ray wave during scattering is the same (namely π) for all scattering events and (iii) each photon is scattered only once, i.e. the diffracted wave is not scattered again inside the crystal. The latter criterion is a realistic approximation if the scattered intensity is much weaker than the incident intensity (Warren, 1990). Regarding the scattering mechanisms, when X-ray photons hit an atom, the center of gravity of the electron-cloud is moved away from the position of the nucleus. This electric dipole vibrates and radiates X-rays. With conditions (i)-(iii) the interference is determined solely by the positions of the scattering centers (electrons in the case of X-ray diffraction). As most electrons are located near the nuclei of atoms, the diffracted intensity distribution is mainly determined by the atomic arrangement in the crystal. This correlation enables the determination of the crystal structure from the position and intensity of the diffraction peaks. If the crystal lattice is distorted and/or the material consists of relatively small ($< 1\mu m$) scattering domains (crystallites), the diffraction peak shape can be well described by the kinematical theory and the analysis of peak profile gives the parameters of the microstructure (type and density of lattice defects, size distribution of scattering domains). The aim of this chapter is to introduce the key concepts and the basic equations of kinematical theory of X-ray diffraction which will be used in the subsequent chapters of this book.

THE INTENSITY SCATTERED BY A CRYSTAL

First, let's investigate the interference of X-rays diffracted from two scattering centers (electrons) in a crystal. One of the scattering centers is selected for the origin of the coordinate system in the crystal (denoted by O in Figure 1). The vector pointing to the second scattering center (point P in Figure 1) is denoted by $\boldsymbol{r}$. The crystal is radiated by a monochromatic primary X-ray beam with the wave-vector $\boldsymbol{k}_o$ which represents the direction of the beam and its magnitude is the reciprocal of the wavelength, λ ($|\boldsymbol{k}_0| = 1/\lambda$). Since the scattering is elastic, the diffracted beam

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