X-ray texture analysis in materials and earth sciences

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Abstract: The texture of a polycrystalline material is quantitatively defined by the orientation distribution function of the crystallites. In addition, higher-order textural quantities may also be considered such as the mis-orientation distribution function which describes the pair distribution of neighbouring crystals, texture fields, and multi-phase textures, thus approaching a comprehensive description of the statistical crystallography of polycrystalline aggregates.

Textures of materials can be measured mainly by X-ray diffraction but also using neutron and electron diffraction. The original textural data are pole density distribution functions from which the orientation distribution function can be calculated.

Textures have an influence on the properties of materials and they originate from all kinds of anisotropic solid-state processes. This establishes the interest in texture in materials science as well as in the earth sciences as illustrated by some examples.

Key-words: texture, materials properties, solid-state processes, powder diffraction, series expansion.

Introduction

The papers of this volume are written on the occasion to commemorate the 100th anniversary of the discovery of X-rays by Wilhelm Conrad Röntgen (1895). Particularly, they are devoted to X-ray crystallography based additionally on the second important discovery by Friedrich, Knipping and v. Laue (1912) of diffraction of Röntgen’s rays in crystals. Thanks to these two discoveries we know today that the vast majority of all anorganic matter surrounding us is in the crystalline state. This applies particularly to virtually all geological materials forming the earth’s crust but also to most of all technologically used materials. Also many organic substances may be crystalline or may at least contain crystalline components.

If we take — at random — a sample of any crystalline material and expose it to an X-ray beam, we may be lucky to obtain one of two essentially different types of diffraction diagrams illustrated in Fig. 1 (right and left). They correspond respectively to a single crystal and to an aggregate of virtually infinitely many small crystals in random orientations.

In the vast majority of cases we shall obtain, however, a type of diffraction diagram illustrated in the middle of Fig. 1. It also represents a polycrystalline sample, as that on the right side but with a non-random distribution of crystallites called a crystallographic texture. In fact, the orientation distribution of the crystallites may span the whole range from all crystals having the same orientation (the diagram is then indistinguishable from that of a single crystal) to completely random. Strictly speaking, the perfectly random state is equally rare in nature as that of a perfectly ordered single crystal. This applies to man-made materials e.g. metals, ceramics, and partly to polymers, as well as to natural ones e.g. geologic and partly also to biologic materials such as teeth, bones, sea-shells, wool or wood. The first texture diagram was observed by Hupka (1913) and Knipping (1913) only one year after the discovery of X-ray diffraction. Texture analysis, as a distinguished field of research, may be dated back to