ON PRACTICAL CALCULATIONS WITH REFLECTION CURVES FOR PERFECT CRYSTALS1)

A. FINGERLAND
Institute of Solid State Physics, Czechosl. Acad. Sci., Prague

The application of the Prins function for practical calculations is rather laborious. In the present article it is shown by analysis of some of the properties of this function that in most experiments with perfect crystals one may use functions of a much simpler form. Such a function is proposed, its use is shown on some examples, a method of simplified calculation of the fundamental constants of the Prins function is given, and finally some numerical examples are added as illustration.

О ПРАКТИЧЕСКИХ РАСЧЕТАХ С КРИВЫМИ ОТРАЖЕНИЙ ДЛЯ СОВЕРШЕННЫХ КРИСТАЛЛОВ

Применение кривых отражений для практических расчетов очень трудоемко. В работе показано на основе разбора некоторых свойств этих функций, что в большинстве экспериментов с совершенными кристаллами можно обойтись с намного более простыми функциями. Такая функция предложена, даны примеры её применения, метод упрощенного расчета основных постоянных кривых отражений и, в заключение, в качестве иллюстрации приведены примеры численных расчетов.

I. INTRODUCTION

The diffraction of X-rays on perfect absorbing crystals according to the dynamical theory is described by the Prins function, which is known in several forms (see e.g. [1], [2]). Many measurements have shown that the properties of selected crystals of calcite, quartz and diamond are very close to those of perfect crystals. Precision measurements with a three-crystal diffractometer on calcite [3], germanium and silicon ([4], [12]) showed very good agreement with dynamical theory even in the shape of the measured curves, and the quantitative evaluation led also to treatment of the theoretical Prins function from a purely practical standpoint.

The use of the Prins function for practical calculations is rather laborious and many experiments deal with only a few properties of this function. We can say, for example, that except for the measurements on the three-crystal diffractometer2) and extremely exact measurements of wavelengths (e.g. [13]), the influence of the asymmetry of the Prins function is negligible. Even on a three-crystal diffractometer, the asymmetry is considerably reduced by the monochromator smearing function [7].

In our considerations, however, we shall start with the Prins function; we shall try to supplement the analysis made of it in [5] by some properties, and we shall introduce a function, which is in a certain sense a good approximation of the Prins function, and on some examples we shall show the possibilities of its application.

1) These curves will be hereafter called Prins functions.

2) See also [15].
As a main reference article we use paper [5], where many important facts about the Prins function are given, and the notation used is a very useful one for further considerations.

In the following text the abbreviation HR and the number following refers to the particular equation in the above-mentioned paper by Hirsh and Ramachandran.

II. SOME IMPORTANT PARAMETERS OF THE PRINS FUNCTION

In most experiments, which deal with the shape of diffraction curves in such detail that one must use the Prins function $P(k, g, y)$, it is usually the symmetrical reflection in which we are interested, i.e. the case where the surface of the crystal is parallel to the diffracting planes. In this case (and for the $\sigma$-component) the constants $g$ and $k$ (see chapter V) lie practically in the intervals

$$0 < k < |g| < 0.1.$$  

We shall use this assumption for deriving some important values of the Prins function. We use the notation from [5]:

$$P(y) = L(y) - \sqrt{(L^2(y) - 1)} = 'P(L) \quad (HR-16)$$

where

$$L(y) = \left\{ y^2 + g^2 + \sqrt{((y^2 - g^2 - 1 + k^2)^2 + 4gy - k^2)} \right\} (1 + k^2)^{-1} \quad (HR-19)$$

where $y$ is an independent variable, $g$ and $k$ constants, fulfilling only the condition (1).

A. Maximum Value of $P(y)$

$y_m = k/g$, as given e.g. in [2]. Putting this in (3), we have

$$L_m = (1 + k^2)^{-1} \left\{ 1 + k^2 + 2g^2 - 2k^2 \right\}$$

and according to (1)

$$L_m = 1 + 2(g^2 - k^2)/(1 + k^2) \approx 1 + 2(g^2 - k^2).$$

In the following auxiliary step we shall assume that

$$L = 1 + 2\varepsilon^2$$

where $\varepsilon > 0$ is a small quantity. Putting in (2)

$$'P(L) = 1 + 2\varepsilon^2 - 2\varepsilon\sqrt{(1 + \varepsilon^2)}.$$ We expand and get

$$'P(L) \approx 1 - 2\varepsilon + 2\varepsilon^2 - \varepsilon^3 + ...$$

and if we keep the quantities only up to the 2nd order

$$'P(L) \approx 1 - 2\varepsilon(1 - \varepsilon)$$