A SIMPLE APPLICATION OF FUZZY ARITHMETIC TO AUTOMATE THE ALIGNMENT OF A CRYSTAL IN CHANNELING EXPERIMENTS

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Abstract

In this paper we present some results concerning the application of fuzzy arithmetic to the alignment of the major symmetry directions of a single-crystal with the ion beam direction. The goniometer settings for the alignment are calculated from the intersection point of the crystal planes plotted on a polar diagram. These planes are represented as straight lines joining the corresponding points of minimal RBS yields of the azimuthal angle φ for different tilts ($\theta \leq 10°$). In our approach, we consider the normalized distribution curves around the minimum RBS yields as fuzzy numbers and we calculate the intersection point of the crystal planes using the concepts of fuzzy subset theory. This technique is proposed as an attempt to automate the crystal alignment procedure, reducing the dependence of the results on uncertainties associated with the experimental data.

1 INTRODUCTION

Ion beam techniques are useful analytical tools to study the atomic structure of materials. In particular Rutherford Backscattering Spectrometry (RBS), in conjunction with ion channeling (RBS-C), is an effective and widely used method to study structural defects in the near-surface regions of single crystals and epitaxial layers [1]. The channeling effect only occurs when the beam is carefully aligned with a mayor symmetry direction of a single crystal, thus is quite important to have an efficient and trustful aligned methodology. At the Instituto de Física of the National University of Mexico (IF-UNAM) [2], the alignment process previous to the RBS-C experiments is performed in a semiautomatic manner. The data acquisition of RBS yields while scanning the azimuthal angle of the sample is performed by a computer system, and the crystal orientation is determined by a direct human intervention. This is a subjective and a time-consuming method that could be improved replacing the human action by an automatic computer system capable of dealing with uncertain quantities associated to the experimental data.

In this work we present a first attempt to totally automate the crystal alignment process in RBS-C experiments using fuzzy mathematics tools. We take advantage of fuzzy number capability to represent uncertainty and we associate fuzzy numbers to the region around the minimum RBS yields obtained when the azimuthal angle is scanning. Fuzzy operators and the Extension Principle [2] allow the evaluation of a simple analytical expression that determines the crystal orientation from experimental data.

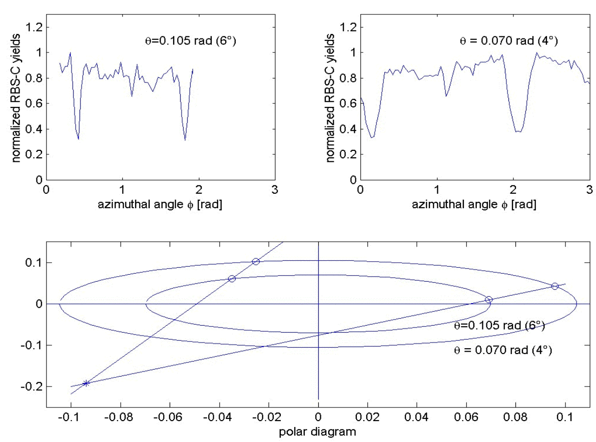

Figure 1. The goniometer settings for the alignment are calculated as the intersection point of the crystal planes, represented as right lines in a polar diagram. These lines are determined by the points φ corresponding to the minimum RBS yield for a fixed θ (θ =6° and θ =4°).

2 CRYSTAL ALIGNEMENT IN RBS-C EXPERIMENTS

Channeling is the steering of an energetic ion beam into open spaces (channels) between close-packed rows or planes of atoms in a crystal. Channeling of MeV ions only occurs when the beam is carefully aligned with a major symmetry direction of a single crystal.

The first step for aligning the crystal mounted on a two-axis goniometer (tilt angle, θ, and azimuthal angle, ϕ) is to tilt it to a small angle, typically 6°. Once a random RBS spectrum is obtained, an energy window is set at just below the maximum energy of the $^4He^+$ ions backscattered from the Si crystal. The RBS-C yields in this window are then collected for a given $^4He^+$ dose as the azimuthal angle φ is increased in steps of 1-2°. The angles φ at which major dips in yield occur correspond to alignment along planar channels. This procedure is repeated for one or more different tilts (θ = 4°, or 5°), the angles for the planar dips are plotted on a polar diagram, and the points are then connected by straight lines. According to the stereographic projection, these lines correspond to planes of the crystal and must intersect at the crystallographic

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axis of the crystal sample. The angles φ and θ at this intersection point are the goniometer settings for the alignment.

3 FUZZY ARITHMETIC APPLIED TO THE CRYSTAL ALIGNMENT

In Physics, experimental measurements present an intrinsic uncertainty associated either to the instrumentation or to the physical processes themselves. Fuzzy subset theory established a new form of dealing with these uncertain quantities representing them as fuzzy numbers.

3.1 Fundamental concepts of Fuzzy Arithmetic

The main feature of fuzzy set theory is the definition of sets with gradual membership, thus fuzzy sets are completely described by a set of pairs, the element *x* and its associated membership value $\mu_A(x)$.
In this work we are concerned with an especial kind of fuzzy sets, *Fuzzy numbers*, also called *Uncertain Numbers*, defined as *convex*, *normal* and *unimodal* fuzzy subsets of $\Re$ [2,3].

A random variable can be transformed to a fuzzy number deriving the membership function from the density function, i.e.

$$\mu_L(x) = \frac{f_L(x)}{\max_x f_L(x)}, \qquad (1)$$

where *max* $f_L(x)$ stands for the max value of $f_L(x)$, $\forall x \in L \subset \Re$, with *x* a random with a density function $f_L(x)$.

Fuzzy numbers can be manipulated using some basic operations defined based on the *Extension principle* [2,3], by which operations on real numbers are extended to operations on fuzzy numbers. Thus, let ⊗ and *A*, *B* denote any of the four basic arithmetic operation (+, -, *, ÷) and two fuzzy numbers defined on $\Re+$ respectively. The fuzzy set C=A$\otimes B$ on $\Re$, is defined $\forall\ z \in \Re$ as

$$\mu_{A\otimes B}(z) = \sup_{z = x\otimes y} \min[\mu_A(x), \mu_B(y)]. \qquad (2)$$

The operators multiplication, ×, and addition, +, of fuzzy numbers, are commutative and associative operators as in the classic case [3]. To extend the definition of fuzzy multiplication and division (eq.2) to fuzzy numbers with support in $\Re$-, we use equivalent operations. The multiplication and division of two fuzzy numbers *A*, *B* such that *Supp A* $\in \Re+$ and *Supp B* $\in \Re-$, can be written equivalently as

$$A * B \equiv -\left(A * (-B)\right), \qquad (3)$$

and

$$A \div B \equiv -\left(A * (-B^{-1})\right), \qquad (4)$$

where the *Supp(-B)*, *Supp (1/B)* $\in \Re+$. Recalling that the function of a fuzzy number is defined as a fuzzy set such that

$$\mu_{f(A)}(x) = \mu(x), \forall x \in A \qquad (5)$$

with $A \subset \Re$, is a fuzzy number and $f(.): \Re \to \Re$ a function defined in reals.

3.2 Application of fuzzy arithmetic to the Crystal Alignment problem.

Crystal alignment parameters, (θ_{al}, ϕ_{al}), are calculated as the intersection point of the two mayor orientation planes of the crystal. Applying basic concept of planar geometry, the polar coordinates of the of the intersection point can be calculated as follows (see fig. 2),

$$\theta_{al} = \sqrt{x_p^2 + y_p^2}, \qquad \phi_{al} = \arctan\left(\frac{y_p}{x_p}\right), \qquad (6)$$

where x_p and y_p are given by,

$$x_p = \frac{b_{24} - b_{13}}{m_{13} - m_{24}}, \qquad y_p = m_{13}x_p + b_{13}, \qquad (7)$$

with

$$m_{13} = \frac{y_3 - y_1}{x_3 - x_1}, \quad m_{24} = \frac{y_4 - y_2}{x_4 - x_2}, \quad b_{13} = y_3 - m_{13}x_3, \quad b_{24} = y_4 - m_{24}x_4, \qquad (8)$$

and x_i, y_i , $i=1,2,3,4$, the projections over the Cartesian coordinate axis of the two principal points of minimal RBS-yield as indicated in figure 2:

$$x_i = \theta\cos\phi_i, \qquad y_i = \theta\sin\phi_i. \qquad (9)$$

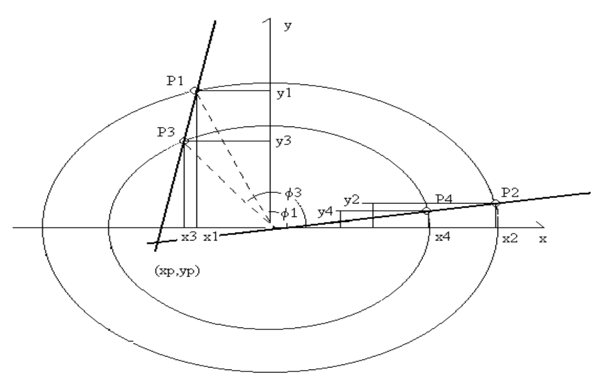

Figure 2. The intersection point of the crystal planes, represented by straight lines, can be calculated easily from the polar projection of the RBS-yield scan using elemental geometric relations. In the case of fuzzy numbers this relations are traduced to fuzzy operators.

The mathematical expressions of equations 6 to 9 have a very simple form and are composed in general of the basic four operations (+, -, x, ÷). However, they couldn't be evaluated directly because the data x_i, y_i are uncertain quantities, with an associated probabilistic distribution. In this case, what a human operator does is to estimate a crispy value for the RBS minimum yield coordinates and then evaluate the equations 6 to 9. Sometimes he calculates the intersection points by means of graphical methods.

Table 1: Alignment parameters calculated applying the fuzzy approach to the experimental data.

θ1, θ2	**Fuzzy**	
	θ_{al}	ϕ_{al}
6°-5°	1.25	51.59
6°-4°	1.15	56.68
6°-3.6°	0.98	43.54
5°-4°	0.56	63.03
5°-3.6°	0.81	48.85
4°-3.6°	1.13	53.72

In order to establish an objective method to calculate de alignment parameters allowing the automatic calculation on line, we apply the formalism of the fuzzy arithmetic. Thus, the uncertain quantities associated to points of minimal RBS-yield are represented as fuzzy numbers (eq. 1) and the equations 6 to 8, are replaced by composed fuzzy operators.

The projection of the minimal yield points to the *x* and *y* axis on the polar diagram are calculated as stated in equation 9, recalling that a function applied to a fuzzy number is defined as in equation 5. The resulting fuzzy numbers are then manipulated to calculate the intersection point (x_p, y_p) as indicated in equations 7 and 8 but using fuzzy operators instead of arithmetic operations.

The crispy values of the intersection point are obtained by defuzzifying [5] the fuzzy sets associated to x_p and y_p using the method of Center-of-Area. Finally, the alignment parameters (θ_{al}, ϕ_{al}) are obtained straightforward from equation 6.

4 EXPERIMENTAL RESULTS

The RBS-C spectra were obtained from Si single-crystals using a 2 MeV $^4He^+$ beam and the backscattered ions were detected with a 13 keV resolution surface barrier detector at a scattering angle of 167°. For this work we scanned the azimuthal angle $\phi \in [0°, 180°]$ at 4 different tilt angles θ=3.6°, 4°, 5° and 6°. The fuzzy algorithm proposed was programmed in *Matlab 5.1* and executed in a PC-*Pentium.*

The alignment parameters (θ_{al},ϕ_{al}) calculated using all the binary combinations of spectra corresponding to different tilts are presented in Table 1.

The values for (θ_{al},ϕ_{al}) calculated using the fuzzy algorithm approach are very close to the alignment parameters estimated independently by an expert: θ_{al_exp}=1°, ϕ_{al_exp}=60°. However they present a dispersion around the mean value due to the precision associated to the experimental measurements, i.e., the fuzzy approach can handle with uncertain quantities but it can't compensate the biased measures associated to the lack of precision.

It is important to mention here that the fuzzy algorithm applied in this work has showed to be a very time consuming method to calculate the alignment parameters.

5 CONCLUDING REMARKS

Based on fuzzy arithmetic, we introduce an automatic method to calculate the alignment parameters of a crystal in RBS-C experiments. This method, together with the already developed semi-automatic data acquisition system can be used to automate the alignment process previous to the RBS-C experiment. The results show the fuzzy approach is useful method to handle with uncertain quantities obtained from experimental processes, allowing an objective calculation of the alignment parameters and then, the implementation of automatic alignment system.

The drawback of this method is the high computation cost required to evaluate the fuzzy algorithm. Further research using approximate operators to optimize the calculating time and exploring the possibility of using a linguistic method instead of a mathematical one is required.

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