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Nonlinear Equations for Geometric Analysis of Linear Crack Patterns in Silicon Crystals

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Abstract

A method is described using nonlinear equations for geometric characterization of triangular surface linear crack patterns in silicon crystals. The proposed equations are solved by an iterative method with several variables. The angle between the surface plane and the (111) crystallographic plane of a silicon wafer is determined from an equation that is a linear combination of the cosines of the angles between the surface plane and the $(\bar{1}11)$, $(1\bar{1}1)$ and $(11\bar{1})$ crystallographic planes. These three unknown angles are the solutions of a nonlinear system of equations dependent on the angles between the directions of linear cracks on the surface plane of the wafer. The method was applied to a silicon wafer and the result compares favourably with the orientation obtained by X-ray diffraction.

Introduction

It is well known that the irradiation of a planar surface of a silicon crystal with a laser beam having a particular value of intensity and frequency brings about a modification of the surface structure. The surface contains a lattice of linear microchannels which are called 'linear crack patterns'. From the work of Tan, Ng & Ong (1984) and Demchuk, Pristrem, Danilovich & Labunov (1987) it is clear that these linear crack patterns (LCP) appear along the crystallographic planes that have the closest-packed atoms.

In his work Fong (1973*a*, *b*, 1986) gives an analytical method of determining cubic-crystal orientations from (111) surface traces and describes other methods and their inconveniences. The method proposed by Fong considers the angles between the first three trace directions and solves a fourth-degree polynomial equation. From these solutions are derived other intermediate quantities. This process of deduction of intermediate quantities is iterated many times. Fong (1986) also describes the possibilities of obtaining the crystal orientation from three or four surface-crack directions.

In their work, Hoekstra, Ohm & Verbraak (1978) give three equations for twins in the austenitic phase of bainitic steel Ni35Cr18 dependent on three measurement quantities and two unknowns. The two unknowns are the angle between a rotation axis *AB* and the projection of the $[\bar{1}11]$ unit vector on the (111) plane and a particular angle of rotation around the *AB* axis. They concluded that there are many solutions, depending on the angle between the twin intersection.

In the present work a method using nonlinear equations is reported. The system of nonlinear equations contains the orientation parameters as unknowns, without intermediate quantities. The solutions are obtained with a numerical method described by Drăgoi (1992). An initial approximate solution is however, required. Also in this paper are reported a theoretical test and an experimental example for analysis of a triangular LCP. A comparison with the X-ray diffraction method is given.

Formation LCP and measurements

The formation of a LCP with a triangular form has been observed by the action of a single pulse of a ruby laser (installed on a laser microanalyser LMA-10 produced in Germany) on a target of single-crystal silicon wafer. The silicon wafer has a misorientation in the [111] direction.

The LCPs were examined with the optical microscope of the LMA-10 and the image was photographed (Fig. 1*a*). The total magnification of the LCP image presented is 2200 times.

The misorientation of the silicon wafer was determined by the X-ray method described in ASTM F26-84 (1984). The value of the misorientation was 1.156°.

The angles between the directions of the LCP are measured by a conventional method. For the triangle indicated in Fig. 1(*b*) the two angles of interest are 59.3 and 60.5°. These values give information about the crystallographic orientation of the wafer. The relationship of these two values to the orientation parameters is given in the next section.

Angular relations of LCPs

With the method of extended stereographic projection (which projects more points beyond both sides of the equatorial circle) and the {111} planes projected onto the plane of the wafer, it is easy to find the projected spherical triangles containing two angles such as *A* and *B*, *B* and *C* or *C* and *A*. *A*, *B*, *C* are the angles between the surface plane of the wafer and the $(\bar{1}11)$, $(1\bar{1}1)$ and $(11\bar{1})$ planes, respectively. The

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first system of equations for a triangular LCP can be derived applying the cosine theorem:

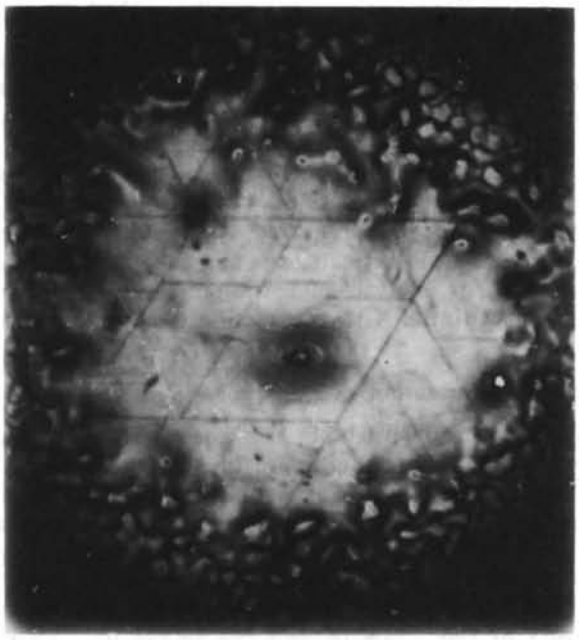
$$\cos x_{12} = (\tfrac{1}{3} + \cos A \cos B)/(\sin A \sin B), \quad (1)$$

then two similar formulae are obtained from (1) by the permutations

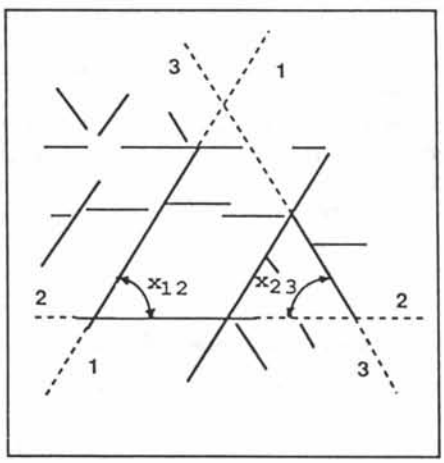
$$1 \rightarrow 2 \rightarrow 3 \rightarrow 1$$

$$A \rightarrow B \rightarrow C \rightarrow A,$$

where the arabic numerals 1, 2 and 3 designate three different directions of lines of the LCP. x_{12}, x_{23} and x_{31} are the angles between the pairs of straight lines 1 and 2, 2 and 3 and 3 and 1, respectively (Fig. 1*b*).



(*a*)



(*b*)

Fig. 1. (*a*) Triangular LCP obtained on a target of silicon wafer with a single pulse of a ruby laser; (*b*) scheme of (*a*) with the definition of the elements.

Table 1. *Test results for equations* (1) *and* (2)

x_{12}	x_{23}	x_{31}	β	ε
60.0000	60.0000	60.0000	30	0
60.0094	60.5256	59.4649	30	1
60.0201	60.5205	59.4594	31	1
60.0378	61.0419	58.9203	30	2
60.0592	61.0322	58.9087	31	2
60.0851	61.5488	58.3661	30	3
60.1171	61.5351	58.3478	31	3
60.1514	62.0465	57.8021	30	4
60.1941	62.0294	57.7765	31	4

The extended stereographic projection of the {111} planes on the (111) plane reveals the known symmetry of the 120° rotation around an axis perpendicular to the (111) plane and from their spherical triangles it is easy to derive the second group of equations, the parametric equations,

$$\cos A = \tfrac{1}{3}[\cos \varepsilon + 2 \times 2^{1/2} \sin \varepsilon \cos \beta]. \quad (2)$$

Two formulae are obtained from (2) by the permutations

$$A \rightarrow B \rightarrow C$$

$$\beta \rightarrow (\beta + 120) \rightarrow (\beta - 120),$$

where ε is the angle between the (111) plane and the surface plane of the wafer and β is the angle between one of the crystallographic directions, ⟨110⟩, and the line obtained from the intersection of the (111) plane with the surface plane of the wafer.

The first system of equations (1) represents the basic relations for determining crystal orientations from the triangular LCP. If one gives values to the parameters (ε, β), it is easy to compute the measurement parameters (x_{12}, x_{23}). In Table 1 the results of a test of (1) and (2) are given, using for ε and β the intervals (0, 4) and (30, 31), respectively.

Table 1 shows that (1) and (2) are satisfactorily checked for nine particular values of ε and β. The sum $x_{12} + x_{23} + x_{31}$ is equal to 180° for all the pairs (ε, β), since it is the sum of the angles of a triangle.

With knowledge, instead, of the pairs of angles (x_{12}, x_{23}) as experimental values, (1) leads to solutions for the unknowns A, B and C. These solutions can be obtained by applying a numerical method, for example the Newton method, for solving a nonlinear system of three equations.

From (2), with A, B and C determined, it is easy to determine the orientation parameters ε and β.

The direct expressions for ε and β in terms of A, B and C are

$$\cos \varepsilon = \cos A + \cos B + \cos C \quad (3)$$

$$\cos \beta = 2^{-3/2}(2 \cos A - \cos B - \cos C) \times [1 - (\cos A + \cos B + \cos C)^2]^{-1/2}. \quad (4)$$

In the following section an example is given of the use of these LCP equations.

Use of LCP equations

In the works of Tan *et al.* (1984) and Demchuk *et al.* (1987), the crack patterns are presented in the (100) and (111) planes. In the present work these patterns are presented in a plane inclined from the (111) crystallographic plane. The procedure for solving the nonlinear equations from (1) was developed in the work of Drăgoi (1992).

The system of nonlinear equations may be solved by two methods: the direct and reverse methods. The direct method uses the values ε and β as independent variables, generating the values x_{12}, x_{23} in Table 1, but with enough values and precision to fit the experimental data. The reverse method solves (1), using the Newton method as described by Kantorovich & Akilov (1977).

According to the Newton method the procedure for solving (1) is the same as that used by Drăgoi (1992) for two equations. The initial value for the start of the iterations was chosen to be $A = B = C = 70°$ and the condition for interrupting the computing process was the difference between two iterative solutions, ZA, ZB and ZC corresponding to the solutions A, B and C, being smaller than a given positive quantity ($\sim 10^{-4}$, denoted by EPS in Fig. 2). In Fig. 2, EPS fixes the precision of all solutions A, B and C by a single condition. The condition given can be considered equivalent to the separate conditions abs $(ZA) < \frac{1}{3}$EPS, abs $(ZB) < \frac{1}{3}$EPS, abs $(ZC) < \frac{1}{3}$EPS. In Fig. 2, P is a column matrix of three functions associated with (1). For example, the first element of P is the function $F1(A, B, C) = \cos x_{12} \sin A \times \sin B - \cos A \cos B - \frac{1}{3}$. The next elements will be $F2(A, B, C)$ and $F3(A, B, C)$ which can be obtained from $F1(A, B, C)$ by the permutation given for (1). I is the 3×3 Jacobian matrix of functions presented like the elements of matrix P. I^{-1} is the inverse matrix of I. The quantities $(I^{-1}P)_1$, $(I^{-1}P)_2$ and $(I^{-1}P)_3$ are the first, second and third elements of (3×1) column matrix $I^{-1}P$.

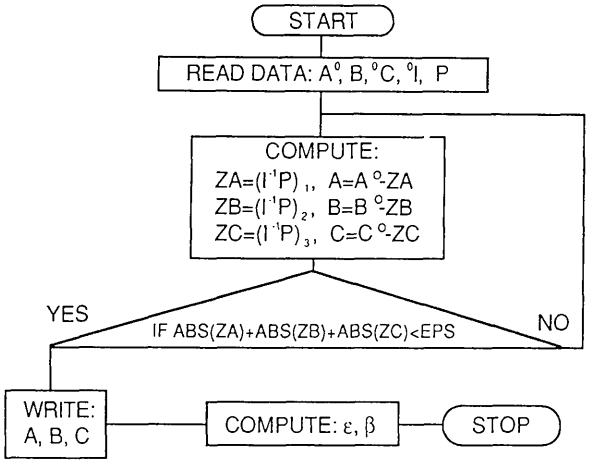


Fig. 2. Schematic diagram for solving LCP equations.

These initial solutions, arbitrarily chosen, were tested and found to be valid not only for misorientation but for high angles of ε, like the angles between crystallographic planes in a crystal with cubic structure.

The theoretical test given in Table 1 was checked satisfactorily using the Newton method. For example, using the values $x_{12} = 60.0851$, $x_{23} = 61.5488$ and solving (1), (2) give $\varepsilon = 3$ and $\beta = 30$, consistent with the values in Table 1. All the numerical values are expressed in degrees.

An experimental test was also performed. Measuring the angles $x_{12} = 59.3$ and $x_{23} = 60.5$ from the photograph (Fig. 1*a*) by a conventional method and applying the Newton method, one finds the value for ε to be 1.162°. This value is in good agreement with $\varepsilon = 1.56°$ measured by the X-ray diffraction method described in ASTM F26-84 (1984). The value of β was ignored in this experiment as it was not required.

Concluding remarks

The groups of nonlinear equations presented make possible the determination of the crystallographic orientation of a silicon wafer near a (111) orientation from the form of crack patterns on the wafer surface produced by a laser-beam pulse.

The accuracy of the obtained orientation is comparable to that achieved by X-ray diffraction.

The method described may possibly be extended to other materials such as GaAs and CdTe.

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