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A study of ion channeling patterns at minor axes in silicon

M. Motapothula [a,b,c,*], Z.Y. Dang [a,c], T. Venkatesan [b], M.B.H. Breese [a,c]

[a] Center for Ion Beam Applications, Physics Department, National University of Singapore, Lower Kent Ridge Road, Singapore 117542, Singapore
[b] NUSNNI-NanoCore, National University of Singapore, Singapore 117576, Singapore
[c] SSLS, National University of Singapore, 5 Research Link, Singapore 117603, Singapore

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ABSTRACT

We present a comprehensive study of channeling patterns showing the angular distributions of 2 MeV protons which are transmitted through a 55 nm thick [001] silicon membrane along, and close to major and minor axes. The use of such ultra-thin membranes allows the relationship between aligned and tilted patterns to be clearly observed and a correlation made between lattice geometry and pattern distribution across many axes. We study the effect of minor planes {1 1 *n*} (*n* odd) at axes which they intersect, where their changing lattice geometry results in a variety of effects. The origin of these patterns is studied with Monte Carlo simulations and we show how one may interpret aspects of the observed patterns to determine the corresponding lattice arrangement. At axes which have a single spacing between atom rows produce the well-known 'doughnut' distribution at small axial tilts. In comparison, axes which incorporate atom rows with a different spacing or geometry produce more complex channeling patterns which exhibit a secondary, inner feature produced by beam incident on these rows.

1. Introduction

Channeling occurs when energetic ions move either parallel, or nearly parallel, to an axis or a plane in a crystal [1]. Channeling causes ions to be repelled by the inter-atomic channel potentials, steering them away from the rows and planes of atoms into the open channels between the rows or planes of atoms. Channeled ions interact with the electron clouds along the channel, resulting in a smearing of their angular distribution which becomes more pronounced with increasing crystal thickness. Lindhard [2] derived formulae for the axial and planar channeling critical angles by introducing stable trajectories which considered that the ions do not come closer than the Thomas–Fermi screening radius, *a*, to the atomic rows or planes in order to be channeled. If they approach closer than this then they become either quasi channeled or randomly scattered [3].

The channeling critical angle, Ψ_c, for row of atoms in the axial case is:

$$\Psi_c = \sqrt{\frac{2z_1 z_1 e^2}{4\pi\varepsilon_0 Ed}}\left|\ln\left(\frac{\mathrm{Ca}}{\rho t}\right)^2 + 1\right|^{\frac{1}{2}} \text{(radians)} \tag{1}$$

$$\mathrm{a} = 0.8853 a_0 \left(Z_1^{\frac{1}{2}} + Z_2^{\frac{1}{2}}\right)^{-\frac{2}{3}} \tag{2}$$

Most studies of channeling phenomena were reported along major axes where the wide, open channels have large critical angles and longer channeling depths. Very few studies have been conducted along high Miller index (minor) axes, where the narrow channels result in smaller critical angles and rapid dechanneling due to interactions with denser electron clouds as well as shallower inter-atomic potentials. These studies were mainly conducted to complement the understanding of ion implantation effects, because channeling of low energy (<50 keV) implanted ions, such as boron and phosphorus, significantly alters the depth distribution of the implanted ions [4,5] and so the device performance. Ref. [6] experimentally located several high and low Miller indices axial/planar channels in a Si crystal for boron and helium ions in a backscattering mode. However, there remains an uncertainty as to whether perfect random alignment is achieved since there may still be a certain channeling effects.

Fig. 1 provides a guide to the angular location of the axes and planes around the Si [001] axis as relevant to the present study.

2. Transmission channeling

In axial alignment, channeling patterns produced by the transmitted beam passing through thick crystals (greater than a few hundred nanometers) resemble a star [7,8] having bright

* Corresponding author at: Center for Ion Beam Applications, Physics Department, National University of Singapore, Lower Kent Ridge Road, Singapore 117542, Singapore. Tel.: +65 83086250; fax: +65 67776126.
E-mail address: malli@nus.edu.sg (M. Motapothula).

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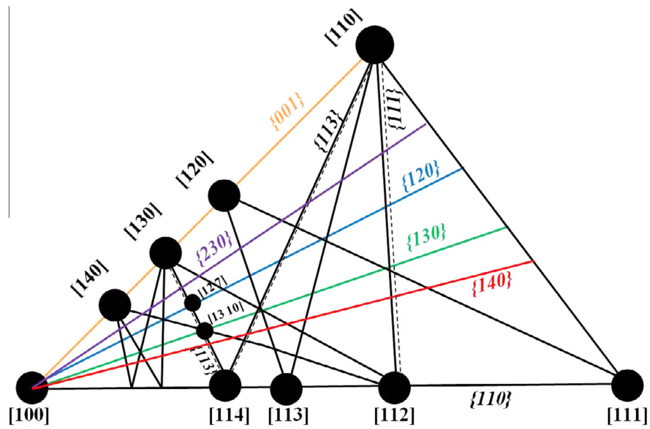

Fig. 1. Stereographic projection of axes and planes in Si lattice along ⟨001⟩, showing the major and minor axes and planes considered here.

regions in the middle, and showing blocking regions along the planes of intersections [1], which can aid the location of an axis. The transmission mode of observing channeling phenomena [9–11] has an advantage in several respects, where one can clearly visualize the angular location of the lattice or image any crystalline defects present such as dislocations and stacking faults, along with observing effects of oscillatory behavior in planar alignment [12,13].

It is now feasible to prepare perfectly crystalline ultra-thin silicon membranes which are only 55 nm thick [14,15]. A description of our sample fabrication and experimental details for fabricating ultra-thin silicon membranes is given in Ref. [14]. Recording such channeling patterns using a simple detection system comprising a YAG scintillator screen and a video camera requires less than a second per image, allowing a wide range of pattern variations from major and minor axes to be compiled under different tilt conditions.

Channeling patterns produced from thick crystals such as the silicon [001] and [111] axes exhibit ring-like shapes on tilting the crystal slightly away from a major axis [16–19] often referred to as "doughnuts", the diameter of the ring increases with tilt angle away from alignment [14]. However, when the crystal is thin (100 nm or less), the axial patterns are more complex [20,21], containing much fine-scale structure arising from the non-equilibrium trajectories which cannot be seen from thicker crystals due to multiple scattering with electrons [22]. For small tilts one observes strong variations from the ring-like shape, in which they appear as geometric shapes such as square and hexagon depending on the axis and the beam tilt [21,23]. For the [011] axis there is additional central feature observed in recorded patterns [21] and simulations [24]. It was previously referred to as the inner of two doughnut distributions.

Here we present a compendium of various pattern shapes and symmetries at minor axes, building on our earlier work [20] where we observed asymmetric axial channeling patterns from axes along the {111} planes, on tilting between the [112] and [110] axis, such as the [213] and [314] axes. The wide {111} plane produced a symmetric pattern both at axial alignment and for a small tilt away, whereas the narrow {111} plane produced an asymmetric pattern owing to the offset between its atom rows.

For materials such as silicon with a diamond crystal structure, all of the {1 *m n*}, *m*, *n* = odd, set of planes have two widths, referred to as wide and narrow. The {111} is the widest among them all, and also it is the only plane where the atom rows of wide channels are opposite each other. Other planes in this family, such as the {113}, also have two widths and since the row atoms of the wide channels are not opposite at most axes which intersect these planes, then one might expect the channeling pattern produced by the wider planes to be asymmetric, as well as that from the narrow planes.

The aims of this study are as follows. First, to provide a compendium of the different channeling patterns observed at various major and minor axes as a reference source, both at axial alignment and for small tilts away. Second, to study the relation between observed pattern asymmetry and the crystal lattice arrangement at minor axes. Finally to derive a generalized behavior across different lattice directions, allowing us to elucidate details of the lattice structure from certain observed pattern attributes.

3. Results

3.1. Axes along major planar directions

Fig. 2a shows a composite set of calculated maps of static interatomic axial continuum potentials, $V(r)$, at various axes using the ZBL universal potential [25], along with the corresponding axially aligned channeling patterns in Fig. 2b, from Ref. [18]. Previously we reported the aligned and tilted case for channeling patterns mainly at major axes [001], [011] and [111] in Refs. [14,20,21]. Here we show the corresponding doughnut patterns obtained from tilting either along, Fig. 2c, or perpendicular to the major planes {001}, {011} and {111}, Fig. 2d, at axes along these directions. One needs to bear in mind that the patterns shown for the [001], [112] and [011] axes (i.e. those at each corner of the triangle) can be considered to be interchangeable between Fig. 2c and d depending on which set of intersecting major planes one is considering, hence both are included in each figure. An initial observation is that each doughnut pattern may exhibit a unique shape, or one that is similar to that observed at other axes, depending on whether the basic atomic arrangement is similar.

Fig. 3 shows a more detailed observation of the evolution of the channeling patterns at the [014], [013] and [012] axes for increasing tilts parallel to (columns a, c, e) and perpendicular to (columns b, d, f) the {001} direction. Fig. 4 similarly shows more detailed evolution of the channeling patterns at the [114], [113] and [112] axes for increasing tilts parallel to (columns a, c, e) and perpendicular to (columns b, d, f) the {011} direction.

3.2. Axially aligned patterns along minor planar directions

Section 3.1 presented channeling patterns which were recorded at axes along major planar directions. We now consider the effect of tilting along minor planar directions, specifically {012} in Fig. 5, {013} in Fig. 6 and {113} in Fig. 7 to provide a comprehensive overview of the relationship between the lattice geometry, mirror symmetry and the observed channeling pattern. Each figure shows an axially aligned pattern at minor axes encountered along a certain planar direction, along with the corresponding FLUX [24] simulated pattern and the atomic arrangement. FLUX is a widely-used Monte Carlo simulation programme for ion channeling, it combines the binary collision model and multi-string approximation, as well as the nuclear and electronic stopping as a function of impact parameter. Where the lattice is symmetric we denote this as 'S' and show the mirror symmetry planes in dashed lines. Note that most of the axes are asymmetric along these directions, as are the corresponding channeling patterns.

4. Analysis and discussion

4.1. Tilts parallel to a major planar direction

Consider the following pattern sequence in Figs. 2–4, starting from [001] to [114] to [012] to [113] to [014]. This sequence