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ON INDEXING OF DIFFRACTING PLANES USING THE KIKUCHI PATTERN

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ABSTRACT

Two types of ambiguity concerning indexing of electron diffraction patterns have been cleared up by making use of the Kikuchi lines. A convenient unambiguous method of uniquely indexing patterns is suggested assuming the beam is always along the viewing direction no matter how the picture is printed. It is shown that there are two completely equivalent ways of indexing the Kikuchi pattern, e.g. [111] or [$\bar{1}\bar{1}\bar{1}$]. The method is also useful in interpreting dark-field pictures when top - bottom contrast is concerned.

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INTRODUCTION

The Kikuchi pattern of a thin foil produced by an electron microscope gives the orientation of the foil uniquely[1,2,3], and maps for indexing all Kikuchi poles in cubic and hexagonal closed packed structures have been published[(2)]. However, in many cases, such as for determination of Burgers vectors or loop types, confusion may still arise concerning the correct assignment of indices to all $\vec{g}$ vectors where the $\vec{g}$ vectors are the reciprocal lattice vectors.

The two ambiguities that may have caused confusion concerning the correlation between the diffraction pattern and the associated $\vec{g}$ vectors are:

1) +g and -g ambiguity: For a given diffraction pattern of a given orientation, e.g. [111] in fcc or dc, and assuming a right handed coordinate system, confusion may have arisen as to assigning +g or -g to the first $\vec{g}$ vector. Even with a Kikuchi pattern, a non self-consistent way of orienting the crystal with respect to its Kikuchi pattern exists. (Fig. 1).
2) Ambiguity in foil normal $\vec{n}$: Fixing one direction, there are still two ways of assigning the other $\vec{g}$ vectors that are consistent with the same Kikuchi pattern but represent different orientations. (Fig.2).

ANALYSIS

For simplicity, we shall only consider the Kikuchi pattern of fcc and dc structures near the <111> orientation (Fig. 3). The tetrahedron of {111} planes is convenient for describing the most commonly used $\vec{g}$ vectors and orientation and will be used hereafter to describe the relationship between the Kikuchi pattern and crystal orientation (Fig. 4).

A [111] crystal orientation will give a $[\bar{1}\bar{1}\bar{1}]$ Kikuchi pattern when viewed above it as shown in Fig. 5. In order to simulate the actual condition when viewing in the electron microscope, we shall assume that the beam is along the viewing direction. The kikuchi pattern is then indexed with reference to the tetrahedron, throughout this paper.

a) Referring to Fig. 6, it can be seen that when the crystal is tilted from [111] orientation to the closest <112>, the movement of poles along the $[2\bar{2}0]$ Kikuchi band is opposite to the tilting direction[1]. This simple relationship clears up the first ambiguity stated in the previous section and it eliminates the possibility of Fig. 1a.

b) From Fig. 7, if we fix one of the direction of a tetrahedron and flip it over, then the two tetrahedra have exactly the same parallel planes, but with the bottom planes reversed in sign. Since the two tetrahedra have parallel planes, they are actually completely equivalent which means they should give the same Kikuchi pattern and that they both represent the same orientation. If we assign indices to them, it is obvious that indeed we can have two general ways of indexing $\vec{g}$ vectors and orientations that are exactly equivalent, both should give the same Kikuchi pattern and both represent the same orientation. So long as all vectors are indexed according to one set or the other, it makes no difference. This explains the second ambiguity.

DISCUSSION AND CONCLUSION

The equivalency of the two tetrahedra shown in Fig. 5, also means that it does not matter from which side the plate (picture) is viewed, (e.g. whether the beam direction is taken correctly or opposite). A typical example is shown in Fig. 8, which is a dark field picture of a P^+ (2×10^{14} nvt) implanted silicon after heat treatment at 750°C for 1/2 hr. The rod-like defects were found to be along <110>[6,7]. Fig. 8a was printed with emulsion side up while Fig. 8b was reversed. The diffraction condition was s>o, hence the bottom of the foil should be in good contrast[(8)] which can be seen to be true on the inclined rods, TB, by assuming the beam was along the viewing direction and that the foil orientation was [111] in both cases.

Hence we come to the following conclusions:

1. For a given Kikuchi pattern, we have two generally equivalent ways of correctly indexing $\vec{g}$ vectors with respect to orientations, e.g. [111] and $[\bar{1}\bar{1}\bar{1}]$. Taking the advantage of assuming that the beam is always along the viewing direction as in the actual case in the electron microscope, we can index the Kikuchi pattern with reference to a suitably oriented tetrahedron. If the orientation is [111] and the top of the tetrahedron is up, the corners of the tetrahedron should point away from the <112> poles. If $[\bar{1}\bar{1}\bar{1}]$ orientation of the foil is assumed up and the top of the tetrahedron is down, then the corners must point towards <112> poles. (Fig. 2).

2. With only small angle tilting or even without any tilting at all in the high voltage electron microscope, one can quickly and easily find the direction of <112> poles by finding the nearest asymmetric pole along a $<2\bar{2}0>$ band near a <111> orientation.
3. Similar arguments can be extended to other foil orientations as well as to other crystal structures.
4. The only limitation in practice is that there has to be a Kikuchi pattern. However, if no Kikuchi pattern is available, then the second Laue zone method[4] can be used to determine the sense of tilting.
5. As long as the bright field (B.F.) or dark field (D.F.) picture is printed in the same manner as the selected area diffraction pattern (S.A.D.), it is immaterial to know the actual direction of the beam. This fact is particularly useful in interpreting D.F. pictures when it is desired to know whether top or bottom contrast is being observed.
6. With this simple correlation of $\vec{g}$ vectors with foil orientation, loop type determinations of perfect dislocation loops in fcc or dc structure near the [111] orientation can be made in a very quick and accurate way[5].

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FIGURE CAPTIONS

Fig. 1. For a given Kikuchi pattern and orientation e.g. [111], there are two ways of arranging the tetrahedron. For simplicity, only the <112> and <111> poles are used to represent the asymmetry on the opposite sides of the <111> pole along <$\bar{2}$20> band. The edges of the tetrahedron are in solid lines if they are on or above the paper, otherwise in dotted lines throughout this paper.

Fig. 2. For a given Kikuchi pattern and a fixed direction ($\vec{g}$ vector), there are two ways of arranging the tetrahedron.

Fig. 3. A complete <111> oriented Kikuchi map. The indices of the poles are assuming a [111] orientation. Note the asymmetry on the opposite sides of the [111] pole along <220> band.

Fig. 4. A complete tetrahedron of {111} planes and their indices as used in this paper.

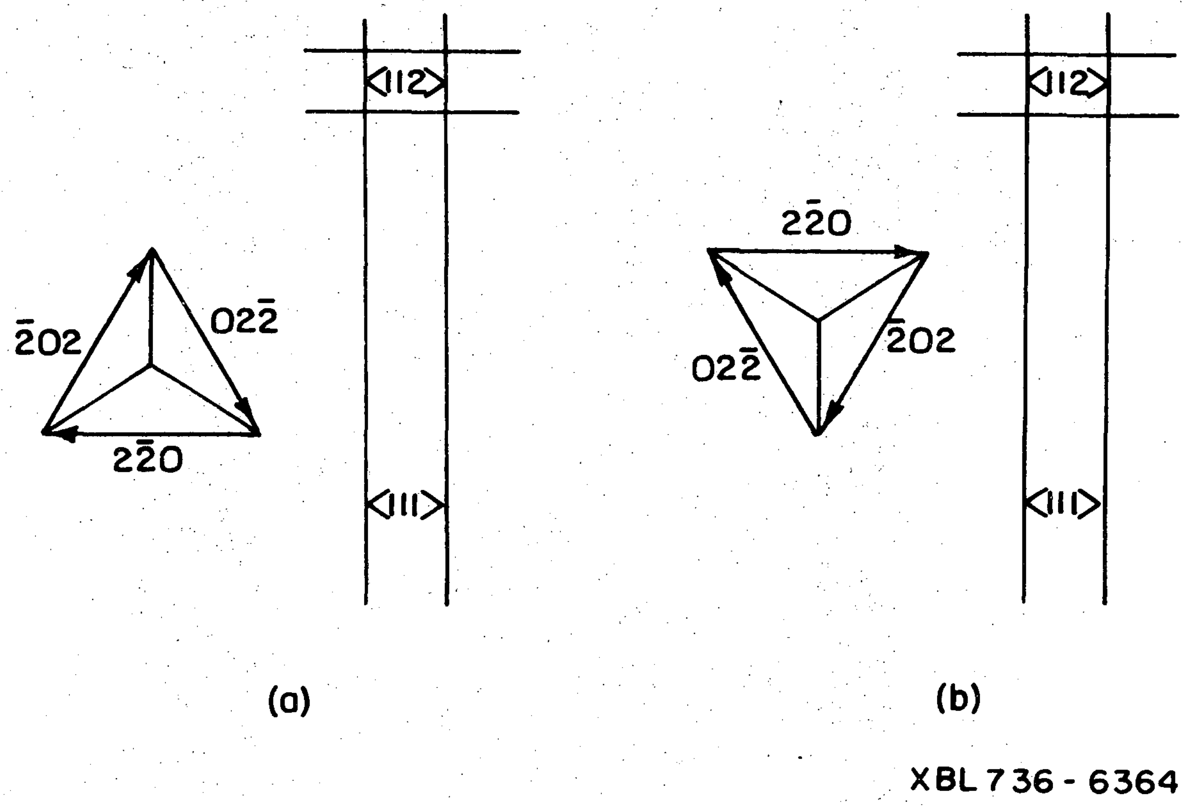
Fig. 5. Relationship between a crystal of [111] orientation and the Kikuchi pattern when viewed from the top.

Fig. 6. Relationship between the movement of Kikuchi poles and the sense of tilting.

Fig. 7. Two equivalent tetrahedra placed with one direction fixed and basal plane flipped over with respect to each other. Hence, there are two generally equivalent ways of indexing $\vec{g}$ and $\hat{n}$ for a given Kikuchi pattern.

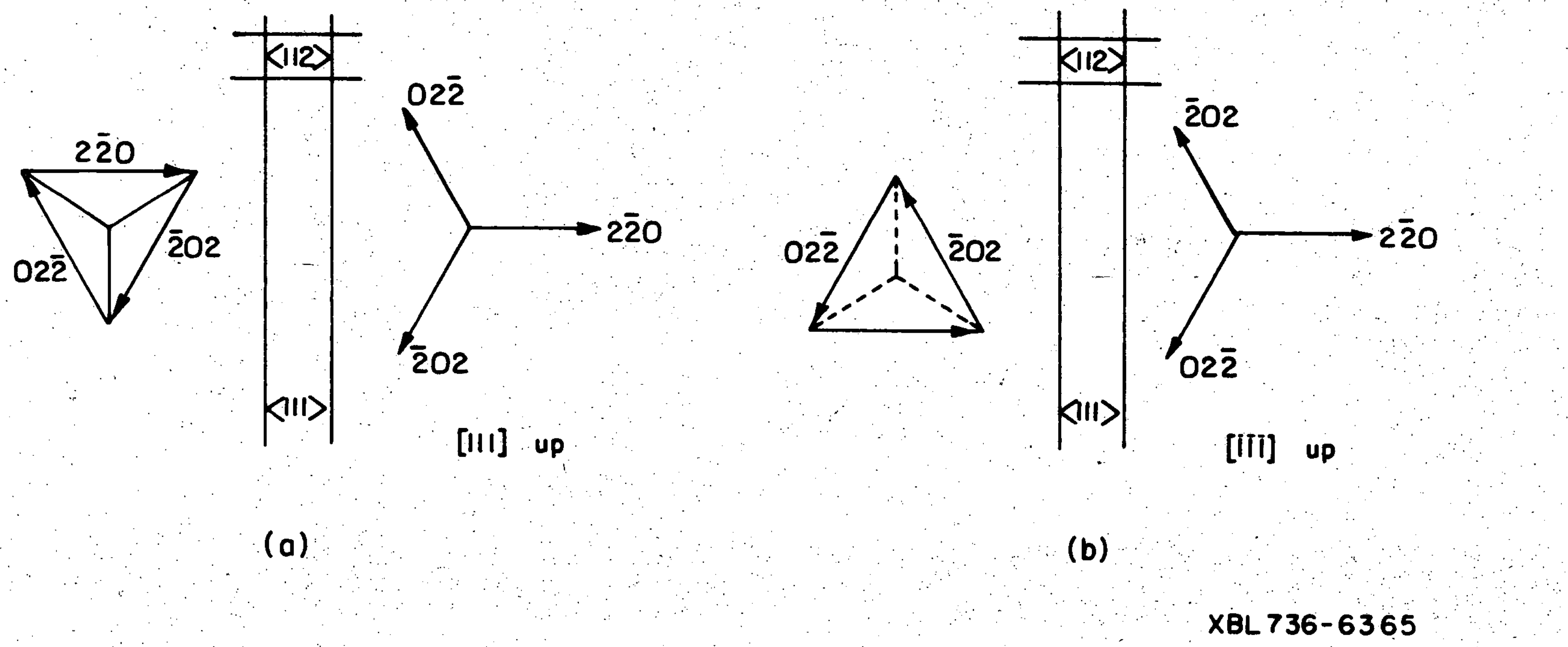
Fig. 8. Dark field picture and its selected area diffraction pattern of a [111] oriented Si implanted with P^+ (2×10^{14} nvt, 100 KeV) and annealed at 750°C for 1/2 hr. a) Printed with emulsion side

up b) Printed with emulsion side down. The rod-like defects are along <110>. If the viewing direction is taken as into the paper, in both cases, it is proved that the determination of top or bottom of the foil is unaffected by how the picture is printed.



$\bar{2}02$
$02\bar{2}$
$2\bar{2}0$
⟨112⟩
⟨111⟩
(a)
$2\bar{2}0$
$02\bar{2}$
$\bar{2}02$
⟨112⟩
⟨111⟩
(b)
XBL 736 - 6364

Fig. 1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0$2\bar{2}$
$\bar{2}$02
<112>
<11>
0$2\bar{2}$
2$\bar{2}$0
$\bar{2}$02
[111] up
(a)
0$2\bar{2}$
$\bar{2}$02
<112>
<11>
$\bar{2}$02
2$\bar{2}$0
0$2\bar{2}$
[$\bar{1}\bar{1}\bar{1}$] up
(b)
XBL 736-6365

Fig. 2.

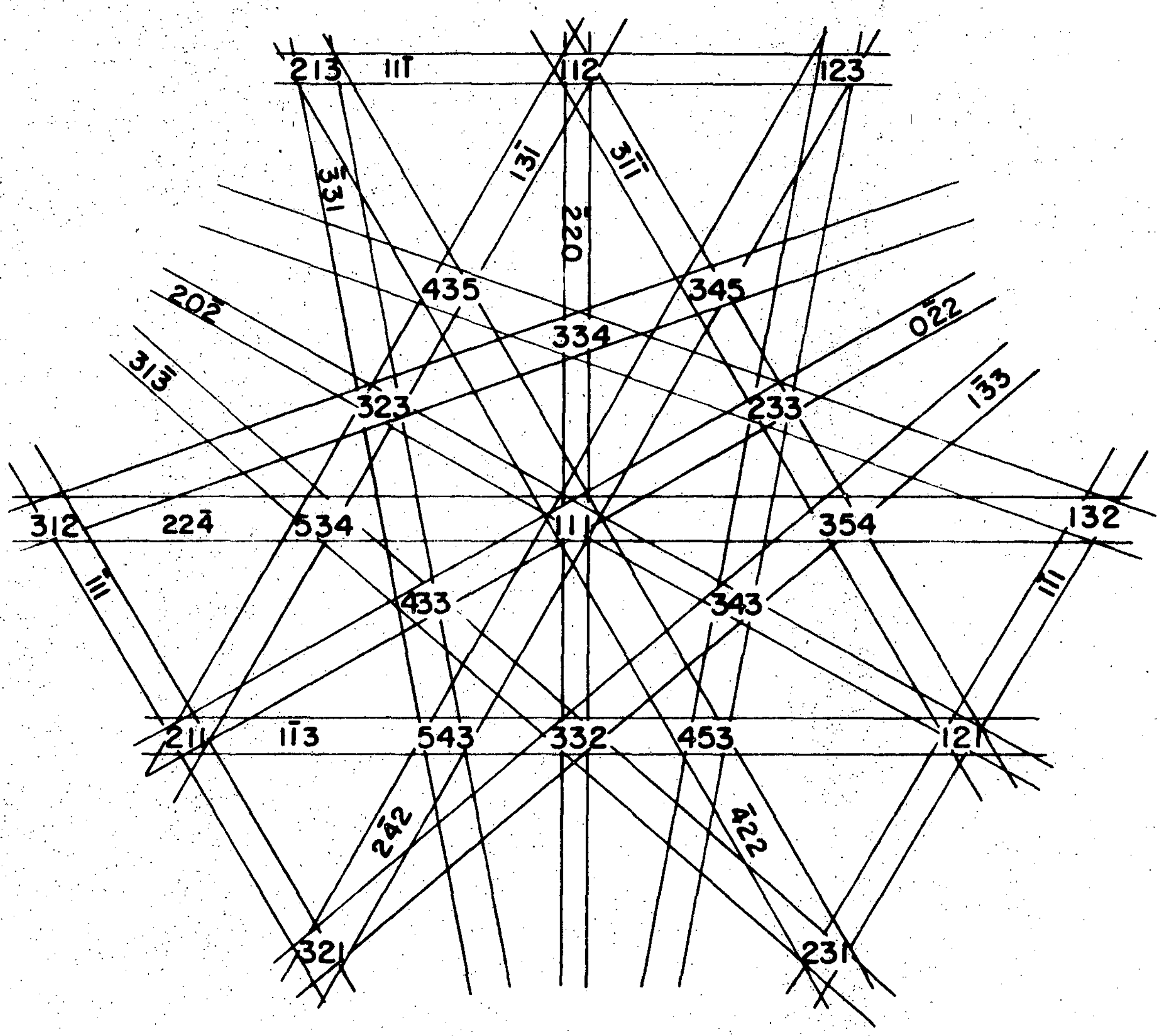

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Fig. 3

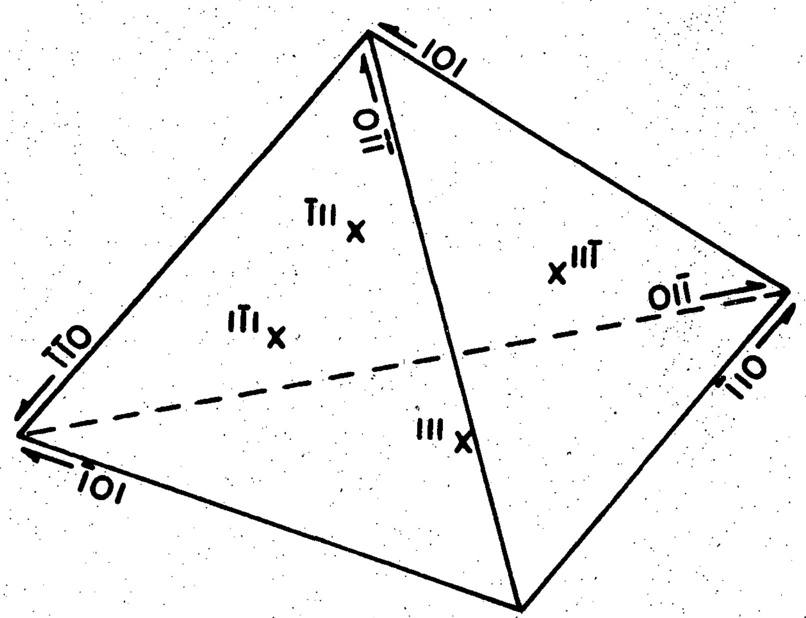

Fig. 4

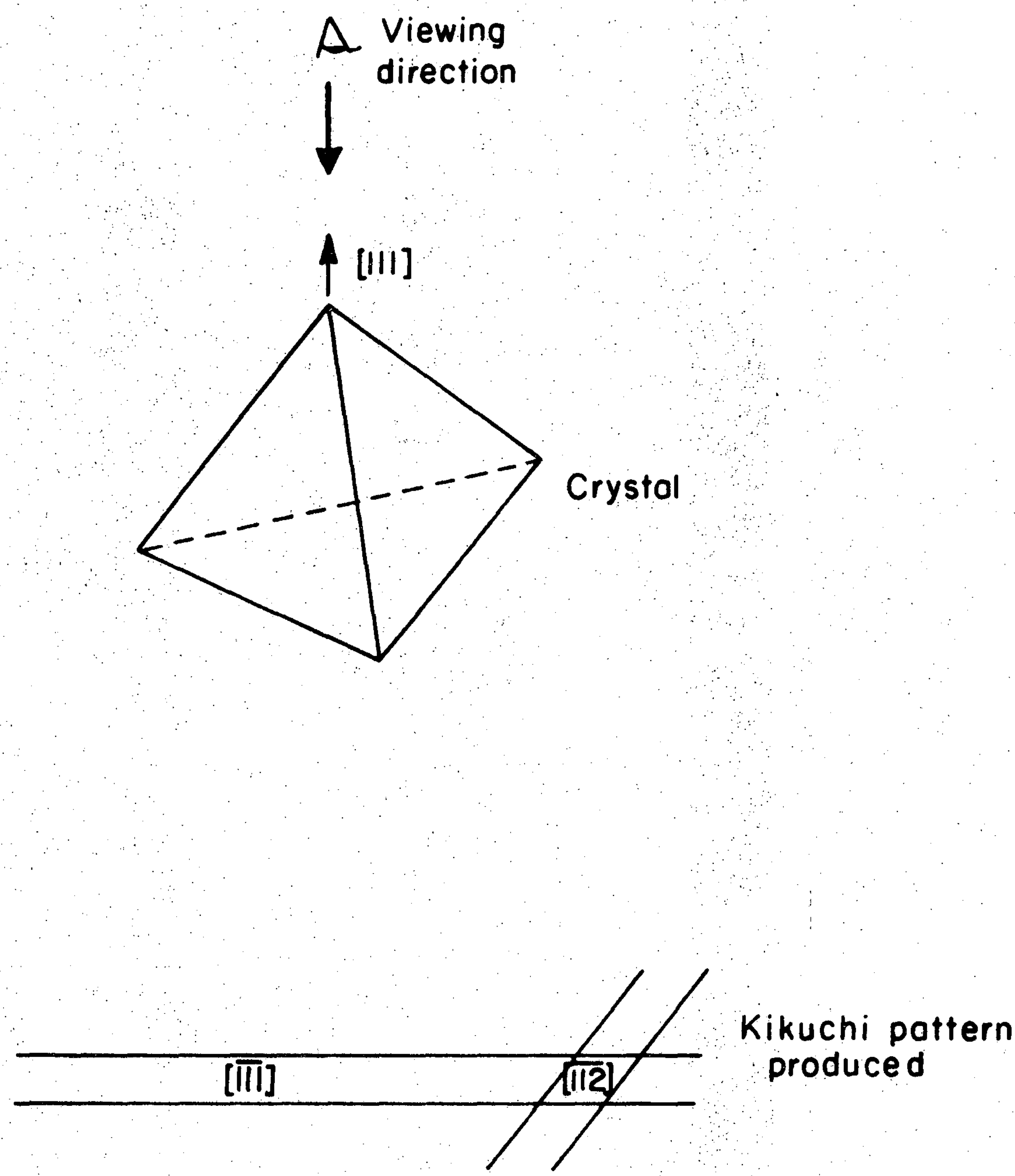

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Fig. 5

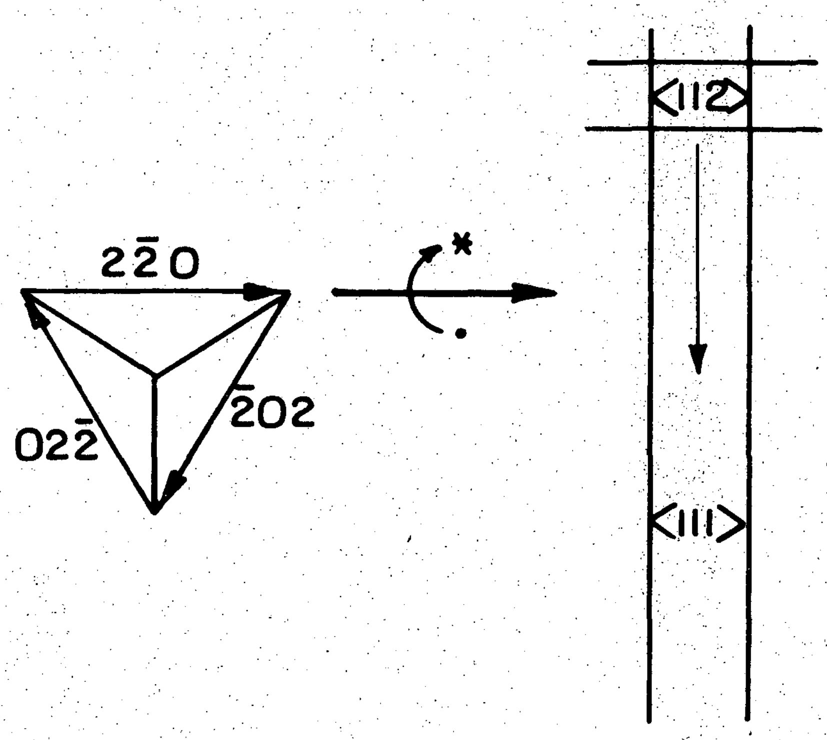

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Fig. 6

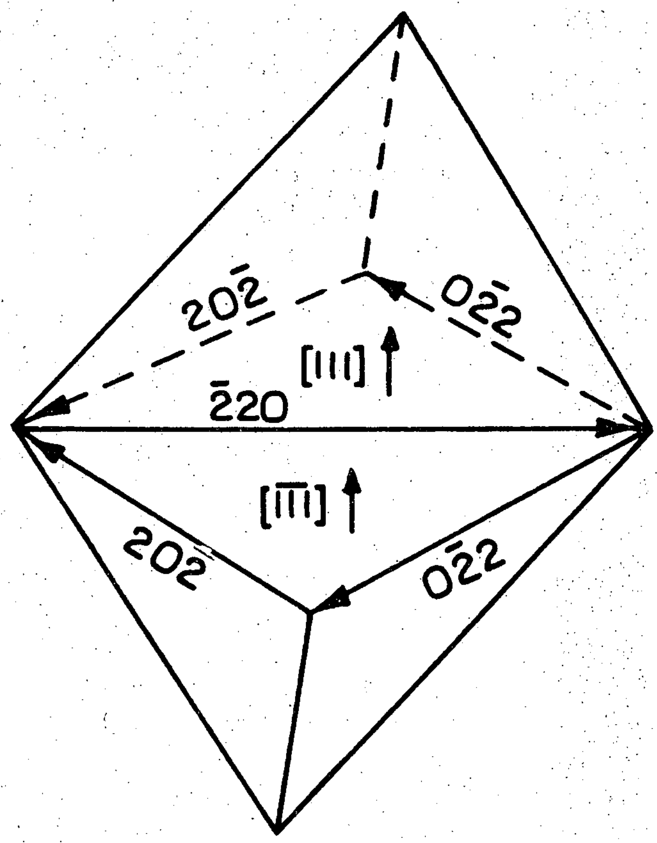

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Fig. 7

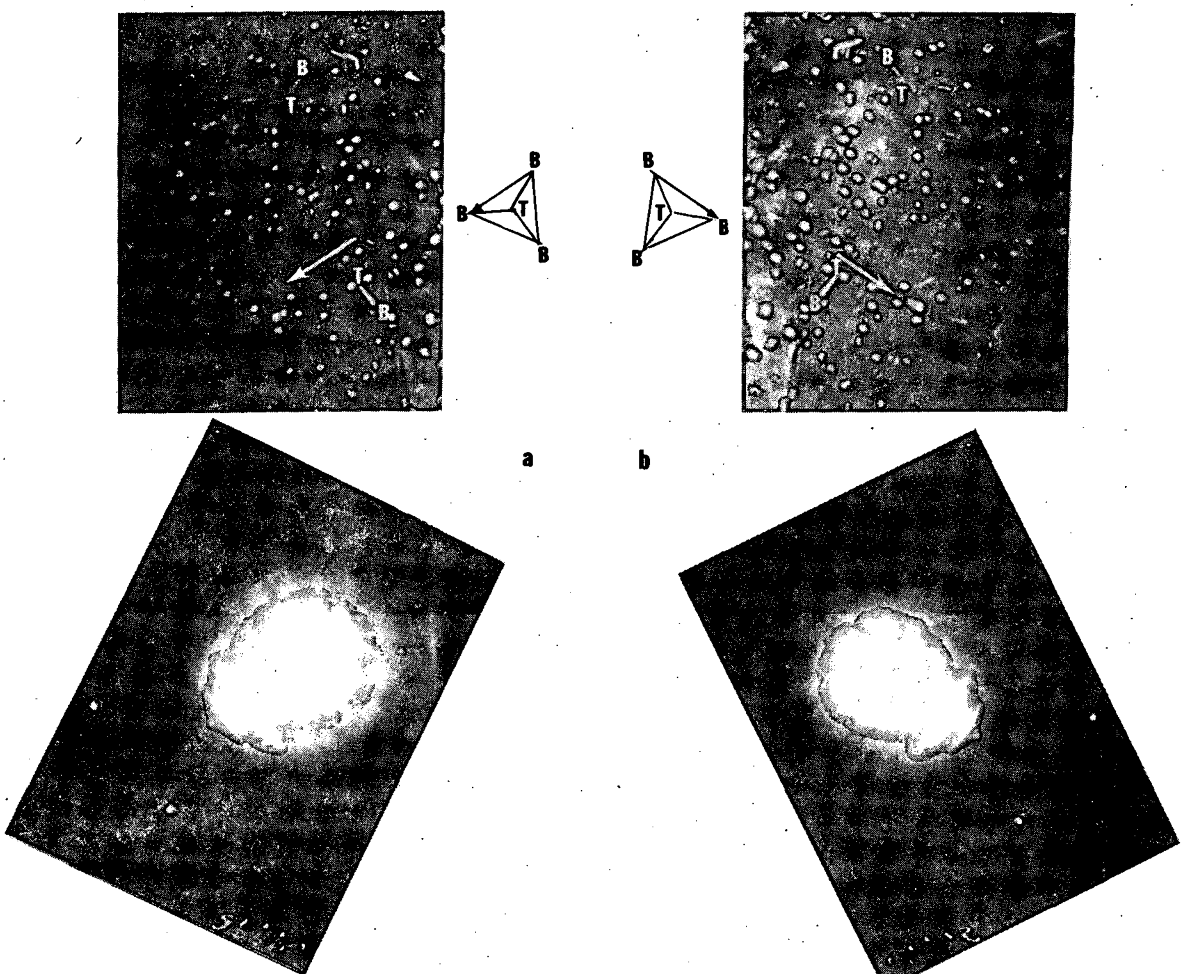

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Fig. 8

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