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Misalignment Sensitivity of an Inclined Crystal Monochromator*

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DISCLAIMER

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abstract

The sensitivity of a novel inclined crystal monchromator design to misalignments has been calculated, and compared to data. Rocking curve line narrowing as well as broadening can occur because the asymmetry factor of dynamical diffraction given by $b = \mathbf{s_0} \cdot \mathbf{n} / \mathbf{s_H} \cdot \mathbf{n}$ can have an absolute value larger or smaller than unity. Here $\mathbf{s_0} \cdot \mathbf{n}$ and $\mathbf{s_H} \cdot \mathbf{n}$ are the direction cosines of the incident and diffracted beams, respectively, and **n** is the inward surface normal. An inclined double crystal monochromator which is perfectly aligned would have $b = -1$ for both crystals , and only then would the diffraction be symmetric. We have computed b and rocking curve widths for inclination angles of 70.53° and 85.00° , and we compare the 70.53° case to data for silicon {111} reflections using 8 KeV ($CuK\alpha_1$) radiation. The 70.53° case applies to $(11\bar{1})$ reflection from a (111) oriented crystal. We report that rotations around the reciprocal lattice vector have the expected effect on b

I. Introduction

The inclined crystal arrangement has recently been tested as a high heat load monochromator[1] and a sensitivity to rotations around $\vec{H}$, the reciprocal lattice vector, was invoked to explain observed rocking curve widths. Rotation around $\vec{H}$ constitutes a degree of freedom available with a symmetric reflection. This degree of freedom, which we have called ρ, is sacrificed in the inclined case, and a misalignment in ρ results in truelly asymmetric diffraction, i.e., diffraction with b not equal to -1.

After deriving the relevant trigonometric relations, we present the supporting data which we have obtained.

II. Asymmetry factor as a function of azimuthal angle

The coordinate system we have used is shown in Fig. 1a. The inclination angle is denoted as β. The $\hat{\mathbf{z}}$ axis lies along $\vec{\mathbf{H}}$, and the $\hat{\mathbf{x}}$ axis lies in the crystal surface along the intersection of a Bragg plane (the x-y plane) with the surface. $\hat{\mathbf{n}}$ is defined to be the inward surface normal. (Chosing the inward instead of the outward normal agrees with the convention of Zachariasen[2].) In our coordinate system $\hat{\mathbf{n}}$ is given by

$$\hat{\mathbf{n}} = \hat{\mathbf{y}}\sin\beta - \hat{\mathbf{z}}\cos\beta \quad . \qquad [1]$$

We consider an incident plane wave with a wavevector along the direction $\hat{\mathbf{s}}_0$ which is shown in Fig. 1b. $\hat{\mathbf{s}}_0$ is given by

$$\hat{\mathbf{s}}_0 = \hat{\mathbf{x}}\cos\theta\cos\rho + \hat{\mathbf{y}}\cos\theta\sin\rho - \hat{\mathbf{z}}\sin\theta \quad . \qquad [2]$$

Here θ is the angle $\hat{\mathbf{s}}_0$ makes with respect to the Bragg plane and ρ is the azimuthal rotation about $\vec{\mathbf{H}}$. The direction of the Bragg diffracted beam, $\hat{\mathbf{s}}_H$, is also shown in Fig.1b and is given by

$$\hat{\mathbf{s}}_H = \hat{\mathbf{x}}\cos\theta\cos\rho + \hat{\mathbf{y}}\cos\theta\sin\rho + \hat{\mathbf{z}}\sin\theta \quad . \qquad [3]$$

From Eqs. 1-3 it is straightforward to write down the asymmetry factor given by $\mathbf{b} = \hat{\mathbf{s}}_0 \cdot \hat{\mathbf{n}} / \hat{\mathbf{s}}_H \cdot \hat{\mathbf{n}}$. The result is

$$\mathbf{b} = \frac{\sin\beta\cos\theta\sin\rho + \sin\theta\cos\beta}{\sin\beta\cos\theta\sin\rho - \sin\theta\cos\beta} \quad . \qquad [4]$$

We note that for $\rho = 0$, we have b=-1 which corresponds to an aligned inclined crystal. (Also, when $\rho = -90^\circ$ we have the conventional asymmetric situation at low incidence angle with $\mathbf{b} = -\sin(\theta - \beta) / \sin(\theta + \beta)$).

We have used Eq.4 to obtain values for b and have used them to calculate values for the FWHM of the Darwin-Prins curves. Values for the FWHM were calculated by dividing FWHM values for symmetric diffraction by $|b|^{1/2}$. Values for Si $(11\bar{1})$ diffraction from a (111) surface at 5 KeV are shown in Fig. 2. For this situation $\beta = 70.529^\circ$ and $\theta = 23.292^\circ$. The same situation at 8 KeV is shown in Fig.3. Here $\theta = 14.221^\circ$. Finally, values for Si $(11\bar{1})$ diffraction for $\beta = 85^\circ$ at 5 KeV are shown in Fig.4. For this latter situation the surface is cut 14.471° from (111). We see that the Darwin width is very sensitive to ρ at large inclination angles.

III. Experimental Verification

We obtained rocking curves in a double crystal arrangement as a function of the azimuthal rotation, ρ ,of the second crystal. The first crystal was set for symmetric (111) diffraction on a tube source and remained stationary. The fixed anode was Cu and we used CuKα radiation at 8.04 KeV. The crystal that we used was float zone Si with a (111) oriented surface, and we made rocking curves for the $(11\bar{1})$ reflection of the second crystal . The results are shown in Fig. 3. Since the zero for ρ was somewhat arbitrary, we have adjusted the data by applying an arbitrary offset to the ρ values. The narrowest rocking curve which we obtained is shown in Fig.4 and had FWHM of 8.4 arcsec. This value is very close to the ideal Darwin-Prins value of 7.5 arcsec, and reveals that at large ρ the FWHM of the second crystal was only 3.8 arcsec since the quadrature addition of 7.5 arcsec for the first crystal and 3.8 arcsec for the second crystal yield the observed result of 8.4 arcsec. The other FWHM values plotted in Fig.3 were obtained in the same way, i.e., by subtracting in quadrature a value of 7.5 arcsec for the first crystal from the observed FWHM.

IV. Summary

Values both larger and smaller than the ideal Darwin-Prins FWHM were obtained by adjusting ρ in our experiments. This observation and the reasonable agreement between rocking curve data on the one hand and calculations on the other hand corroborate Eq. 4 .

Acknowledgements

We would like to acknowledge the considerable input of D.M. Mills concerning alignment issues for an inclined crystal monochromator.

[1] A.T. Macrander, W.K. Lee, R.K. Smither, D.M. Mills, S. Rogers, and A. Khounsary, . these proceedings

[2] W.H. Zachariasen, "Theory of X-ray Diffraction in Crystals", (Dover , NY, 1945).

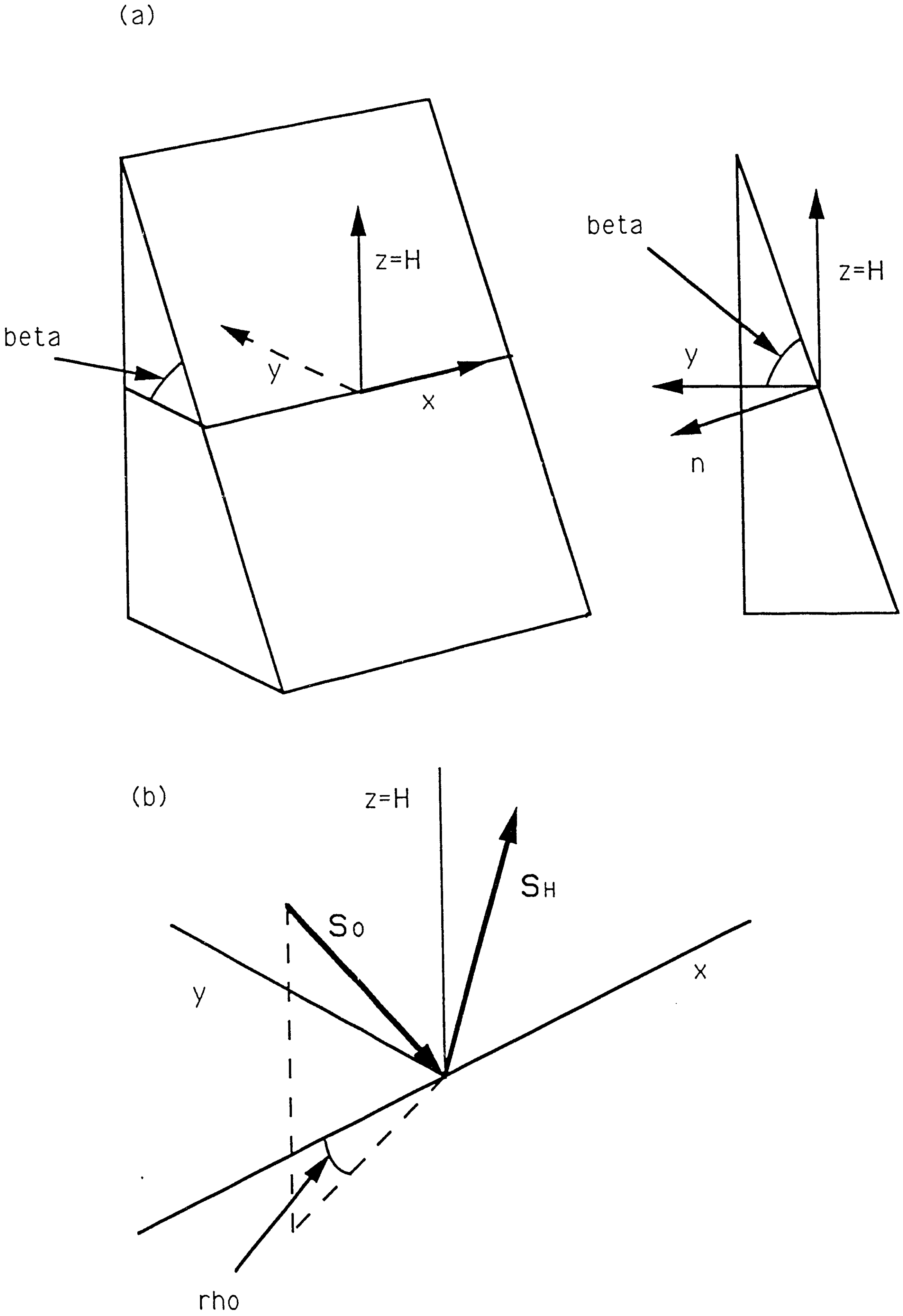
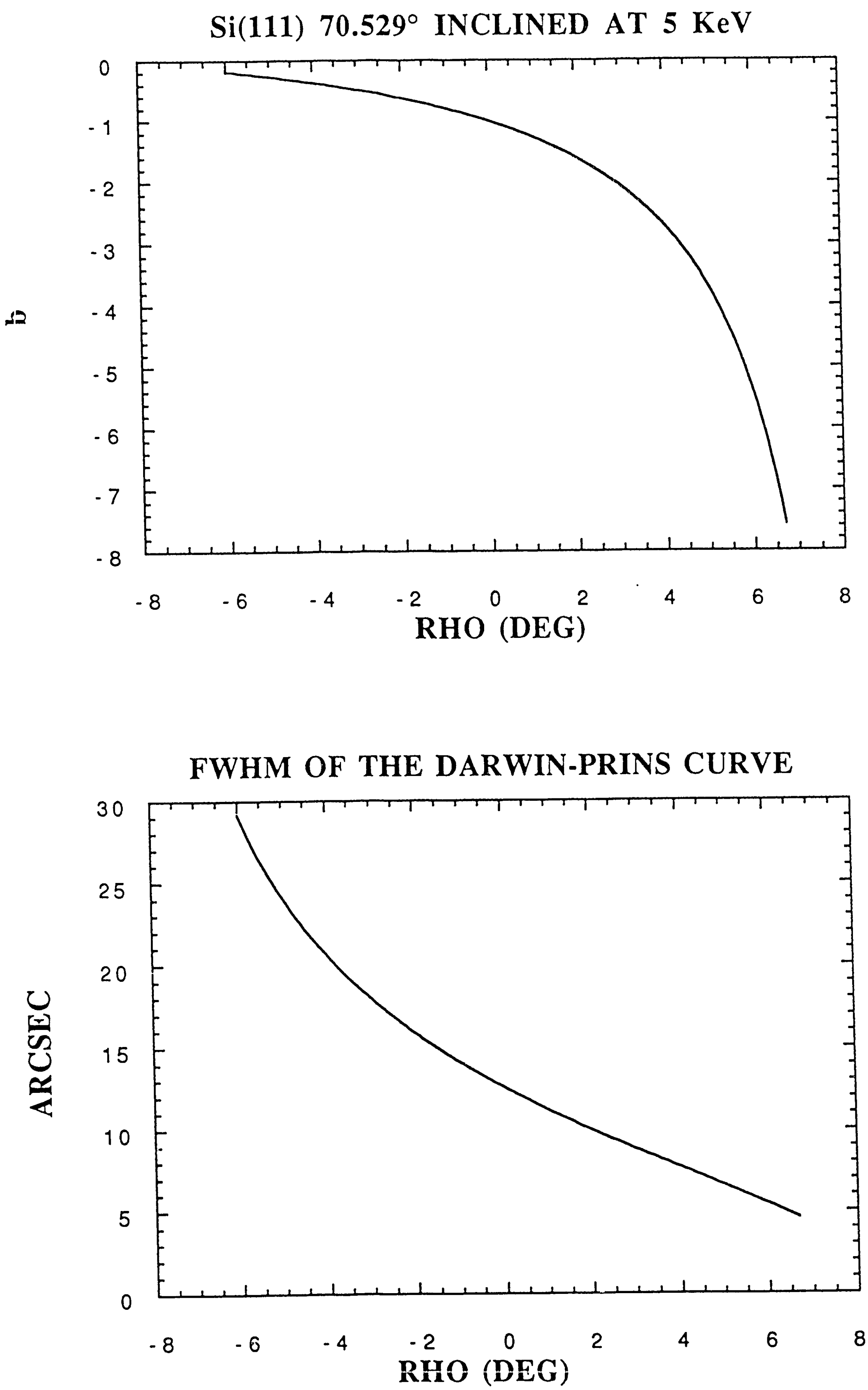


Fig.1



Si(111) 70.529° INCLINED AT 5 KeV
b
0
-1
-2
-3
-4
-5
-6
-7
-8
-8
-6
-4
-2
0
2
4
6
8
RHO (DEG)
FWHM OF THE DARWIN-PRINS CURVE
ARCSEC
30
25
20
15
10
5
0
-8
-6
-4
-2
0
2
4
6
8
RHO (DEG)

Fig. 2

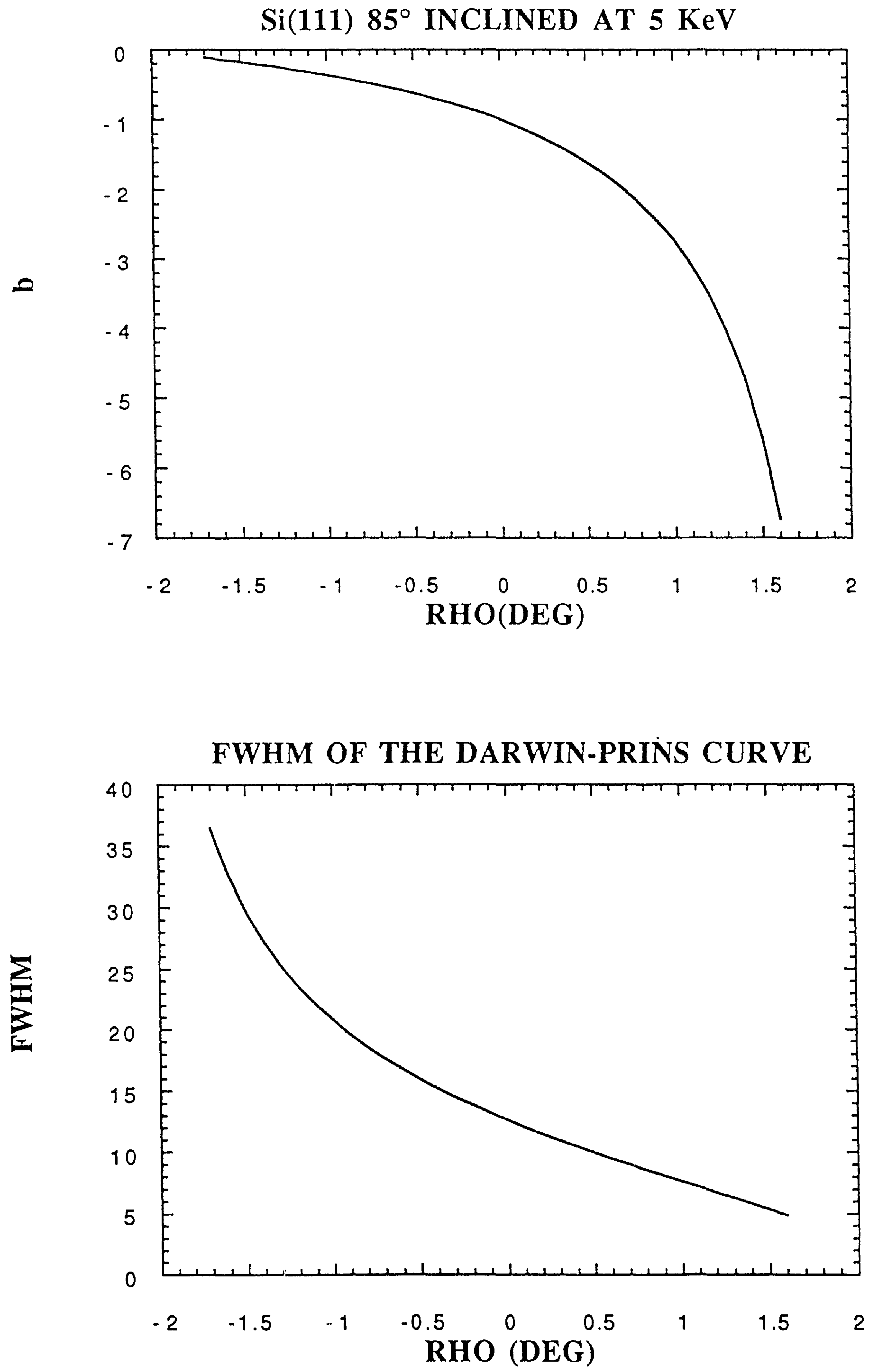
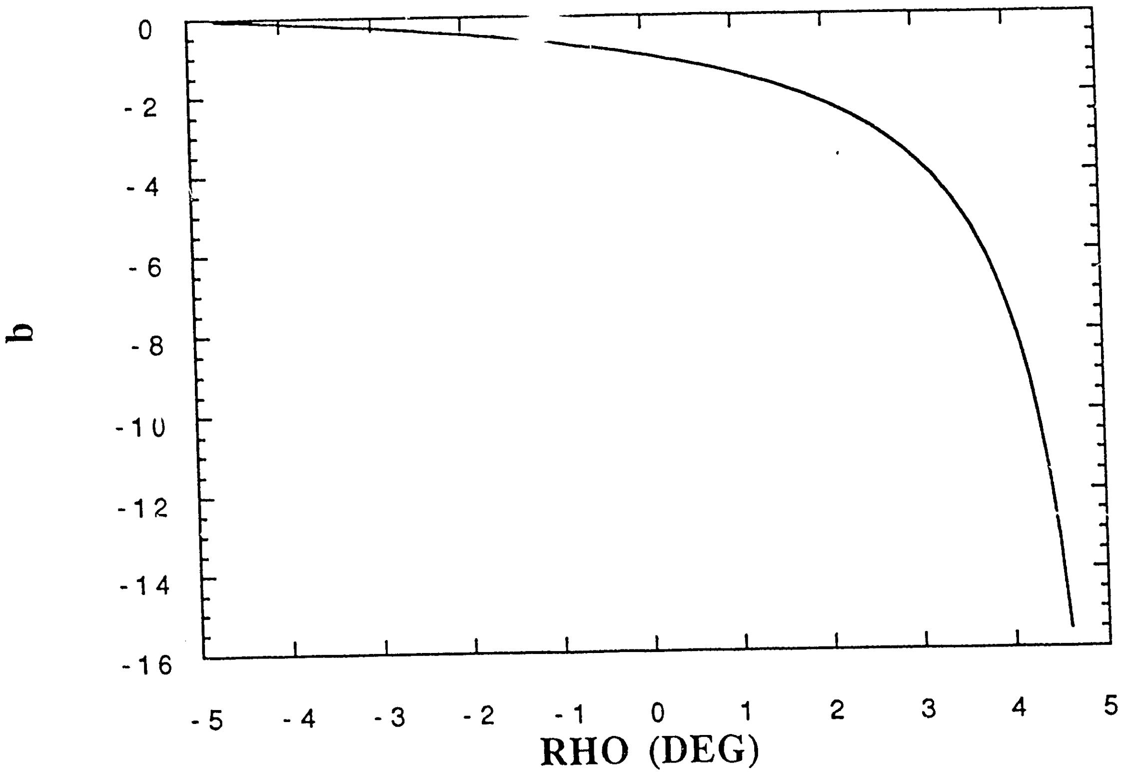

Si(111) 85° INCLINED AT 5 KeV
b
0
-1
-2
-3
-4
-5
-6
-7
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2
RHO(DEG)
FWHM OF THE DARWIN-PRINS CURVE
FWHM
40
35
30
25
20
15
10
5
0
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2
RHO (DEG)

Fig. 3

SI(111) 70.529° INCLINED AT 8 KEV



FWHM OF DARWIN-PRINS CURVE
AND 8 KEV DATA

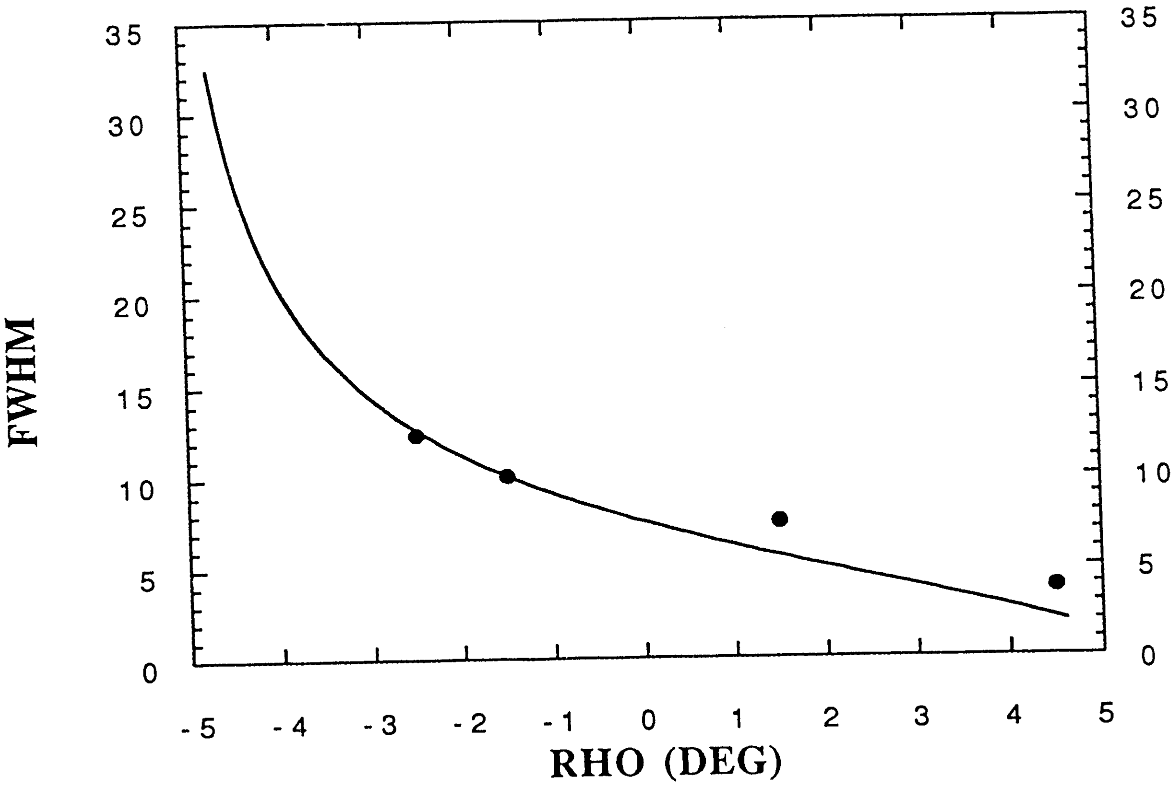


Fig. 4

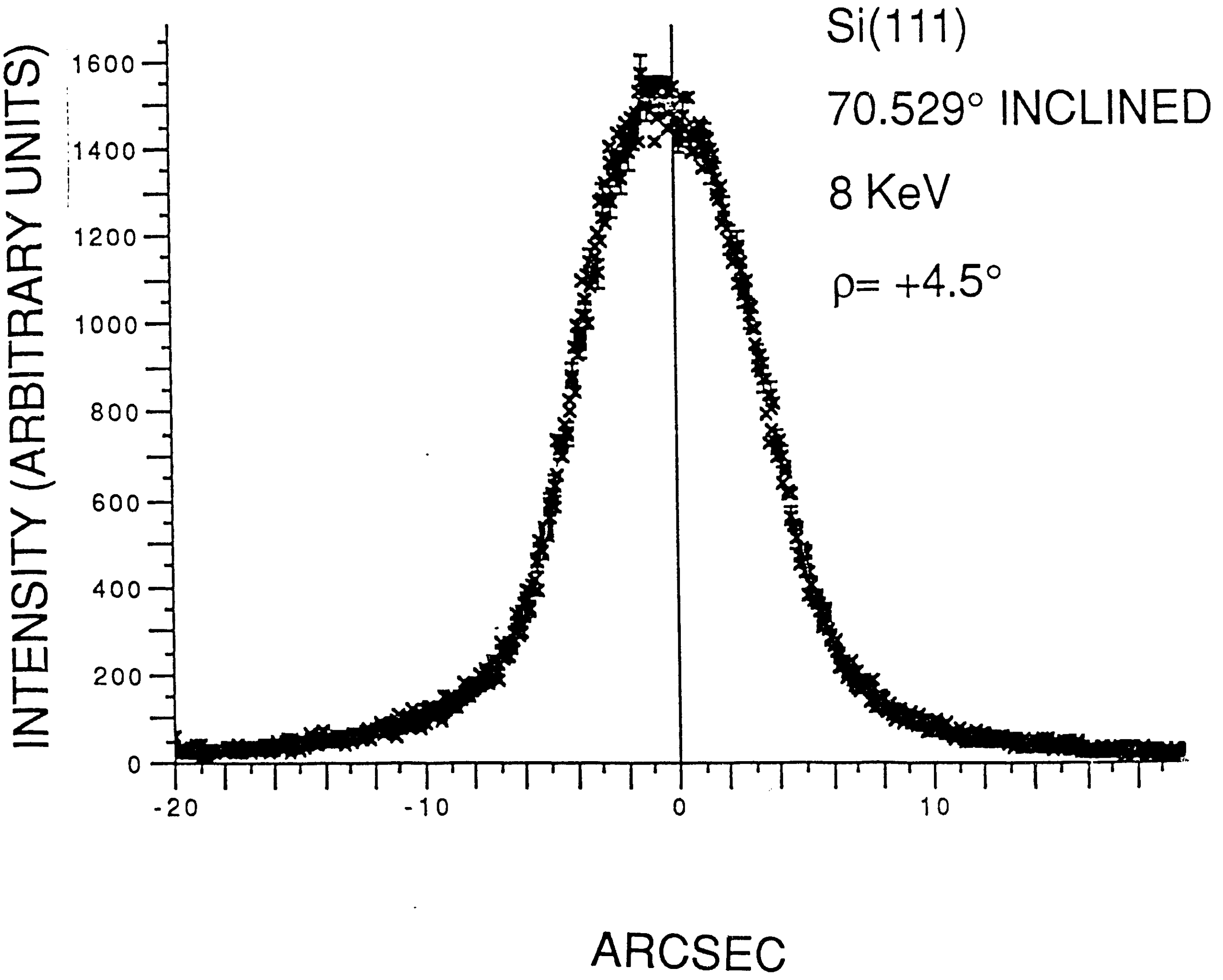

Si(111)
70.529° INCLINED
8 KeV
ρ= +4.5°
INTENSITY (ARBITRARY UNITS)
1600
1400
1200
1000
800
600
400
200
0
-20
-10
0
10
ARCSEC

Fig. 5

END

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