

Diamond Assessment Run at Chess 11/2007

10/31

2007

We now have a new asymmetric crystal monochromator installed in the beam line. Both crystals are cut from the same silicon sheet, as shown below.

Two asymmetric silicon(331) monochromator crystals

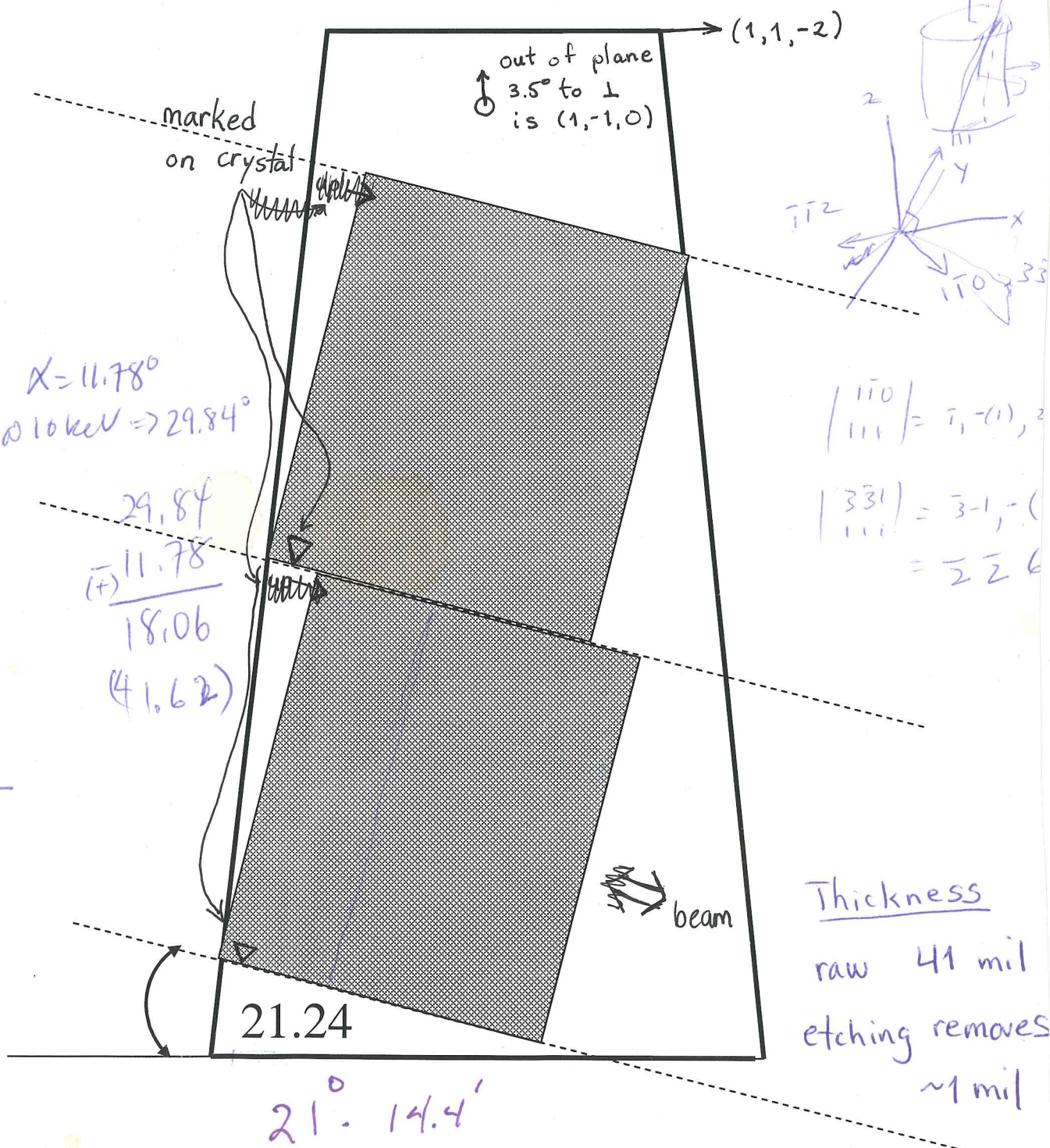
K.D. Finkelstein

10-05-07

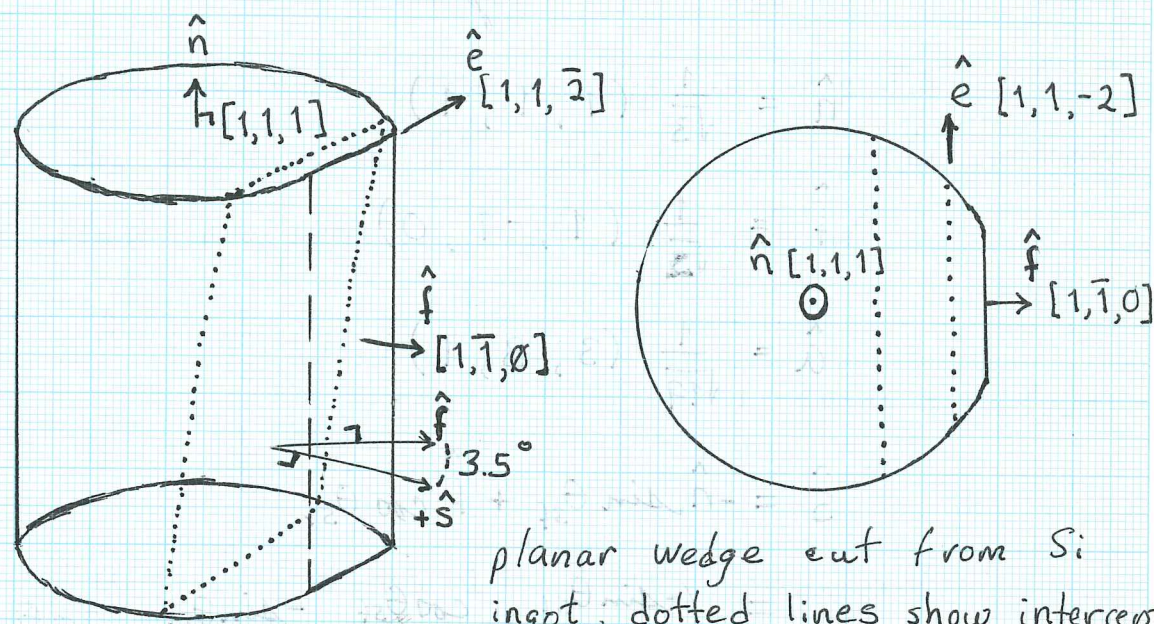
Cut 2 rectangular crystals out of one tall slice provided.

(Drawing is NOT to correct scale.)

Crystals have finished size 2" X 2.75" with 2" side along dashed lines. Position rectangles in the best way for cutting, & corners may be clipped. PLEASE MAINTAIN ORIENTATION SO WE KNOW WHAT SIDE IS "UP"!



The original wedge was cut from a 111 silicon ingot as shown below. The ingot is a cylinder with one flat side.



planar wedge cut from Si ingot; dotted lines show intercepts with the boundaries of the ingot

The planar wedge was cut so that the intercepts with the 111 planes at the ends of the cylinder form lines that are parallel to the flat edge, as shown. The tip angle away from the vertical is 3.5° as shown. The precision of this number is not stated, but is probably good to 0.1° or so.

Some definitions:

$\hat{a}$: direction normal to the 331 planes

$\hat{n}$: [1,1,1] unit vector

$\hat{f}$: [1,-1,0] unit vector

$\hat{s}$: normal to the crystal surface, defined such that $\hat{s} \cdot \hat{a} > 0$ but $\hat{s} \cdot \hat{f} \geq 0$.

$\hat{v}$: unit vector in plane of $\hat{s}$ and $\hat{a}$ such that $\hat{a} \cdot \hat{v} < 0$ and $\hat{s} \cdot \hat{v} = 0$, $\hat{v}$ is beam axis.

$\hat{u}$: unit vector $\hat{v} \times \hat{s}$

$\hat{e}$: unit vector $\hat{n} \times \hat{f} = [1, 1, 2]$

1. check the cut angle 21.24°

$$\hat{n} = \frac{1}{\sqrt{3}} (1, 1, 1)$$

$$\hat{f} = \frac{1}{\sqrt{2}} (1, -1, 0)$$

$$\hat{a} = \frac{1}{\sqrt{19}} (3, 3, 1)$$

$$\hat{s} = -\hat{n} \sin \theta_{sf} + \hat{f} \cos \theta_{sf}$$

$$= \left(\frac{-\sin \theta_{sf}}{\sqrt{3}} + \frac{\cos \theta_{sf}}{\sqrt{2}}, \frac{-\sin \theta_{sf}}{\sqrt{3}} - \frac{\cos \theta_{sf}}{\sqrt{2}}, \frac{-\sin \theta_{sf}}{\sqrt{3}} \right)$$

where I use angle notation θ_{ij} for the angle between directions i and j . I always take the angle θ_{ij} to be in the interval $[0, 180^\circ]$. Furthermore, let

$$S_{ij} \equiv \sin \theta_{ij} \quad \text{and} \quad C_{ij} = \cos \theta_{ij}$$

Then the cut angle above is θ_{eu}

$$\hat{v} = \alpha \hat{s} - \beta \hat{a} \quad \text{with} \quad \hat{v} \cdot \hat{s} = 0 \Rightarrow \alpha = \beta \cos \theta_{as}$$

$$= \beta (\hat{s} \cos \theta_{as} - \hat{a})$$

$$\hat{v} \cdot \hat{v} = \beta^2 (1 - \cos^2 \theta_{as}) = (\pm \beta \sin \theta_{as})^2$$

choosing $\beta > 0$ to ensure that $\hat{a} \cdot \hat{v} < 0$ gives

$$\hat{v} = \frac{1}{\sin \theta_{as}} (\hat{s} \cos \theta_{as} - \hat{a})$$

$$= \frac{1}{\sqrt{19} \sin \theta_{as}} \left(\left[\frac{-S_{sf}}{\sqrt{3}} + \frac{C_{sf}}{\sqrt{2}} \right] C_{as} - \frac{3}{\sqrt{19}}, \left[\frac{-S_{sf}}{\sqrt{3}} - \frac{C_{sf}}{\sqrt{2}} \right] C_{as} - \frac{3}{\sqrt{19}}, \frac{-S_{sf} C_{as}}{\sqrt{3}} - \frac{1}{\sqrt{19}} \right)$$

$$= \frac{1}{S_{as}} \left(\left[\frac{-S_{sf}}{\sqrt{3}} + \frac{C_{sf}}{\sqrt{2}} \right] C_{as} - \frac{3}{\sqrt{19}}, \left[\frac{-S_{sf}}{\sqrt{3}} - \frac{C_{sf}}{\sqrt{2}} \right] C_{as} - \frac{3}{\sqrt{19}}, \frac{-S_{sf} C_{as}}{\sqrt{3}} - \frac{1}{\sqrt{19}} \right)$$

The angle θ_{as} is the asymmetry angle for the crystal

$$\cos \theta_{as} = \hat{a} \cdot \hat{s} = \frac{-1}{\sqrt{19}} \left(\frac{7}{\sqrt{3}} S_{sf} \right) = -\sqrt{\frac{49}{57}} \sin \theta_{sf}$$

Obviously this is wrong! because θ_{sf} is only 3.5° which would put θ_{as} close to 90° . Let see if another variation on crystal plane assignments might be found.

$$\left. \begin{aligned} \hat{n} &= \frac{1}{\sqrt{3}} (1, 1, 1) \\ \hat{f} &= \frac{1}{\sqrt{2}} (1, -1, 0) \end{aligned} \right\} \text{ same as above}$$

$$\hat{a} = \frac{1}{\sqrt{19}} (-3, +3, -1) \leftarrow \text{changed!}$$

$$\begin{aligned} \hat{s} &= -\hat{n} S_{sf} + \hat{f} C_{sf} \\ &= \left(-\frac{S_{sf}}{\sqrt{3}} + \frac{C_{sf}}{\sqrt{2}}, -\frac{S_{sf}}{\sqrt{3}} - \frac{C_{sf}}{\sqrt{2}}, -\frac{S_{sf}}{\sqrt{3}} \right) \end{aligned} \quad (\text{same as above})$$

$$\hat{a} \cdot \hat{s} = \frac{1}{\sqrt{19}} \left(\frac{S_{sf}}{\sqrt{3}} - \frac{6}{\sqrt{2}} C_{sf} \right) = \frac{S_{sf}}{\sqrt{57}} - \sqrt{\frac{36}{38}} C_{sf}$$

This should be positive, so I again change my choice of $\hat{a}$.

$$\hat{a} = \frac{1}{\sqrt{19}} (+3, -3, 1) \leftarrow \text{changed again!}$$

$$\hat{a} \cdot \hat{s} = \sqrt{\frac{36}{38}} C_{sf} - \frac{1}{\sqrt{57}} S_{sf} = \sqrt{\frac{18}{19}} C_{sf} - \frac{1}{\sqrt{57}} S_{sf}$$

$$= 0.963427, \quad \theta_{as} = 15.54^\circ \leftarrow \text{not what Ken has}$$

But if $\hat{a} = \frac{1}{\sqrt{19}} (+3, -3, -1) \leftarrow \text{changed again!}$

$$\hat{a} \cdot \hat{s} = \sqrt{\frac{18}{19}} C_{sf} + \frac{1}{\sqrt{57}} S_{sf} = 0.97960$$

$$\theta_{as} = 11.59^\circ \leftarrow \text{this is what Ken has!}$$

So the cut angle is θ_{eu}

$$\begin{aligned} c_{eu} &= \hat{e} \cdot \hat{u} = -\hat{e} \cdot (\hat{s} \times \hat{v}) \\ &= -\hat{e} \cdot \left(\hat{s} \times \left(\frac{\hat{s} c_{as} - \hat{a}}{s_{as}} \right) \right) \\ &= \frac{1}{s_{as}} (\hat{e} \cdot \hat{s} \times \hat{a}) \end{aligned}$$

$$\hat{s} \times \hat{a} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{s_{sf}}{\sqrt{3}} - \frac{c_{sf}}{\sqrt{2}} & \frac{s_{sf}}{\sqrt{3}} + \frac{c_{sf}}{\sqrt{2}} & \frac{s_{sf}}{\sqrt{3}} \\ +3 & -3 & -1 \end{vmatrix} \quad \frac{1}{\sqrt{19}} \quad \frac{\hat{s}}{s_{as}}$$

$$= -\frac{1}{\sqrt{19}} \left(+\frac{2}{\sqrt{3}} s_{sf} - \frac{c_{sf}}{\sqrt{2}}, +\frac{4}{\sqrt{3}} s_{sf} - \frac{c_{sf}}{\sqrt{2}}, +\frac{6}{\sqrt{3}} s_{sf} \right)$$

$$c_{eu} = \frac{1}{\sqrt{6}\sqrt{19}s_{as}} \left(-\frac{18}{\sqrt{3}} s_{sf} + \frac{2}{\sqrt{2}} c_{sf} \right) \leftarrow \text{see p. 130}$$

$$N = 10.953548, \theta_{eu} = \begin{cases} 102.47^\circ \\ 197.53^\circ \end{cases}$$

~~$180^\circ - \theta_{eu} = 17.53^\circ$, then's value is about 49~~

He verified that in his notes: a ϕ displacement of $\sim 4^\circ$ was needed to put the scattering plane into the vertical plane.

11/01

2007

after some more searching, we found what we think is the 331 reflection of the monochromator. A "burn" of the beam spot is shown below. There is a large low-intensity spot and a second more intense stripe through the middle.



I think that the large square is 15 keV X-rays from the $\bar{3}3\bar{1}$ reflection, and the central stripe is from another Laue spot that happens to fall nearly in angle. These crystals are very large, so "nearly" is not a very stringent requirement. The fact that it is so short indicates that the angle must be fairly large and give a b-factor not so different from 1.

Now that I think of it, what possibly keeps us from seeing all of the Laue spots in the upper hemisphere? These crystals are very large. Of course, only the 15 keV component will diffract off the diamond, so maybe we don't really care.

Still, it would be nice to have a clean monochromatic beam to work with.

* We aligned the second monochromator crystal by fixing the first in its nominal position and then rocking the second one in θ and χ ("tilt").

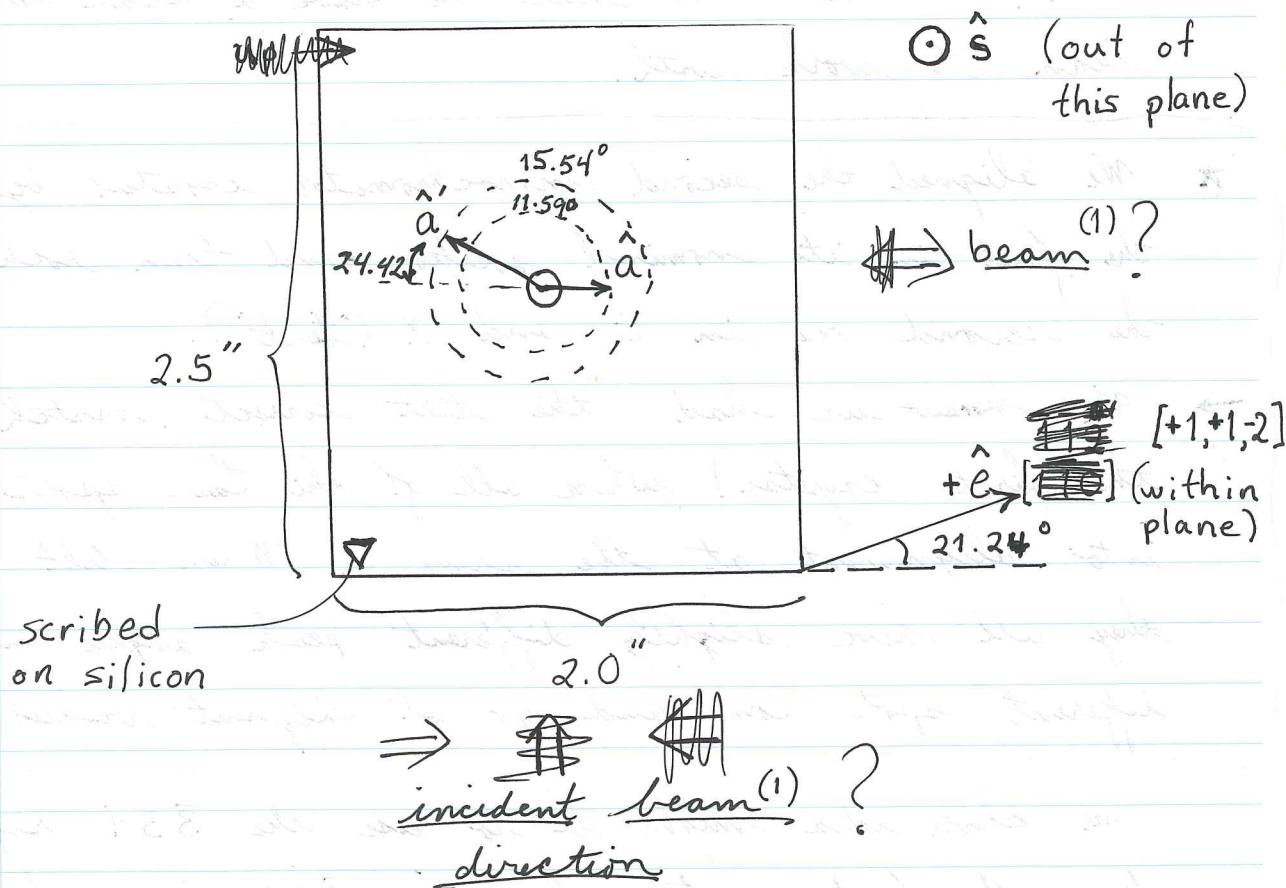
→ We knew we had the tilt correct (match to the first crystal) when all of the Laue spots came into alignment at the same θ . When tilt is off they all have slightly different peak angles and the different spots come and go at different values of θ .

One clever idea might be to use the $\bar{3}3\bar{1}$ reflection from the first crystal, but the $\bar{3}31$ from the second and get rid of all of the other energies that come from other Laue peaks. Lets try it.

$$\left\{ \begin{array}{l} \hat{a} = \frac{1}{\sqrt{19}} (+3, -3, -1) : @ 15 \text{ keV } \theta_B = 19.52^\circ \\ \Rightarrow \beta = 7.93^\circ, b = 3.75 \\ \hat{a}' = \frac{1}{\sqrt{19}} (+3, -3, +1) : \beta = 3.98^\circ, b = 8.28 \end{array} \right.$$

We will lose another factor ~ 2 in intensity, but the beam will be essentially pure 331 radiation and the spot image will be what the diamond will "see".

One change is that the ϕ angle must be changed quite a lot. In terms of the wafer cut as shown on p. 123, the following image shows the projections of $\hat{a}$ and $\hat{a}'$ onto the machined surface of the crystal.



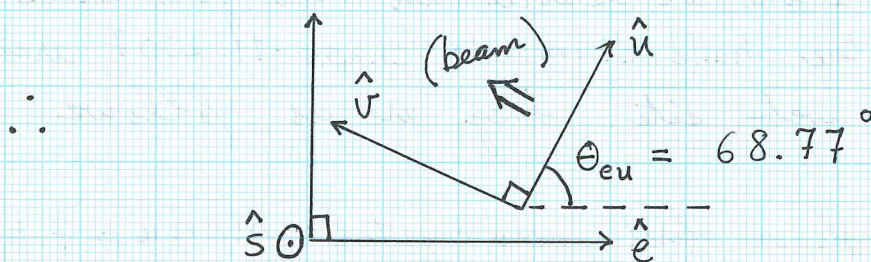
¹ See p. 132-133 for the answer to this conundrum.

To find the beam direction, I reprise here the calculation from p. 127 where I went wrong.

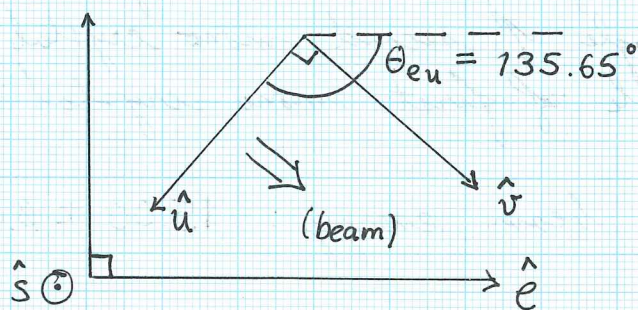
$$\begin{aligned}
 \hat{u} \cdot \hat{e} &= (\hat{v} \times \hat{s}) \cdot \hat{e} = \frac{1}{\sin \theta_{as}} (\hat{e} \cdot \hat{s} \times \hat{a}) \\
 &= \begin{vmatrix} 1 & 1 & -2 \\ -\frac{S_{sf}}{\sqrt{3}} + \frac{C_{sf}}{\sqrt{2}} & -\frac{S_{sf}}{\sqrt{3}} - \frac{C_{sf}}{\sqrt{2}} & -\frac{S_{sf}}{\sqrt{3}} \\ 3 & -3 & -1 \end{vmatrix} \frac{1}{\sqrt{19} \sqrt{6} S_{as}} \\
 &= \frac{1}{\sqrt{19} \sqrt{6} S_{as}} \left\{ -\frac{2}{\sqrt{3}} S_{sf} + \frac{C_{sf}}{\sqrt{2}} - \frac{4}{\sqrt{3}} S_{sf} + \frac{C_{sf}}{\sqrt{2}} - \frac{12}{\sqrt{3}} S_{sf} \right\} \\
 &= \frac{1}{\sqrt{19} \sqrt{6} S_{as}} \left(-\frac{18}{\sqrt{3}} S_{sf} + \frac{2}{\sqrt{2}} C_{sf} \right) = 0.362188
 \end{aligned}$$

To resolve the direction, I need the sign of

$$\begin{aligned}
 \hat{v} \cdot \hat{e} &= \frac{1}{\sin \theta_{as}} (\hat{e} \cdot \hat{s} C_{as} - \hat{e} \cdot \hat{a}) \\
 &= \frac{1}{S_{as}} \left\{ \frac{C_{as}}{\sqrt{6}} (0) - \frac{1}{\sqrt{6}} \frac{1}{\sqrt{19}} 2 \right\} < 0
 \end{aligned}$$



then if I replace $\hat{a} \rightarrow \hat{a}$ then the angles change.



Nov. 3
2007

There seems to be some disagreement about the direction the beam is supposed to be going in this figure. I say it should be going along $\hat{v}$ and Ken showed me that it is actually going contrary to $\hat{v}$, according to the scribe marks on the crystal.

see note
on facing
page

I guess I will just assume that it is a reverse sign convention on the notation $(h k l)$ for a particular reflection. If the crystallographers use the opposite convention from me then all of my results carry over, except that $\hat{f}, \hat{e}, \hat{n}$ is a left-handed coordinate system, the vector $\hat{e}$ of a particular reflection points along $\hat{k} - \hat{k}'$ instead of $\hat{k}' - \hat{k}$, my convention. Then we are in agreement. This seems plausible; all other alternatives are ruled out or unlikely based on the good agreement of measured and expected X-ray energy of $15.00 \text{ keV} \pm .05 \text{ keV}$

I worked out the relations of the monochromator. The calculations are saved in the file chess-11-2007.xls on the hald/diamonds/chess-11-2007 area of the group web site. They are as follows.

incidence angle on first mono crystal: $\text{monu} = 7.683^\circ \pm 0.1^\circ$
tip angle θ of 2nd " " : $\text{mond} = 31.133^\circ \pm 0.1^\circ$
azimuthal angle of first mono crystal: (no motor) = $4^\circ \pm 1^\circ$
azimuthal angle of second mono crystal: $\text{mp2} =$
tilt angle of second mono crystal: $\text{tilt} =$
tilt angle of first mono crystal: (no motor) = $0^\circ \pm .1^\circ$

Selected beam energy: $15.00 \pm 0.08 \text{ KeV}$

Note: The sign convention hypothesis is not valid. If I reverse the sense of any of the given planes then the r.h. coordinate system convention I use for $(\hat{f}, \hat{e}, \hat{n})$ will continue to ensure that any physical predictions I make from this analysis remain valid.

Example 1: let $\hat{f} \rightarrow -\hat{f}$ but $\hat{n} \rightarrow -\hat{n}$ also

then $\hat{e} \rightarrow +\hat{e}$ (r.h. coordinates)

$$\hat{s} \rightarrow -\hat{f} c_{sf} + \hat{n} s_{sf} = -\hat{s}$$

$$\hat{a} \rightarrow -\hat{a}, \quad \hat{s} \cdot \hat{a} \text{ invariant}$$

$$\hat{u} = \hat{v} \times \hat{s} \rightarrow +\hat{u}, \quad \underline{\hat{v} \rightarrow -\hat{v}!}$$

So that $\hat{e} \cdot \hat{u}$ is invariant

and $\hat{e} \cdot \hat{v} \rightarrow +\hat{e} \cdot \hat{v}$ is not invariant

ambiguous
orientation
specification
?

Example 2: let $\hat{f} \rightarrow +\hat{f}$ but $\hat{n} \rightarrow -\hat{n}$ this time

then $\hat{e} \rightarrow -\hat{e}$

$$\hat{s} \rightarrow \cancel{\hat{s}} + \hat{f} c_{sf} + \hat{n} s_{sf} \equiv +\hat{s}'$$

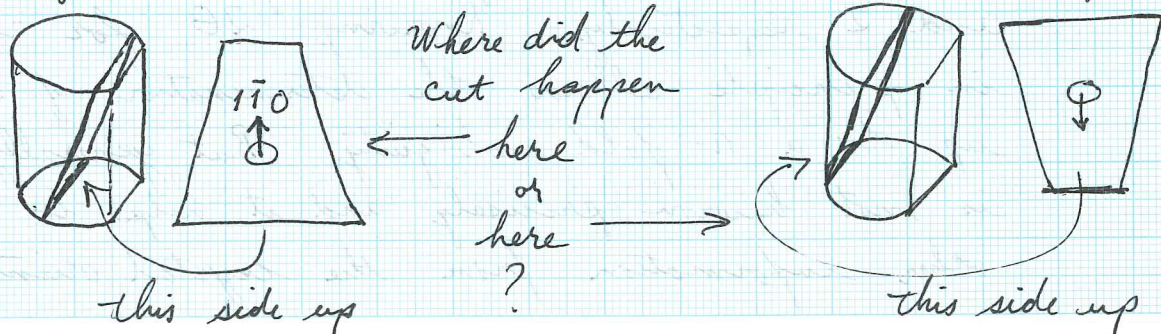
$$\hat{a} \rightarrow +\hat{a}', \quad \hat{a}' \rightarrow +\hat{a} \text{ (exchange these)}$$

$$\hat{u} = \hat{v} \times \hat{s} = \frac{1}{s_{as}} (\hat{s} \times \hat{a}) = \frac{1}{s_{as}} (\hat{s}' \times \hat{a}')$$

$\Rightarrow \hat{u}' \leftarrow$ checked in $\hat{f}, \hat{e}, \hat{n}$ basis

$$\hat{v} = \hat{s} \times \hat{u} \rightarrow \hat{s}' \times \hat{u}' = \hat{v}'$$

So Example 2 merely exchanges the two solutions $\hat{a}$ and $\hat{a}'$ while Example 1 identifies a new ambiguity in the spec. of the crystal orientation that I did not notice before.



This ambiguity is exemplified by example 1. It proves the opposite from what I wanted it to! One cannot tell by looking at the indicator on the surface of the wedge which side of the wedge we are looking at. Which side does make a difference; the two sides are not equivalent. I was unlucky to choose the wrong possibility and think I had proved Ken has mis-oriented the crystal. The ability to get a good beam in this orientation shows Ken has the right choice.

11/5/2007 Finding the orientation of a new diamond

I decided to work out a general procedure to determine the crystal orientation of a new diamond. To do it, I need 2 independent diffraction peaks with measured goniometer settings. The peaks must be oriented in the vertical scattering plane. Under these conditions, it can be done.

Let R_x : rotation operator from crystal frame to goniometer zero reference frame
 R_1 : rotation from goniometer zero frame to the lab frame with the crystal oriented to diffract at peak 1
 R_2 : same as R_1 , for peak 2.

Let $\vec{g}_1, \vec{g}_2$ be the two momentum vectors that are responsible for the diffraction at peaks 1 and 2 respectively. Knowing 2θ for each peak in principle allows the determination of $\vec{g}_1$ and $\vec{g}_2$ up to a n -fold ambiguity. But generally 2θ is not known precisely and it helps to have other information from the crystal orientation.

Let $\vec{q}_1, \vec{q}_2$ be the crystal momentum vectors that correspond to $\vec{g}_1$ and $\vec{g}_2$.

$$\vec{g}_1 = R_1 R_x \vec{q}_1 \quad \text{and} \quad \vec{g}_2 = R_2 R_x \vec{q}_2$$

R_x is unknown but we can solve for it. Define

$$\vec{p}_1 = R_1^{-1} \vec{g}_1 \quad \text{and} \quad \vec{p}_2 = R_2^{-1} \vec{g}_2$$

Both $\vec{p}_1$ and $\vec{p}_2$ are known or can be guessed by hypothesis. One can then check it as follows

$$\vec{p}_1 \cdot \vec{p}_2 = \vec{q}_1 \cdot \vec{q}_2 \quad \text{if the hypothesis is correct}$$

This is an accurate check because R_1 and R_2 are measured very precisely. We do not need to know the absolute goniometer position because the goniometer offsets are common to R_1 and R_2 and can be buried inside R_x . It is then easy to solve for R_x by solving simultaneously

$$\vec{p}_1 = R_x \vec{q}_1 \quad \text{and} \quad \vec{p}_2 = R_x \vec{q}_2$$

Knowing R_x , we can then find a goniometer setting when the crystal is in a normal orientation and read off the crystal axis directions $\hat{a}_1, \hat{a}_2, \hat{a}_3$ in the lab as $\hat{u}_1, \hat{u}_2, \hat{u}_3$

$$\hat{u}_i = R_0 R_x \hat{a}_i$$

where R_0 is the goniometer rotation that puts the crystal in some known orientation with respect to its faces and edges in the lab frame.

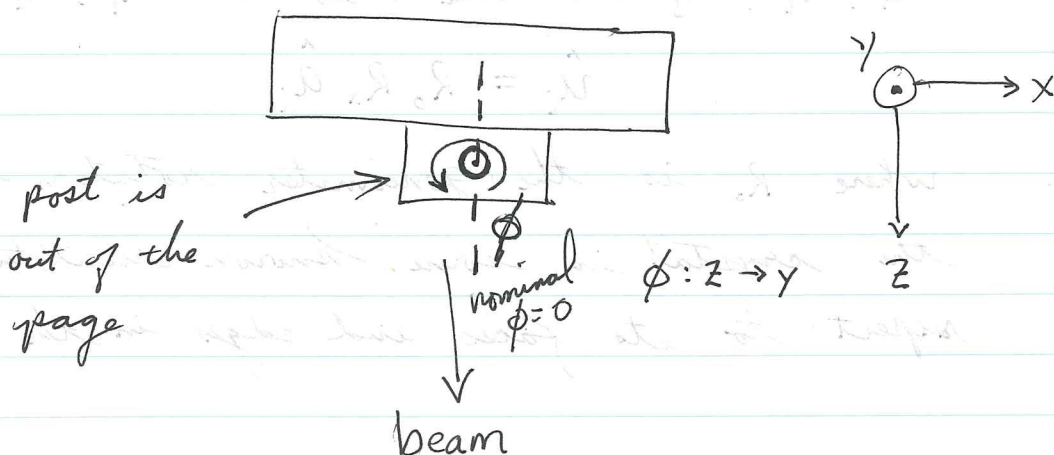
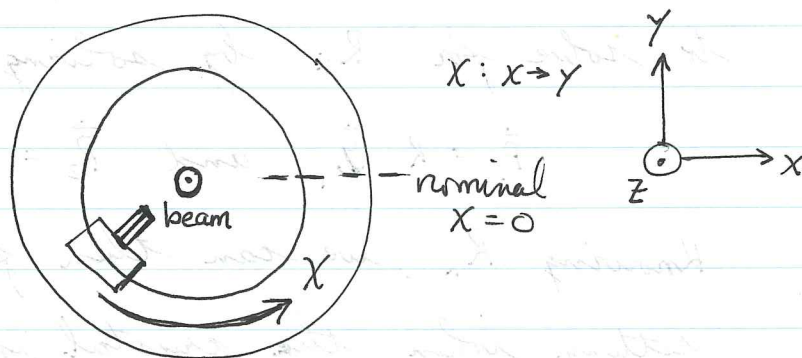
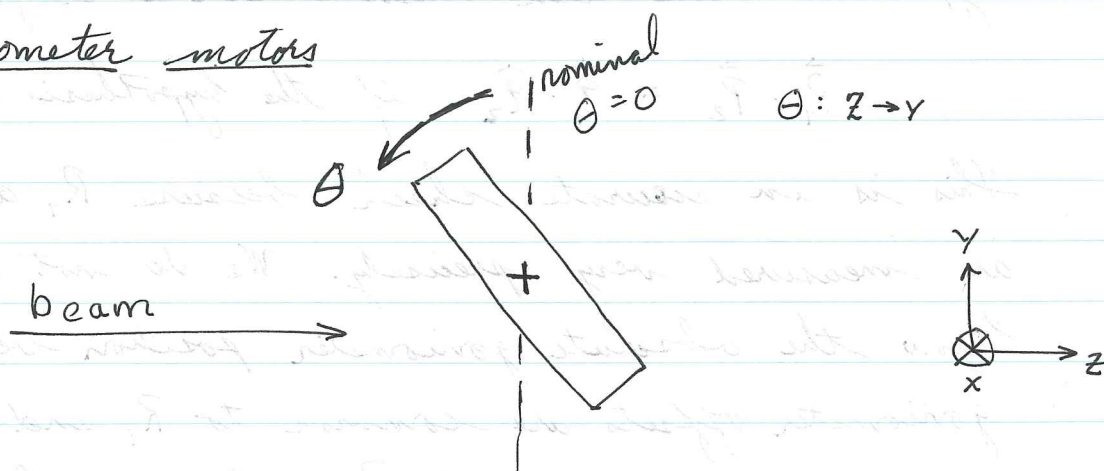
11/6/2007

all of this has been coded up and is found in the program

axisfinder.cpp

The program is in C++. It has a full set of test functions inside that validate its computation modules. I saved a copy of it in ~/physics/kinematics/Bragg

Soniometer motors



The goniometer is controlled from a machine c1.chess.cornell.edu using a program called spec. This has many commands and features. The most common are

SPEC/FOURC Cheat Sheet - (K. Finkelstein 12/20/06)

Bold=>commands (all commands use lower case letters except the E in section 4)

Italics=>arguments

(FOURC: type FOURC in place of SPEC)

1) Getting Started from the UNIX Shell

Command	Definition
%spec	Start SPEC program
SPEC>^d	Exit SPEC
SPEC>startup	Self guided macro for setting up to use SPEC
SPEC>config	For access to the config. file

Configuration File Structure:

Pg 1	Motor Definitions	(See operator)
Pg 2	Used by staff only	(See operator)
Pg 3	Used by staff only	(See operator)
Pg 4	Counters/Timers	(See operator)

To define monitor scaler:

SPEC>**mon**=*chosen monitor mnumonic*

To define timer scaler:

SPEC>**det**=*chosen detector mnumonic*

SPEC>**counters**

Command returns name and # of each counter and lets user assign mon, det

2) Moving motors and counting (*mn*=>a motor mnumonic, *#*=>a number)

SPEC> mv <i>mn #</i>	Moves motor <i>mn</i> to position <i>#</i>
SPEC> mvr <i>mn #</i>	Move motor <i>mn</i> a distance <i>#</i>
SPEC> tw <i>mn #</i>	Tweek motor <i>mn</i> in <i>#</i> user unit steps
SPEC> ct <i>±#</i>	Count all detector signal for: + <i>#</i> => time in sec., - <i>#</i> => number of monitor counts

3) Scanning with motors (*s*=starting point, *f*=finishing point, *int*=steps)

Scan between absolute motor positions

SPEC> ascan <i>mn s f int ±cts</i>	Scan with one motor
SPEC> a2scan <i>mn1 s1 f1 mn2 s2 f2 int ±cts</i>	Scan with two motors
SPEC> a3scan similar arguments	Scan with three motors

Scan relative to the start position and then return

SPEC> dscan or d2scan or d3scan	(Same syntax as ascans)
--	-------------------------

Other types of scans

SPEC> mesh <i>mn1 s1 f1 int mn2 s2 f2 int ±cts</i>	Mesh or nested scans
FOURC> th2th <i>s f int ±cts</i>	Theta-twotheta scan with twotheta in relative units

Controlling scans

SPEC>^c	Stops the scan in progress
SPEC> scan_on	Restarts scan from stop

4) Monochromator macros

SPEC> get_E	Displays Mono energy in KeV
SPEC> move_E <i>#</i>	Moves mono to energy <i>#</i> KeV
SPEC> set_E <i>#</i>	Defines mono energy to be <i>#</i> KeV
SPEC> Escan <i>s f int ±cts</i>	Scans energy from <i>s</i> to <i>f</i> in <i>int</i> steps
FOURC> Escan <i>s f int ±cts (fixQ)</i>	Scan energy (at fixed sample Q)

5) Getting and setting motor positions

Each motor has 2 defined positions:

DIAL POSITION & USER POSITION = ($\pm$ DIAL POSITION) + offset

SPEC> wm <i>mn1, mn2, ..., mn6</i>	Lists information on 1-6 motors
SPEC> wa , or we	Lists all motors positions
SPEC> lm	Lists limits and positions
FOURC> wh	Lists 4-circle angles

The next two macros change the offset in performing their tasks

SPEC> set mn #	Set motor mn to USER position = #
SPEC> set_dial mn #	Set motor mn to DIAL position = #
SPEC> set_lm mn low high	Set the USER low & high limits of motor mn

6) Other useful macros

SPEC> history	Displays a list of previous commands
SPEC> !!	Repeat last command
SPEC> !-5	Repeat 5 th command back in the list
SPEC> !-10	Repeat 10 th command in history
SPEC> !xxx (xxx=first few letters of a previous command)	Repeat that command
SPEC> !dscan	Will repeat last dscan defined

7) Macros

Optical table position/angle are moved with table macros.
See www.chess.cornell.edu/spec/optical.htm or ask operator.

Example 1

SPEC> def 2up 'mvr m1 a;mvr m2 b'	Define a macro called 2up that moves m1 by +a units and m2 by +b units
SPEC> 2up	Executes the macro 2up

Example 2

SPEC> def step2 'mvr th \$1;mvr tth \$2'	Step2 Define macro with 2 arguments input as follows:
SPEC> step2 2.5 5.0	Executes the macro that moves th +2.5 and tth +5.0 units

Data Files

SPEC (and **FOURC**) create ascii data files with the file names assigned when the **STARTUP** macro is run. (You can name and begin a new file by typing **newfile**.)

Unless otherwise specified, each scan is appended to the data file. In the data file each scan begins with a header containing motor positions and other information about the experiment. This is followed by recorded values of motors and counters at each step in the scan.

We offer several ways to examine the data files:

cplot is a powerful command line driven program that can be opened in a new window by typing **cplot**. A manual for CPlot is available at each station or from the CHESS operator. The program can produce publication quality output, but is not user friendly for those with little UNIX experience.

newplot (typed at the command line) is a simple GUI based program for examining and comparing scans. It has a number of built in functions for visualization and for limited analysis.

spec data files can also be copied to your own computer for further analysis.