HIGH RESOLUTION MONOCHROMATOR SYSTEMS
USING THERMAL GRADIENT INDUCED VARIABLE BRAGG SPACING*

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CONF-850734--5

July 1985

DE85 018446

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*Work supported by the U. S. Department of Energy

Submitted to the International Conference on Synchrotron Radiation
Instrumentation, Stanford, CA, July 29-August 2, 1985.

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Abstract

The vertical divergences of bending magnet and wiggler synchrotron sources are generally considerably larger than the acceptance angles of typical monochromator systems. This is particularly true at high energies ($E \geq 14$ keV) where the Darwin widths of perfect crystals are of the order 10^{-6} radians. By imposing a thermal gradient on the crystal, an efficient, wide acceptance angle monochromator can be obtained. The necessary condition being that the resulting $d \cdot \sin\theta$ is a constant across the beam. Gains in intensity of 3-100 can be realized relative to standard flat crystal systems. A number of possible designs are presented for both two and four crystal monochromator systems. The use of Si, Ge, and quartz monochromators are discussed.

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Variable d-spacing monochromators offer some interesting possibilities for the designer of x-ray optical systems. The variable spacing can be achieved in a number of ways including doping, strain, and thermal gradients.¹ The use of thermal gradients seems to be the simplest and most precise method. By proper application of a thermal gradient it is possible to match the acceptance angles of the monochromator to the vertical divergence of a synchrotron beam. Previously Smither¹ has discussed the use of thermal gradients for both flat and curved monochromator systems. We apply the ideas to certain synchrotron applications.

Darwin widths of perfect single crystals are quite small, varying from 5×10^{-5} to 10^{-6} radians, (1 sec to 0.2 sec) depending on the energy and orientation of the crystals. The magnitude of the vertical opening angle, $\Delta\theta$, of bending magnet and wiggler beams is $1/\gamma$ where γ is the ratio of the beam energy to the rest mass energy of the electron. For the National Synchrotron Light Source (NSLS) this is approximately 2×10^{-4} radians.

In fig. 1 we show a diagram of a two crystal beam line where thermal gradients have been applied to both crystals, ("A" and "B"). The crystals have a thermal expansion coefficient of " α " so that

$$\frac{\Delta d}{d} = \alpha \Delta T \quad (1)$$

where d is the Bragg spacing, Δd the change in the Bragg spacing and ΔT is the variation of temperature across the beam. Combining Eq. 1 with Bragg's law we get

$$\Delta T = \frac{1}{\alpha} \frac{\Delta d}{d} = \frac{1}{\alpha} \cot \theta \Delta \theta \quad (2)$$

*Work supported by the U. S. Department of Energy.

The acceptance angles of the crystals will match the vertical divergence of the beam if eq. 2 is satisfied.

The heat, W , necessary to impose this gradient is

$$W = KA \frac{\Delta T}{\Delta l} \quad (3)$$

where K is the thermal conductivity of the crystal, A is the cross section area, and Δl is the length of the beam across the crystal. If the source is a distance L from the crystal then

$$\Delta l = \frac{L \Delta \theta}{\sin \theta} \quad (4)$$

By substitution we get

$$\frac{\Delta T}{\Delta l} = \frac{\cos \theta}{\alpha L} \quad (5)$$

and

$$W = KA \frac{\cos \theta}{\alpha L} \quad (6)$$

Interestingly, the thermal gradients and heats are independent of the opening angle, only ΔT depends on it.

The Darwin width of a perfect crystal depends on the material, energy and crystal orientation. Here we are going to discuss a number of different crystals and a number of orientations so we will use the simple, approximate formulation of Berreman². Ignoring absorption,

$$\delta \theta = 2 \left| \frac{F_{re}}{F_o} \right| \frac{(1 - N_{re})}{\sin \theta \cos \theta} \quad (7)$$

and

$$\frac{\delta E}{E} = 2 \left| \frac{F_{re}}{F_o} \right| \frac{(1 - N_{re})}{\sin^2 \theta} \quad (8)$$

where $\delta \theta$ is the Darwin width, $\left| \frac{F_{re}}{F_o} \right|$ is the real part of atomic scattering factor and n_{re} is the real part of the index of refraction. The opening angle

(FWHM)³ of the synchrotron is

$$\Delta\theta = \frac{0.94}{\delta} \left(\frac{\lambda}{\lambda_c} \right)^{0.425}$$

where λ is the wavelength of synchrotron light and λ_c is the critical wavelength.

In fig. 2 we show the opening angle of NSLS (solid line) and the Darwin widths for a number of crystals at three energies (5.41, 8.05, and 17.48 keV). Note that at the low energies, the opening angles are only 3-10 times greater than the Darwin width whereas at the higher energies they are almost two orders of magnitude larger. The gain in intensity is the approximate ratio of the Darwin widths to $\Delta\theta$. In Table 1 we summarize the relevant parameters for a number of crystals. Note that in all cases the temperature differences, gradients, and heat loads are quite modest and should not provide difficult engineering challenges.

For high and ultra high resolution experiments a four crystal design of the type described by Heald⁴ seems superior to the two crystal designs. From Table 1 it can be seen that the highest resolution is achieved using a Si(14,6,0) crystal. The gradients and heats required are quite small, consequently, it is clear that the white beam from the synchrotron must not be allowed to fall on this crystal. The beam heating would clearly detune the crystal. It seems that it would be better to use Si(4,0,0) or Si(8,4,0) crystals for the first ("A" and "B") and the Si(14,6,0) for the second pair ("C" and "D") (See Fig. 3). In certain applications quartz crystals have better resolution than Si but they are generally not used because of their sensitivity to radiation damage. The radiation damage would be minimized by using the four crystal design with Si crystals for the first pair ("A" and "B") and quartz for the second ("C" and "D"). Currently many beam lines are using sagittal focusing⁵ to account for the horizontal divergence of bending magnet radiation. Nothing discussed above precludes such focusing. Only one crystal would need to be bent. Another approach is to bend the first crystal, "A", in the horizontal plane and apply a thermal gradient to it as shown in fig. 4. In this case, Smither has shown that a parallel, monochromatic beam results. In fig. 4 we show one such arrangement, where the first crystal is followed by two flat high resolution crystals to further monochromatize the

beam. The fourth, crystal "D" is bent to obtain sigittal focusing. A two crystal design would also work well.

The use of thermal gradients adds some complexity to the design of a beam line. However, it results in certain simplifications. It eliminates the need for complex, expensive focusing mirrors. If harmonic rejection is needed a flat mirror will suffice. Pizoelectric positioners are also not needed since simple adjustment of the average temperature can bring a crystals reflection energy into coincidence with the other crystals. Temperatures can easily be measured and adjusted to hundreths of a degree, which allows energy adjustments of tenths of a meV.

The application of thermal gradients can be done in a variety of ways. Perhaps the simplest is water or freon cooling at one and electrical heating at the other controlled by analog feedback systems. Considerable work will be required to develop the best methods. We plan to test some of these concepts at NSLS in the near future.

Acknowledgments

The authors would like to acknowledge helpful discussion with P. Georgopoulos, S. Heald, A. McKale, P. A. Montano, and G. Shenoy.

Table 1

Crystal	E(keV)	$\Delta T(^{\circ}\text{K})$	$\frac{\Delta T}{\Delta l(^{\circ}\text{K/cm})}$	W(watts)	$\delta(\theta)$ (10^{-5} radians)	δE (meV)	Gain
Si(1,1,1)	5.4	212	323	162	6.7	920	3
Si(2,2,0)	5.4	112	279	139	4.1	221	5
Si(4,0,0)	5.4	53	187	83	3.6	125	6
Ge(2,2,0)	5.4	48	114	28	7.4	569	3
Quartz(2,0,1)	5.4	22	52	2.6	1.32	100	15
Quartz(3,1,0)	5.4	1.8	7.7	0.4	6.34	41	3
Si(1,1,1)	8.0	263	336	168	4.4	1,375	4
Si(4,0,0)	8.0	100	285	143	1.6	187	10
Si(6,2,0)	8.0	24	154	77	1.6	62	10
Ge(4,0,0)	8.0	51	116	29	2.6	326	8
Quartz(2,0,3)	8.0	23	53	13	1.2	145	16
Quartz(2,4,2)	8.0	0.6	2.4	0.6	5.0	14	4
Si(4,0,0)	17.5	182	335	167	.66	417	18
Si(8,4,0)	17.5	68	282	140	.14	33	87*
Si(14,6,0)	17.5	5.1	36	18	.19	3.5	61*
Ge(8,5,0)	17.5	29	112	28	.24	63	48*
Quartz(0,0,9)	17.5	12	51	2.5	.096	23	123*

Table Caption

The relevant parameters (defined in the text) for various crystals at three different energies. The values were calculated assuming the crystals are 12 meters from the source, the crystals are 0,1 cm thick, 1 cm long and 5 cm wide. The thermal conductivities are 1., 0.5 and 0.1 watts/K-cm for Si, Ge and quartz respectively. The thermal expansion coefficients are 2.4×10^{-6} , 6×10^{-6} and 13×10^{-6} $^{\circ}\text{K}^{-1}$ for Si, Ge and quartz respectively.

*The gains in intensity were calculated assuming a vanishing source size. For NSLS to source size of 0.1mm would limit the gains to approximately 20.

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Figure Captions

- Fig. 1 Schematic drawing of a two crystal system for monochromatizing a synchrotron beam. Both crystals are flat and have a thermal gradient applied to them so that the value of $d \sin \theta$ is a constant.
- Fig. 2 A graph comparing the opening angle solid line θ of a synchrotron beam width with the Darwin width of various planes in Ge(squares), Si(circles) and Quartz (triangles).
- Fig. 3 Schematic drawing of a four crystal system to monochromatize a synchrotron beam. All four crystals have thermal gradients applied to them.
- Fig. 4 Schematic drawing of a four crystal system to monochromatize and focus a synchrotron beam. Only crystal "A" has a thermal gradient applied to it.