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MODELING OF X-RAY BEAMLINES AND DEVICES

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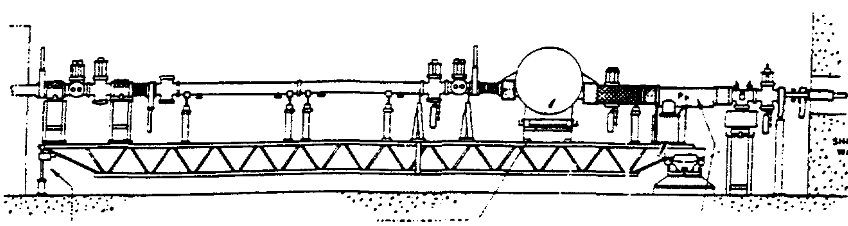
ABSTRACT

X-ray beamlines on synchrotron sources are similar in size and complexity to beamlines at state-of-the-art neutron sources. The design principles, tools, and optimization strategies for synchrotron beamlines are also similar to those of neutron beamlines. We describe existing design tools for modeling synchrotron radiation beamlines and describe how these tools have evolved over the last two decades. The development of increasingly powerful modeling tools has been driven by the escalating cost and sophistication of state-of-the-art beamlines and by a world-wide race to exploit advanced synchrotron radiation sources.

INTRODUCTION

X-ray beamlines on synchrotron sources are expensive and complicated instruments. First generation (parasitic operations) and second generation (dedicated small emittance) beamlines are ~20 m long with ~1/4 inch of steel shielding and cost ~$1-2 M [1]. Third generation (undulator) sources require beamlines ~60 m long with ~1" of lead shielding and cost ~$4-7M [2]. Typical beamline layouts are illustrated in Fig. 1. As shown in Fig. 2, new beamlines often contain expensive and complicated first-of-their-kind components. These new components demand careful modeling before fabrication. In addition, as the cost of beamlines has risen, beamline developers have increasingly relied on modeling to develop confidence that each beamline will be optimized for its mission.

1st/2nd Generation ~1/4" steel/ (20 m long)/ $1-2M



3rd Generation ~1" lead/ (60 m) long $4-7M

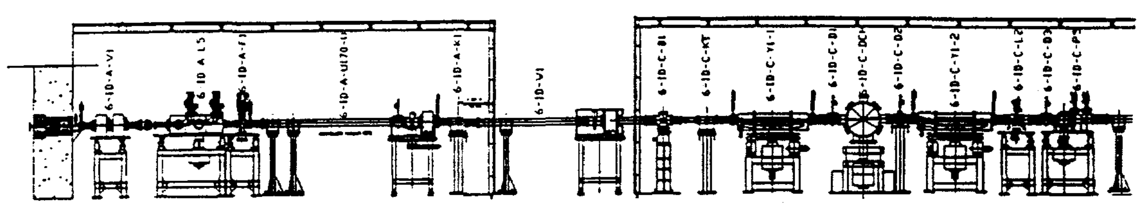


Fig. 1 Typical beamlines on synchrotron sources.

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Fig. 2 Sagittal focusing double crystal monochromator on beamline X14 at the NSLS. The photograph shows some of the 12 in-vacuum motors used to align the two crystals and dynamically bend the second crystal to a cone. This device was the first of its kind.

In general, beamline modeling is an iterative process. As shown in Fig. 3, modeling begins by defining a beamline mission. Beamline mission sets the beamline requirements: energy resolution, momentum transfer resolution, flux, tunability, harmonic rejection, and sample volume. Other factors also guide (restrict) synchrotron beamline design such as shielding requirements for personnel protection, background considerations, vacuum for beam transport, and thermal considerations.

Modeling is an iterative process

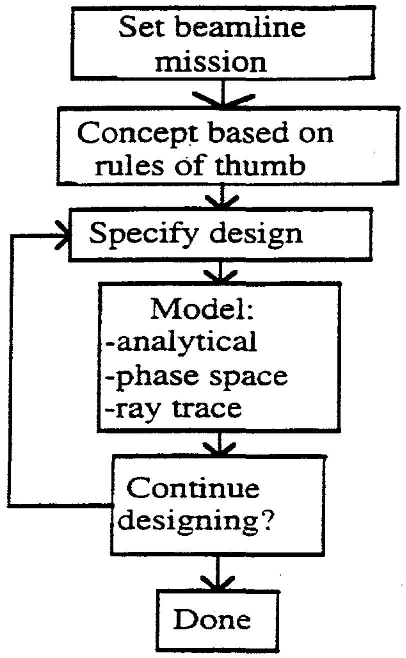

Fig. 3 Flow diagram for beamline design.

After defining the beamline mission and required characteristics, the next step in beamline modeling is to conceptualize the beamline based on simple "rules of thumb." For example, sagittal focusing (Fig. 4) can collect more radiation than meridional focusing, but the aberrations are more difficult to control. Similarly, the 20 times larger scattering angles of crystals relative to total-external-reflection mirrors means that crystal optics can be about 20 times shorter than mirrors.

Since synchrotron optics are dominated by a small number of optical elements, it is possible to rule out certain designs quickly and rapidly narrow-in on the most likely optical components. Figure 5 shows the designs of seven beamlines at the Advanced Photon Source as conceived in late 1994. As can be seen in Fig. 5, the beamlines designs are dominated by a small number of components.

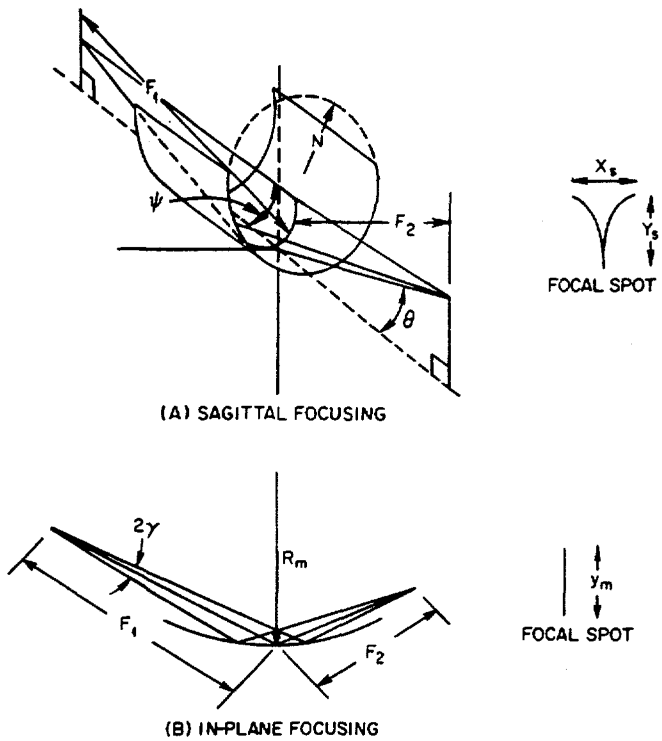

Fig. 4 Sagittal (out-of-plane) and meridional (in-plane) focusing.

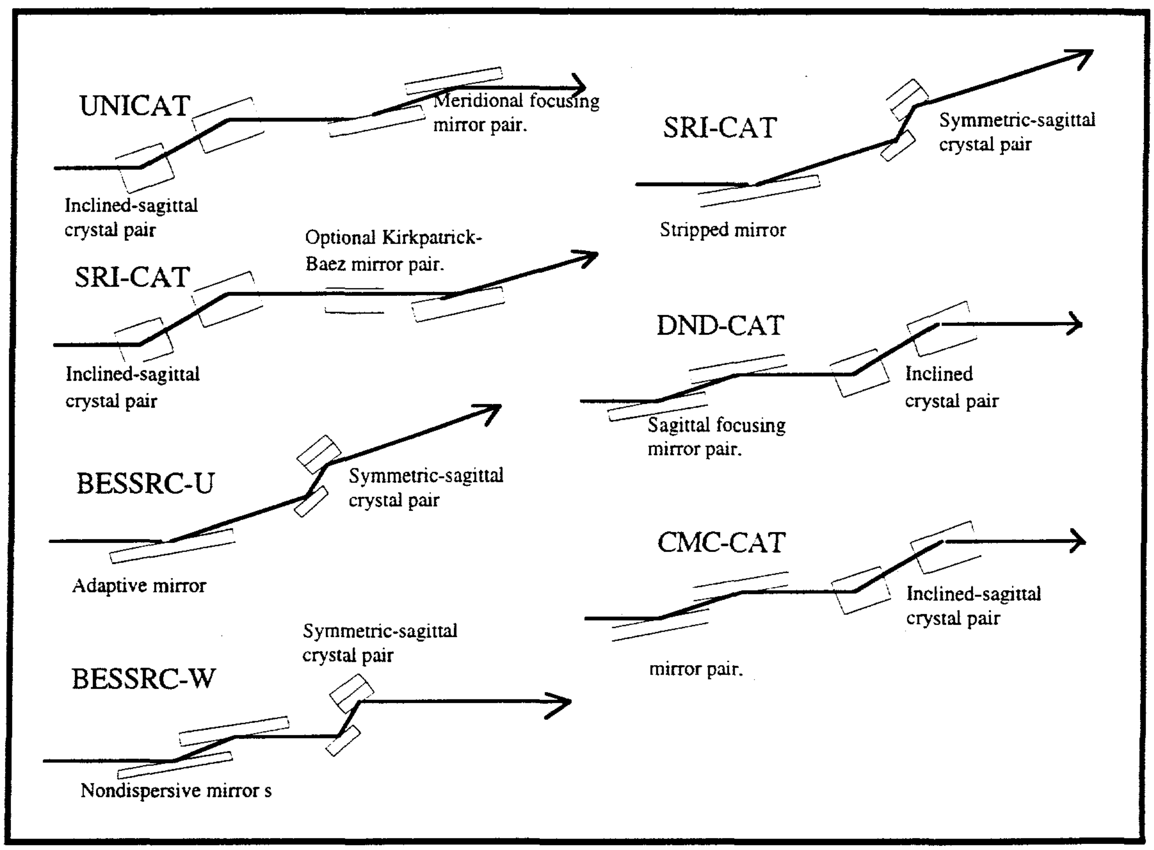

Fig. 5. Conceptual beamline designs at the APS.

The next step in beamline modeling involves specifying beamline parameters for modeling. This is followed by detailed modeling of component performance, and modeling of the overall beamline with analytical, phase space or ray trace models. The estimated beamline performance is then compared to alternative designs and the process is iterated until the designer is satisfied as illustrated in Fig. 3.

FOUNDATIONS OF X-RAY OPTICS

Early modeling of x-ray instrumentation built on x-ray optical principles developed for conventional x-ray sources and on x-ray astronomy. For example, the basic theory of x-ray focusing with mirrors [3,4] and x-ray focusing with crystals, [5-7] has a long history of use with conventional sources and Kirkpatrick and Baez [3] demonstrated the principles of an x-ray microscope/microprobe with crossed meridional mirrors (Fig. 6) long before the discovery of synchrotron radiation. The introduction of x-ray synchrotron sources in the 70s however, led to synchrotron specific instrumentation papers and to whole conferences devoted to synchrotron radiation instrumentation [8,9]. These conferences and papers began addressing the new challenge of utilizing tunable and extremely intense x-ray sources.

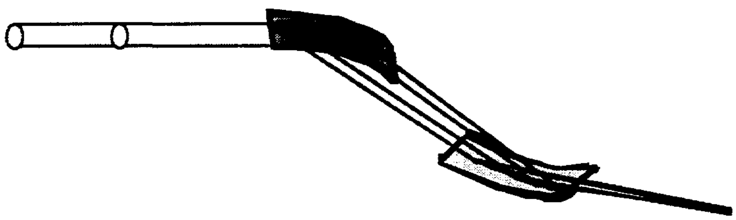

Fig. 6 Kirkpatrick-Baez mirror pair.

The First International Conference on Synchrotron Instrumentation and Developments was held in Orsay France in 1977 [8]. This conference attracted over 170 participants and was extended to a three day meeting with over 65 papers. In 1978 a Workshop on X-ray Instrumentation for Synchrotron Radiation Research at the Stanford attracted over 150 participants and again more than 65 papers. These early conferences introduced scientists to many new concepts including mosaic crystal focusing monochromators, synthetic multilayers, phase space optics, and x-ray induced mirror damage. Conference proceedings and refereed journal articles were augmented with synchrotron facility reports. For example, thermal analysis of components [10] (Be windows, etc.), software and experimental design [11], source properties[12], and a host of other topics of great interest to beamline designers were treated through facility reports. In addition synchrotron radiation books began to be published which included detailed considerations on instrumentation design [1].

ANALYTIC MODELING

For individual beamline components it is often possible to study their behavior through analytical techniques. These techniques are fast and can be integrated into ray-tracing programs which combine multiple components. Mirror reflectivity (Fig. 7) can be calculated from fairly simple programs to estimate the dependence on surface coating, x-ray energy and glancing angle [13]. Surface roughness, its spectral density function and contamination can also be treated by analytical models to estimate their effect on mirror performance [14-16]. Analytical models are also used to estimate the aberrations associated with various focusing schemes [3,17]. With a Kirkpatrick-Baez mirror system, a simple analytical formula estimates the divergence which can be collected before aberrations dominate the demagnified image size. Analytical models have also been used to study the Bragg angle matching between x-ray crystals with a flat-crystal sagittal-crystal pair. Sparks, et al. [18] were able to show that a cylindrically curved crystal set for M~1/3 intercepts a fan of radiation at a nearly constant Bragg angle. A nondispersive flat-crystal sagittal-crystal pair were also found to match Bragg angles for a wide range of magnifications when the focusing crystal was bent to a conical (Fig. 8) shape [19].

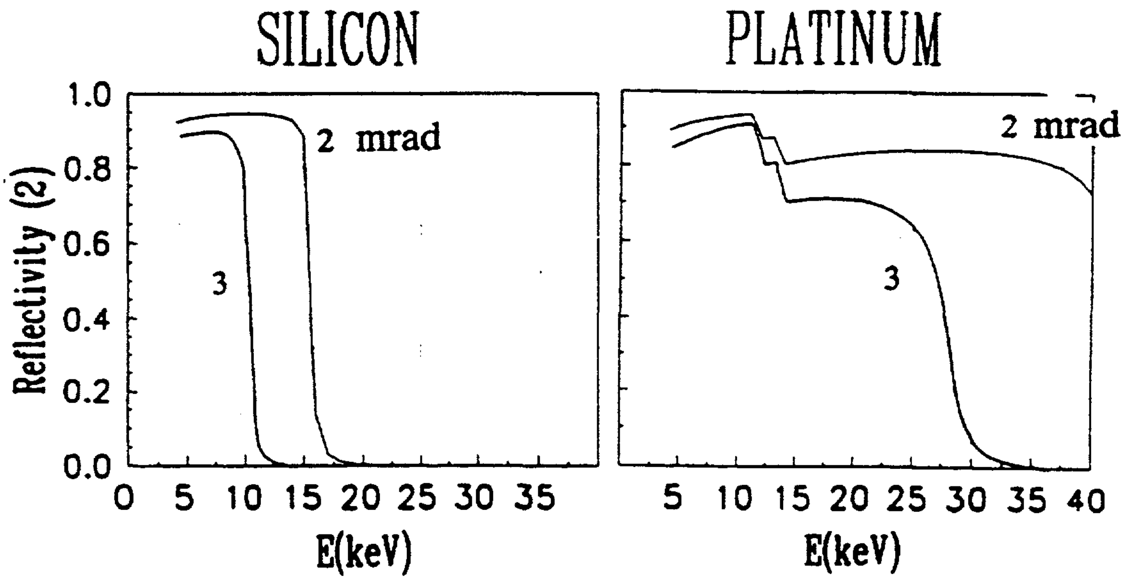

Fig. 7 Mirror x-ray reflectivity through a pair of non-dispersive mirrors as a function of x-ray energy, coating, and glancing angle.

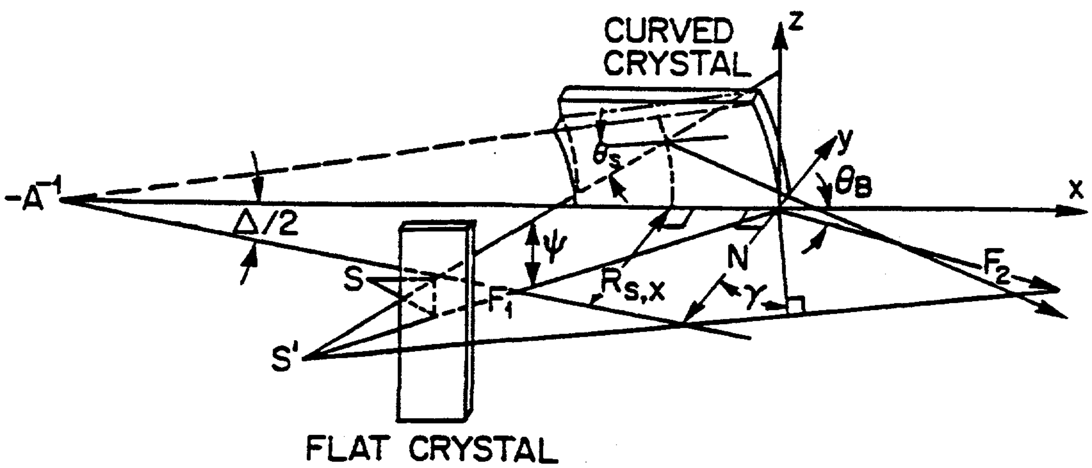

Fig. 8 Conical crystal geometry.

PHASE SPACE OPTICS

Powerful phase space modeling techniques are also often used to study the behavior of synchrotron beamlines and components. Phase space optical approaches originated with charged particle optics of the accelerator based sources. Within the phase space description, it is possible to follow the beam from the source through optics and then map the fraction of the source which is transported to the experiment. The key advantage of phase space optics is the ability to predict performance limits of various optical schemes. In addition, phase space optics can be used to estimate the deleterious effects of apertures and surface roughness. With phase space optics, it is fairly easy to estimate the surface roughness required to preserve x-ray brilliance (Fig. 9). Although the general techniques are very powerful, they are difficult to use with complicated optics. The best publication is somewhat difficult to find [20].

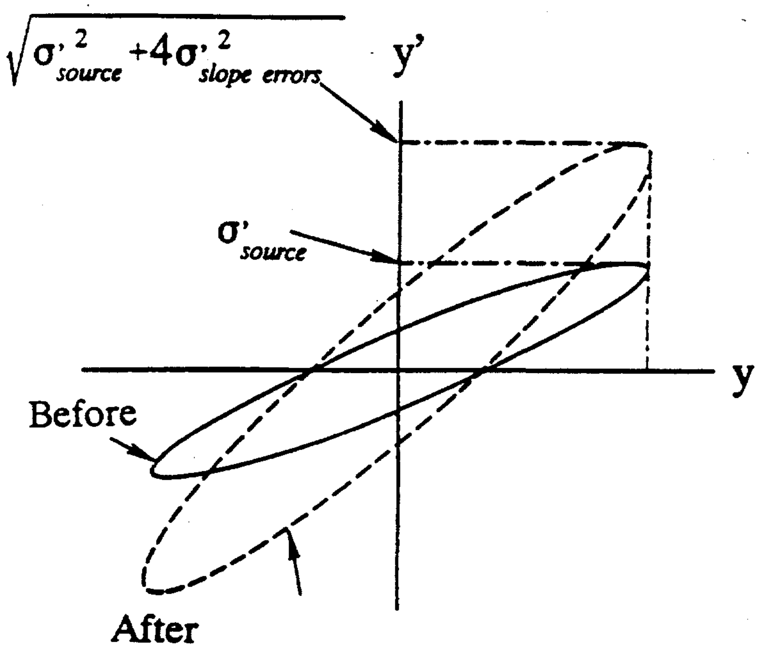

Fig. 9 Surface roughness effect on x-ray brilliance.

RAY TRACING

Modeling of complicated x-ray components and beamlines is most often done using ray tracing techniques. An early suite of ray tracing programs was introduced by Darsbury around 1982. These were soon followed by the program SHADOW [21] around 1985. SHADOW has become the x-ray standard because it accurately handles many different optical elements. In particular SHADOW, unlike some other programs, handles asymmetric crystals and rough surfaces.

One problem with SHADOW is its cumbersome interface. Early versions of SHADOW also suffered from a limited number of rays, and a limited number of computer platforms. These problems have restricted routine use of SHADOW. Most often SHADOW is used to *verify* beamline designs. Beamline designers tend to use faster and more use-friendly ray-trace programs to develop beamline concepts.

Specialized ray-tracing programs are often fast and flexible but are not as well tested and hence not as convincing as SHADOW. For example, a suite of programs have been coded at ORNL to help in the design of x-ray microbeam and x-ray diffraction beamlines. These programs are very fast, can handle 10^6 rays easily and can be configured for simple optimization of beamline design. However these programs cannot easily handle diffraction limited conditions, are only accessible to expert programmers, and are not stable (i.e. the code changes at the users whim). Nevertheless, even simpler ray tracing programs have been used to discover these and new ray optical designs.

The discovery of the cylindrical crystal focusing geometry is a good example of an application of a simple x-ray ray-tracing program. Sparks, et.al. [18] studied the Bragg angles of rays reflected through a flat-crystal cylindrical-crystal nondispersive pair (Fig. 8). To their surprise, at a magnification near 1/3, the Bragg angles matched for a large divergence out of the diffracting plane. This discovery led to the development of dynamical sagittal crystal focusing optics which have been widely adapted for focusing synchrotron radiation. (Fig. 10).

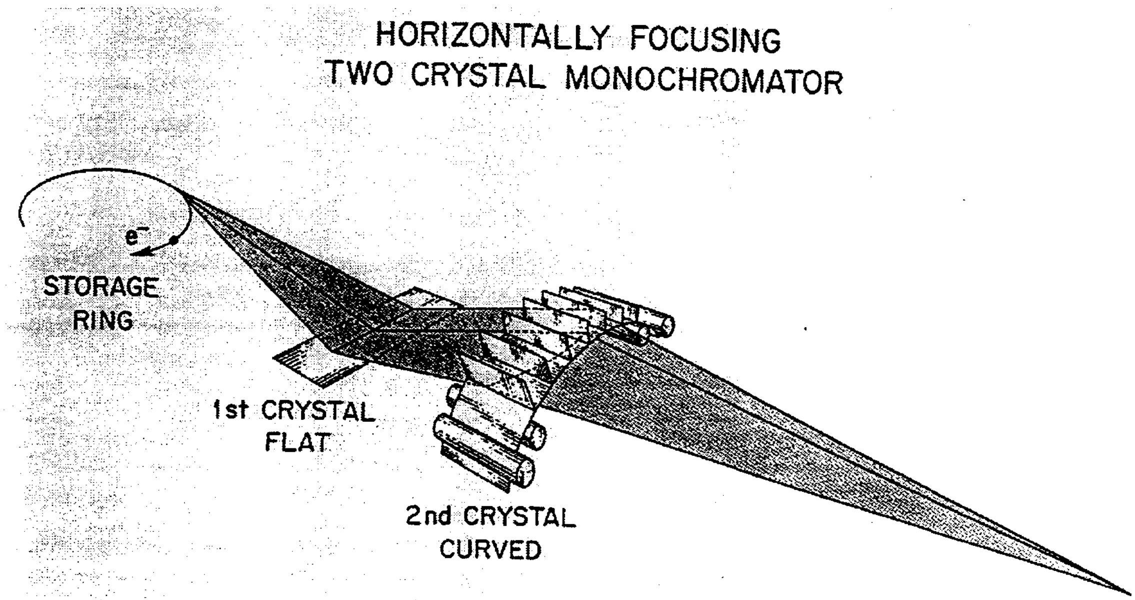

Fig. 10. Beamline optics for beamline X14 at the NSLS. The double crystal monochromator focuses the horizontal beam divergence with a dynamically-bent sagittal-focusing Si crystal.

A simple ray-tracing program was also used to discover that sagittal crystal focusing could be improved by going to a conically bent crystal [19]. This program was designed to search for an optimum cone angle at various magnifications. The program found that near M=1 the aberrations resulting from sagittal crystal focusing were minimized. This discovery led to the development of beamline X14 at the National Synchrotron Light Source (NSLS) which was the first beamline designed to use a dynamically bent two-crystal monochromator [22].

A simple ray-tracing program also found that a so called "inclined crystal" could be used to focus the out-of-plane synchrotron radiation divergence from an undulator. The inclined geometry[23] is designed to distribute the thermal load from a small high-intensity x-ray beam. The crystal surface is cut at an angle relative to the reflecting Bragg planes, but unlike an asymmetric geometry, the cut is perpendicular to the diffracting plane (Fig. 11). A ray tracing program was used much like an experiment to test the focusing properties of a sagittally focusing inclined crystal pair [24]. It came as a complete surprise that for an inclined crystal, the radius of curvature increases inversely with the cosine of the cut angle. This property greatly extends the tunable range of an inclined crystal of a given thickness compared to a sagittal focusing symmetric crystal. The program also mapped out the range over which aberrations were small (Fig. 12).

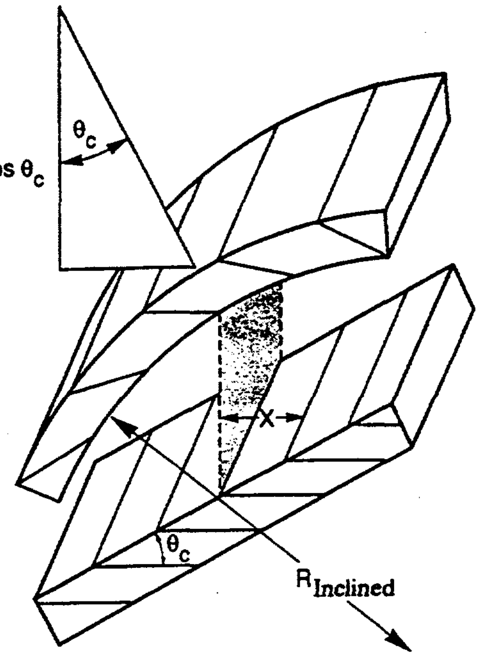

Fig. 11. Inclined crystal geometry showing the diffraction plane, Bragg planes and crystal surfaces. The second crystal is cylindrically curved to focus the beam horizontal divergence.

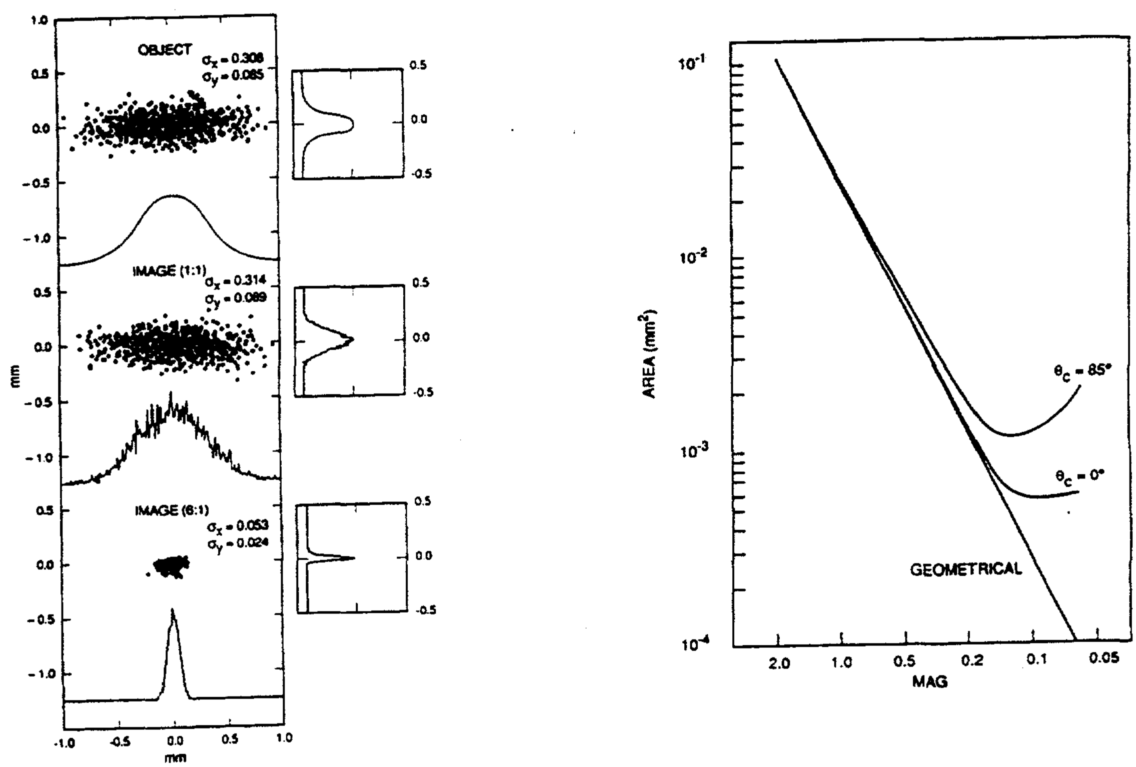

Fig. 12. Aberrations as a function of magnification for an undulator source and with a sagittal focusing inclined monochromator.

OTHER BEAMLINE MODELING RESOURCES

Source properties are critical to synchrotron beamline design. Analytical calculations and numerical recipes have evolved to accurately predict the source properties of bend magnet, wiggler and undulator synchrotron sources. Undulator source properties are particularly complicated and the program URGENT has provided the community with a fast, well documented program to predict the source properties of most undulator devices [23].

Shielding also presents a very important aspect of beamline design for high energy synchrotron sources. Although analytical models exist for shielding design, these are complicated to apply. Numerical codes based on the analytic models allow rapid verification that the analytic model predicts adequate shielding under all possible conditions [26,27].

CONCLUSION

There are many design tools available for modeling the performance of synchrotron radiation beamlines. These tools have evolved rapidly over the last two decades and allow beamline designers to predict the performance of new beamline concepts. Because of a vigorous and growing community interested in the design of synchrotron radiation instrumentation, design tools are constantly being tested and improved. The availability of several standard tools has simplified the task of verifying beamline designs.

ACKNOWLEDGEMENT

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