

POPULAR SCIENCE ABSTRACT

Student: Johan Eckdahl

Lund University Master Programme in Physics

Synchrotron radiation facilities are some of the world's largest machines, yet they are built for exploring its smallest processes. These ring shaped facilities can reach over 1 kilometer in circumference but produce beams of light thin enough to examine materials at the atomic scale. From computer chips to the structure of proteins, synchrotrons are revolutionizing how science is done.

To produce an X-ray beam suitable for any given experiment an array of high precision optics is needed. The optics include focusing mirrors, filters, attenuators, collimators, and more. However, one of the most important though harshly treated elements is the monochromator. Monochromators in hard x-ray beamlines commonly consist of two silicon crystals which reflect only frequencies of light satisfied by the Bragg condition. The Bragg condition is met by the comparability of the silicon lattice spacing and hard X-ray wavelengths. Rejected wavelengths deposit their energy as heat. The sensitive lattice of the silicon will endure relatively large amounts of stress and begin to distort under the heat load. This distortion inevitably affects the crystal lattice in a way that alters the Bragg condition over the range of the beam incidence. In this case the reflected wavelengths will significantly deviate from expected values. This can include a wider or smaller range of wavelengths and/or reduction of flux in reflected beams. It is important to understand these effects and their significance if one is to mitigate or compensate for them.

The easiest, and most necessary, way to reduce these effects is to cool the silicon. The silicon can also be adjusted to an effective Bragg angle to reflect the proper frequency. Further frequency tuning can be performed by reflection from the second crystal. The second crystal will lack many of the challenges of the first, since most energy from the beam has already been transferred to the first crystal.

In order to predict the magnitude of these effects, and thereby prevent myopically producing an ineffective design, an engineer can employ finite element analysis (FEA). In this experiment the program COMSOL is used to make predictions of the lattice strain in a model of the monochromator in the NanoMAX and BioMAX beamlines at the MAX IV facility in Lund, Sweden.

There are limits, however, to what software like COMSOL can do. In the case of ray tracing, that is, approximating the energies and paths of photons in 3-dimensional space as they travel from the insertion device to the crystal, it falls short. Software called Shadow3 can be used to model this process. It can also model the reflected beam based on the deformation in the silicon crystal. However, some effects are not built into Shadow3 and must be added by the user or else proven to be insignificant. In this case it is important to have a grasp of theory so that one can extend the reach of software into the realms of calculation that have yet been left only to the mind.

Of course predictions are only valuable if they correspond to reality. It is important that consistent validation is performed to ensure that real life measurements correspond to those found in simulation. The more aligned these values are, the more one can trust the simulation and the more flexible it becomes. In the case of monochromators one can measure such things as the heat of the crystal and the cooling fluid, the wavelengths and position of the reflected beam, and total reflected flux. Upon obtaining these values one can return to the trusted simulations, where tweaks can be made to improve the system and then again be validated. This process can repeat until the user is satisfied with the results. This paper outlines simulation efforts and concludes with a valuable model for current and future beamlines.