TWO-COLOR SELF-SEEDING AND SCANNING THE ENERGY OF SEEDED BEAMS AT LCLS*

F.-J. Decker, Y. Ding, Y. Feng, M. Gibbs, J. Hastings, Z. Huang, H. Lemke, A. Lutman, A. Marinelli, A. Robert, J.L. Turner, J. Welch, D. Zhang, D. Zhu, SLAC, Menlo Park, CA 94025, USA

Abstract

The Linac Coherent Light Source (LCLS) produces typically SASE FEL pulses with intensities of up to 5 mJ and at high photon energy an FEL bandwidth 0.2% (FWHM) [1]. Self seeding with a diamond crystal reduces the bandwidth by a factor of 10 to 40. The range depends on which Bragg reflection is used, or the special setup of the electron beam like over-compression. The peak intensity level is lower by a factor of only five, giving the seeded beam an advantage of about 2.5 in average intensity over the use of a monochromator with SASE. Some experiments want to scan the photon energy, which requires that the crystal angle be carefully tracked. At certain energies and crystal angles different Bragg lines cross which allows seeding at two or even three different colors inside the bandwidth of the SASE pulse. Out-of plane lines come in pairs, like [1 -1 1] and [-1 1 1], which can be split by adjusting the yaw angle of the crystal, allowing two-color seeding for all energies above 4.83 keV.

INTRODUCTION

Hard x-ray self-seeding with a crystal was introduced just three years ago at the FEL 2010, Malmö, Sweden [2]. A year and a half later the LCLS was upgraded with a chicane to bend the electron beam around a diamond crystal, which provides the necessary seed using Bragg reflections [3]. Understanding the exact setup of the crystal with its many possible Bragg reflections and using them in unforeseen ways will be discussed.

SEEDING CRYSTAL BRAGG LINES

The crystal stage was designed having mainly the Bragg reflection at the $[0\ 0\ 4]$ plane in mind, so the main crystal angle (pitch) can be moved from 45° to 90° plus a few degrees on each side which allows for misalignments (Fig. 1).



Figure 1: Side view of the HRXSS chicane setup. Undulator 16 (out of 33) was removed to make space for a small chicane (magnets in blue), which bend the electron beam about 2 mm into the paper plane, while the SASE photons go straight through the diamond crystal. The yaw angle axis is vertical when the pitch angle sits at 90° and can move about $\pm 2.5^{\circ}$.

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Soon it was recognized that there are more lines like the [2 2 0] Laue line [4] where the "reflection" actually goes through the diamond crystal. Figure 2 shows a few more in-plane lines which were used. At the crossing of the two lines at 54.74° and 8.51 keV it is possible to get seeding on two (or more) lines, which was quickly verified (Fig. 3). A long range angle scan from 45° to 75° at 7.2 keV showed that there are more lines to be explained (blue dots in Fig. 2).



Figure 2: Seeding lines for Bragg reflections with photon energy versus crystal angle for a few basic planes. In blue the [0 0 4] plane corresponds to the surface plane of a cube; its line minimum energy is at 90° (pitch) to the FEL beam. The crystal cube sits then on one of its edges. The [2 2 0] plane cuts diagonally through four corners and its seeding line has a minimum at 0° pitch angle, since its plane would be then 90° to the beam. The [1 1 1] plane cuts through three corners and its perpendicular axis goes through the top, front corner (at 90° pitch). To reach its minimum the pitch angle needs to go further to about 145°. It should be mentioned at this point that with the pitch angle at 90° there are three more corners which have the same angle to the FEL beam and there should be four red lines crossing at the 90° point, the other in-plane line of [-1 -1 1] and the two lines from the out-of-plane planes [-1 1 1] and [1 -1 1]. The perpendicular axes of these outof-plane planes lie on a cone instead of a plane.



Figure 3: At 8.5 keV the [2 2 0] and the [0 0 4] lines cross each other and seeding on both lines is observed around 54.6°. Here the energy location of the highest peak in the spectrum is plotted versus the crystal angle revealing that there are two preferred energies at angles between 54.54° to 54.64°. Scattered dots are peaks of SASE background.

MORE CRYSTAL LINES

To calculate more crystal lines we started first one by one and discovered that we don't have to extend the crystal rotation angle much beyond 90° to reach the lowest energy, but instead use the [-1 -1 1], which has its minimum near the low of 42° of our range. Figure 4 shows all crystal lines from 3 to 11 keV, which should be reachable.



Figure 4: All reachable seeding crystal lines between 3 and 11 keV. Each family of the same indices has the same color, like all combinations of [3 3 1] are magenta. The solid and dashed lines are in-plane lines [a a b] with the distinction that the dashed ones have a negative sign on the first two indices, e.g. [-1 -1 1] which goes all the way down to 3 keV. The dash-dotted lines are the out-of-plane lines like [-1 1 1] and [1 -1 1]. They should lie perfectly on top of each other, or get shifted apart in energy with a small yaw adjustment. Here the best known roll and yaw offsets of -3.73° and -0.61° are used, which makes all the dash-dotted lines cross at about 81°.

Out-of-Plane Lines

The out-of-plane or dash-dotted lines from Fig. 4 are the most interesting for two-color self-seeding, since they allow the generation of two seeded spectral lines close together at any energy above 4.83 keV. Due to a small roll error of the crystal of -3.73° the two lines don't just separate with yaw angle, but cross each other at certain pitch angles. The data in Fig. 5 was achieved at our FEE (Front End Enclosure) spectrometer energy of 8.45 keV and adjusting the crystal angle and yaw angle to put the four different out-of-plane line pairs on top of each other. Two black pairs ([1 -1 3], [-1 1 3] and [-1 -3 1], [-3 -1 1]) at 49° and 61°, one magenta pair ([-1 -3 3], [-3 -1 3]) at 65° and the green pair ([2 0 2], [0 2 2]) at 78^{\circ}. Making the overlap work in the code required the above mentioned offsets of -3.73° for roll and -0.61° for yaw offset. This explains also all the blue dots of Fig. 2 and 4; they lie perfectly on the lines now.



Figure 5: Yaw angle to put out-of-plane lines on top of each other at 8.45 keV. The point at 62° comes from a 7.2 keV setup and falls right on the curve.

Two-Color Self-Seeding

Besides crossing points of the many Bragg lines, the out-of-plane line pairs allow the production of two-color seeded FEL pulses (Fig. 6.) within the SASE bandwidth, which is typically about 30 eV. The FEE spectrometer used in the figure has an acceptance limitation of about 15 eV around the center. The high SASE content is not typical for a well tuned up seeded setup, the test was mainly to test this configuration and get the data for Fig. 5.

The spectrum of a more tuned two-color seeded beam pulse, where the photons of around 7.1 keV were sent to a photon experiment [5], is shown in Fig. 7. Their separation is about 40 eV. To achieve two-color seeded pulses much beyond the SASE bandwidth the newly tested pulse-stacked FEL setup can be used, where two bunchlets within one RF bucket generate two SASE pulses of different energy and variable delay [6].



Figure 6: Averaged spectrometer distributions of twocolor seeded beams for different yaw angles for the [-1 -3 1], [-3 -1 1] line pair. The crystal angle is 60.5° for the typical energy of 8.45 keV. A small angle change of 0.02° yaw will separate the lines by about 3 eV more.

ENERGY TRACKING

Some photon experiments require a slow scan of the energy over a range of their interest. A small script to scan the electron energy already existed, but at the same time the crystal angle has to be moved to keep the seeded line following the required energy. To test a tracking code first a desired energy parameter was changed in a saw tooth like pattern by 200 eV around 9.6 keV (Fig. 8).



Figure 7: Two-color energy distribution of a single shot at 7.1 keV. After tuning up for a wide SASE bandwidth (low L1X amplitude) to get the 40 eV wide separation.

Then a vernier energy script changes the electron energy to get the required photon energy and finally the crystal angle tracks the photon energy, which might be capped so the beam is not outside the energy acceptance. When tuning up seeding, we intended to be on the [2 2 0] line, but were accidentally on the nearby nearly horizontal out-of-plane line [-3 1 3], which was not known at that time. By tracking with the slope of the [2 2 0] line we were parallel to [2 2 0] but never hitting it. Later we tuned up to see two peaks assuming that one is the [2 2 0] and got the expected tracking result where SASE and seeded peak move together in time (Fig. 9.)



© Figure 8: Energy tracking. The green energy vernier follows and caps the desired energy (red). The crystal angle (blue) follows too, but undershoots at the start of each saw tooth to avoid backlash.



Figure 9: Tracking energy of seeded FEL. The peak of the $[2 \ 2 \ 0]$ line and the underlying SASE "background" move together to the right going from top to bottom in about a minute. The slope for $[2 \ 2 \ 0]$ is about 250 eV/deg. The middle picture show the appearance of a second line $[-3 \ 1 \ 3]$ (magenta in Fig. 4), which moves much slower and in the opposite direction.

To verify that the second line was the only known nearby line at the time [1 1 3] we changed the tracking direction (down in energy and up in crystal angle) to fit that line. The energy was adjusted till we were hitting the line, but it turned out that we slowly wandered away too. Later analyses with the help of archived data showed that we lowered the energy by about 250 eV and were nearly tracking the [-1 -1 5] line (yellow in Fig. 6). Figure 10 shows a typical crystal angle scan while looking at the peak value of the spectrum. It demonstrates nicely that with coarse scans with like 0.1° step sizes, you might miss a narrow line with a width of only 0.028° rms.



Figure 10: Typical crystal angle scan at the [2 2 0] line to find the peak performance for the current energy setting.

SUMMARY

Tracking the seeding crystal to follow a Bragg line in the energy-vs-crystal angle diagram is tricky, especially at very high energies where there are many other lines and their crossings to consider. The average seeded intensity is typically a factor of 2.5 higher than SASE with a monochromator. The in-detail study of the crystal revealed the possibility of two-color self-seeding, which was quickly used in an upcoming bio-imaging experiment with one of the two photon energies below and the other above the iron K-edge [5].

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