Calibration of IR Spectrometer.
ALICE shifts # 2749 to # 2757

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During the FELIS experimental run between 10th & 13th November 2011, the SpectroSense IR spectrometer was used in conjunction with a 1-D PyroArray detector from Delta Developments to determine the IR wavelength the FEL was tuned for and to measure the shot-shot stability of the intensity and wavelength of the FEL pulse. To aid the calibration a Nicolet polystyrene standard (Ref. No. 011945) was taped to the entrance slits of the spectrometer.

1 Optical Layout of IR-FEL Beam

The optics box of the IR beamline has been fitted with a beamsplitter to allow IR radiation to be transmitted simultaneously to the experiment on the optical table (the SNOM) and also to the spectrometer for diagnosis. Figure 1 shows the relative layout. Not shown is a \( f = 300\text{mm} \) focal length IR lens in the optics box which focusses the collimated IR light on to the entrance slits of the spectrometer. The spectrometer is designed to take IR light focussed on its entrance slit, collimate the beam to the grating, and then refocus it to the exit slit. Behind the exit slit is a single element pyro-detector. This can be used in scanning mode to measure the spectrum of the incident IR light. Alternatively, the mirror in front of the exit slit can be remotely flipped out of the way to allow the dispersed spectrum to pass through a large aperture at the back of the spectrometer and onto a 1-D detector array to collect a broad spectrum without the need to scan the spectrometer grating. This rear port is where the Delta Developments pyroarray is mounted.

A LabView virtual instrument (VI) was written to read the digitised signals from all 32 channels of the pyroarray and record the measured spectrum. The National Instruments ADC card is set to use the Laser Trigger signal in the diagnostics room to trigger the data collection. The VI can therefore record a complete spectrum of each FEL macropulse. A screen shot of the VI is shown in Figure 2. On the left hand side is a tabbed pane giving an oscilloscope like screen of the waveform seen by a selected channel of the pyroarray. On the right hand side is the resulting spectrum. At the time of the experiment, the VI was not integrated with the SpectraSense spectrometer, so the abscissa of the displayed spectrum is shown in units of channels of the pyroarray. The VI has since been modified to read the selected wavelength from the spectrometer and apply this to the spectral display. It also calculates the grating dispersion to convert from detector channels to wavelength.

The beamsplitting design of the optics box allows for continuous monitoring of the wavelength and intensity of the FEL radiation whilst experimental data is also being
Figure 1: Sketch of the optical layout of the optics box showing how the IR-FEL beam is split between pathways to the SNOM experiment and simultaneously to the Spectrometer. The PyroArray detector can be seen as the rounded object affixed to the rear of the spectrometer.

Figure 2: A screen shot of the LabView VI used to record the IR spectrum measured by the pyroarray.
Figure 3: FTIR spectra of the Nicolet Polystyrene standard. As measured by a Perkin Elmer instrument at University of Liverpool.

collected.

2 Polystyrene Standard

The Nicolet standard reference was taped to the entrance slits of the spectrometer. Following the initial calibration run the IR absorption spectrum of the standard was measured using a Perkin Elmer FTIR instrument in one of the teaching labs at University of Liverpool by Gareth Holder. This is the same instrument used for measuring the FTIR signature of the Liverpool biological samples and so will provide a good correlation between the FTIR absorption measurements and the calibration of the IR-FEL beamline. As the Perkin Elmer instrument is used routinely by students to measure well calibrated test samples in the course of their studies, it can be assumed that the instrument itself is kept in good calibration. The FTIR measurement was conducted at a resolution of 4.0 cm$^{-1}$ and is shown in Figure 3.

The standard gives a number of lines of different intensity in the wavelength range accessible by the FEL. For ALICE operating at 25 MeV, this is $\lambda = 6.5 - 9.0 \mu m$ and $\lambda = 5.5 - 7.8 \mu m$ at 27.5 MeV. For these measurements ALICE was operated at 25 MeV.
3 Calibration of the Spectrometer

The spectrometer has a turret containing three dispersion gratings and for the wavelength range of interest is operated using Grating 3. This has a line density of 75 l/mm and a 10 µm blaze. The dispersion of the grating for a user given wavelength can be looked up on the Princeton Instruments website. Mark Roper has tabulated a selection of dispersions for both 75 l/m and 150 l/mm gratings. These are shown in Figure 4. The data points can be empirically fitted to quadratic curves which then allow a value for dispersion to be obtained for any wavelength. The relationship for the dispersion \(D\) found are:

\[
D_{75} = 26.319 - 0.11252\lambda - 0.023255\lambda^2
\]  
(1)

for 75 l/mm gratings (gratings 2 and 3) and:

\[
D_{150} = 13.16 - 0.11252\lambda - 0.004651\lambda^2
\]  
(2)

for the 150 l/mm grating of Grating 1. The dispersions are quoted in terms of wavelength per mm of horizontal displacement along the detector plane and in units of nm/mm. The Delta Developments pyroarray has tis channels on a pitch of 0.635 mm.

The spectrometer was optically aligned using the upstream HeNe laser from the FEL, transported down the IR-FEL beamline and shone onto the entrance slits of the spectrometer. The instrument was then physically moved to ensure that the HeNe alignment beam shone onto the centre of the grating, the alignment was then fine tuned to take the reflected zero-order HeNe light out through the exit slit (the single element pyro-detector being removed for this alignment). Grating 1 gives better reflection in the visible and so was used for this setup procedure, however the zero-order reflection in the visible is still dim and this alignment requires care.

The alignment of the spectometer was done initially with the optics box vented as the mirrors in the box were being aligned at the same time. It was subsequently noticed that the IR-FEL beamline moved as it was evacuated due to unbalanced atmospheric loading on the vessels and pipework. This had the effect of moving the IR-FEL beam significantly. The alignment of the HeNe beam through the spectrometer was also observed to be significantly different after the beamline was evacuated. Curiously, the alignment of the IR-FEL and coincident HeNe alignment beams with the entrance slits of the spectrometer remained unchanged, although the optical alignment through the spectrometer was changed significantly, leading to a large spectral calibration shift. This seemingly odd behaviour is attributed to the effect of the focusing lens in the optics box, which retained its focus position as the angle of the incident light on it changed. As the spectral calibration appeared insensitive to adjustment of the mirrors and beamsplitter in the optics box, it was decided to correct the alignment using the angle of the upstream mirror M6. This alignment work was done in early September and left unchanged until the FELIS experiment started in mid-November.

Figure 5 shows a measurement of the zero order position for the IR-FEL beam using Grating 3, an undulator gap of 12 mm and a machine energy of 25 MeV at the start of the November FELIS experiment. It is measured in scan mode using the single element pyro detector. A calibration shift of approximately 1.5 nm is observed in the recorded wavelength of the zero order transmission of the IR-FEL beam. To correct for this using the steering of mirror M6 would require an adjustment in the roll of the mirror by about
Figure 4: The theoretical dispersion of the spectrum across the detector plane of the spectrometer.
-400 steps. As the IR-FEL beam had already been aligned on the optical table, this adjustment was not made as any adjustment of the optics upstream of the optics box affects both the spectrometer alignment and that to the instrument on the optical table. On setting up the FEL to obtain $\lambda = 7 \mu m$ radiation on 10/11/11 using a 15 mm undulator gap and 25 MeV, an absorption line was noticed in the pyroarray response. This was attributed to a possible absorption line in the polystyrene standard that was affixed to the entrance slits of the spectrometer. On 11/11/11 it was decided to measure this more accurately. However, setting the undulator gap to 15 mm did not show this feature. The gap was stepped between 14.80 mm and 15.30 mm in increments of 0.05 mm before the absorption feature was found using a gap of 15.22 mm. It is clear therefore that the absolute electron energy of ALICE varies from day to day, needing a retuning of the undulator gap by $\pm 0.2$ mm to obtain the same radiated wavelength. As the actual electron energy is determined by the RF phasing and other factors as well as the dipole field strengths, it is dependant upon the precise tune of ALICE and is expected to be variable. The value to any spectroscopy experiments of a well calibrated spectrometer to measure the IR wavelength generated is clear.

Figure 6 shows the spectral absorption line recorded by the pyroarray. It shows two spectra, one with the polystyrene standard in place on the entrance slits of the
Figure 6: The absorption line in the polystyrene standard as seen using the pyroarray. The red spectrum is of the unattenuated FEL output, the blue spectrum features a strong absorption line from the polystyrene.

spectrometer (blue), the other is the unattenuated FEL beam with the standard removed (red). Repeating the absorption measurement using the spectrometer in scanning mode with the single element pyro-detector gives a measurement of $\lambda = 6.89\mu$m radiation for the generated FEL radiation. This gives an absorption line at $\lambda = 6.87\mu$m, or about 1455 wavenumbers. Each measurement in Figure 6 is the average of approximately 600 individual spectra from the pyroarray recorded over a 30 second period. The FTIR analysis of the polystyrene standard (Figure 3) gives a pair of intense lines at 1452 and 1492 wavenumbers. We therefore see good agreement between the observed absorption line in Figure 6 and the expected line at 1452 wavenumbers. In looking for this absorption line, the undulator gap was decreased to 14.8 mm (approximately $\lambda = 7.15\mu$m) giving a decrease of $\sim 50$ wavenumbers in the measured IR wavelength. It is therefore reasonable to conclude that the lower wavenumber absorption line of the 1452/1492 pair was the one found in Figure 6.
4 Conclusions

With care the spectrometer can be correctly aligned with the beamline to give good wavelength calibration. Any adjustment of the beamline optics upstream of the optics box should be done with care as it will impact on the calibration / alignment of the spectrometer.

The polystyrene standard should be used to confirm the calibration of the spectrometer by using an absorption line that is close to the spectral line of interest in the sample. This calibration should be checked at least daily as the nominal machine energy and the selected undulator gap are not sufficient to generate a predetermined wavelength and some adjustment of the gap is necessary to allow for variation in the actual energy of the electron beam.

Alignment of the beamline can be confirmed by measuring the zero order calibration of the spectrometer. Any noticeable error (certainly if greater than the line width of the FEL) should be cause for concern.

To confirm the wavelength reported by the pyroarray software it is recommended to also collect a spectrum in scan mode using the single element pyro-detector.