DXS 4f-HRM: Misalignment with Random Data Distribution and Optimization of Heat Compensation

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Introduction

1. Motivation

The 4f-High Resolution Monochromator (4f-HRM) is an indispensable part to the LCLS-II-HE-DXS upgrade, providing the science opportunities such as:

•Characterization of collective modes of metastable materials phases (e.g. via laser/field manipulations or other transient stimuli)

•Characterization of collective modes in complex materials in the critical energy resolution range ~2-25 meV (~kT)

•Expected impacts in quantum materials, condensed matter chemistry, and amorphous materials, as a result of the high-resolution capabilities being developed

However, due to its complexity (numerous optical components), flexibility (fully tunable bandwidths and pulse duration), and precision (high-resolution capabilities), multiple testing of robustness and optimizations need to be conducted before physical production.

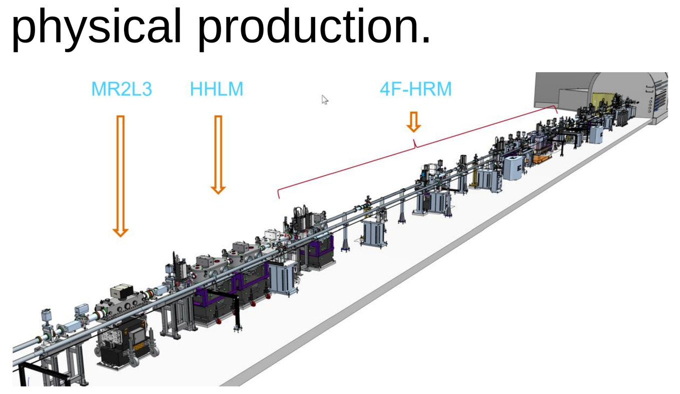
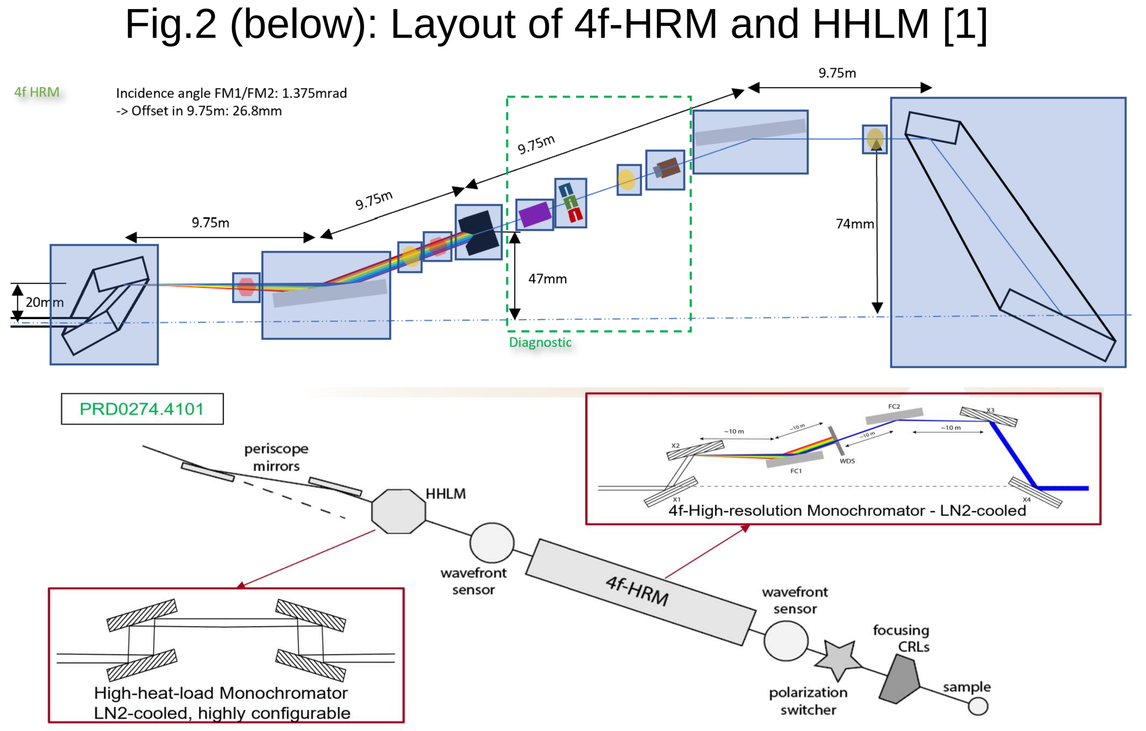


Fig. 1(left): Location of the MR2L3, HHLM, and 4f-HRM. (Note: Other telescope devices, including MR1L3, MR1L0, and MR2L0, are not shown in this figure due to its distant location.) [1]

Fig.2 (below): Layout of 4f-HRM and HHLM [1]



2. Problem Statements

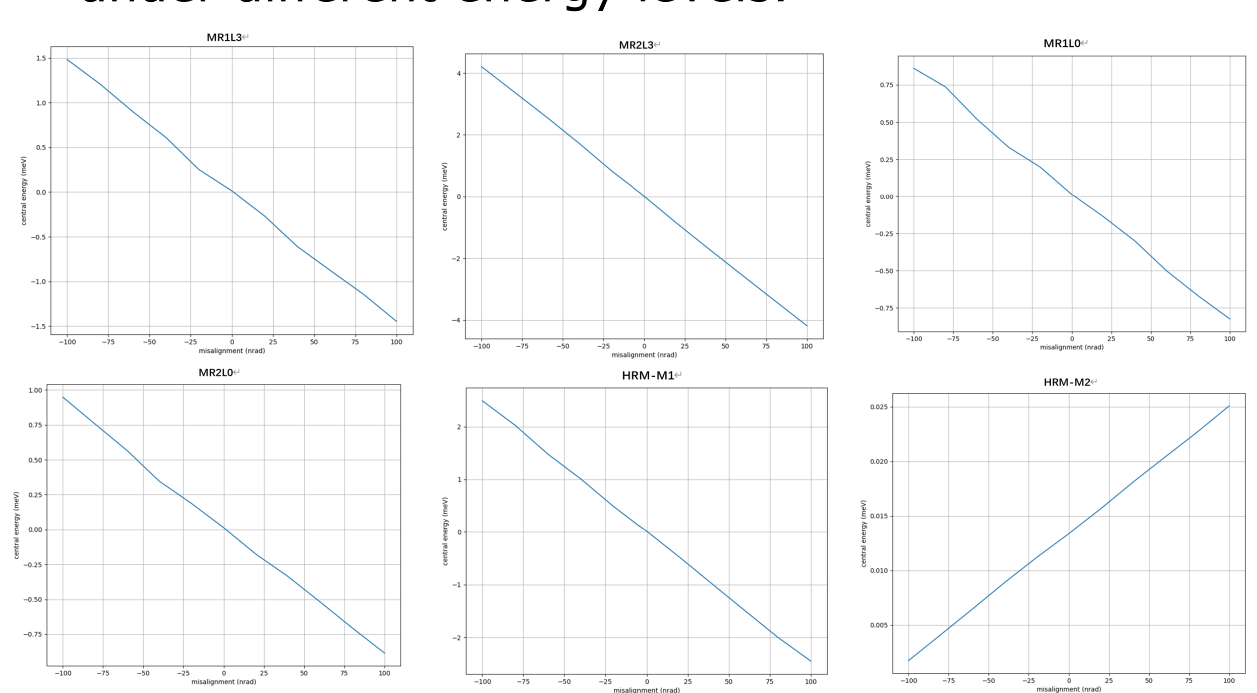
- The alignment tolerance of the components (i.e., How sensitive are the optical components during the beam propagation, and how accurate are the results after the propagation with misalignments of the optical components)
- The optimization of the mirrors' foci compensating for the crystals' heat deformation under high-power beams (i.e., What is the best focus value for the mirror to compensate for the crystals' heat deformation caused by the high-power beam)

Methods & Results

I. Alignment Tolerance

1. Linearly Distributed Alignments

- To begin with, the testing of the alignment tolerance of the HRM is conducted in a simple case: examining the relation between linearly distributed angles of the components and the resulting beam's central energy under different energy levels.



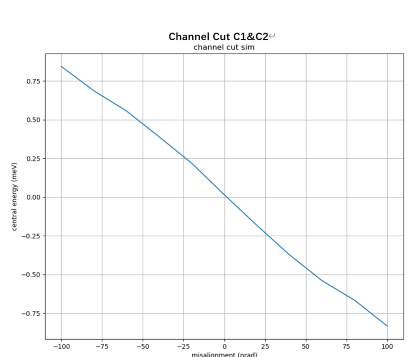


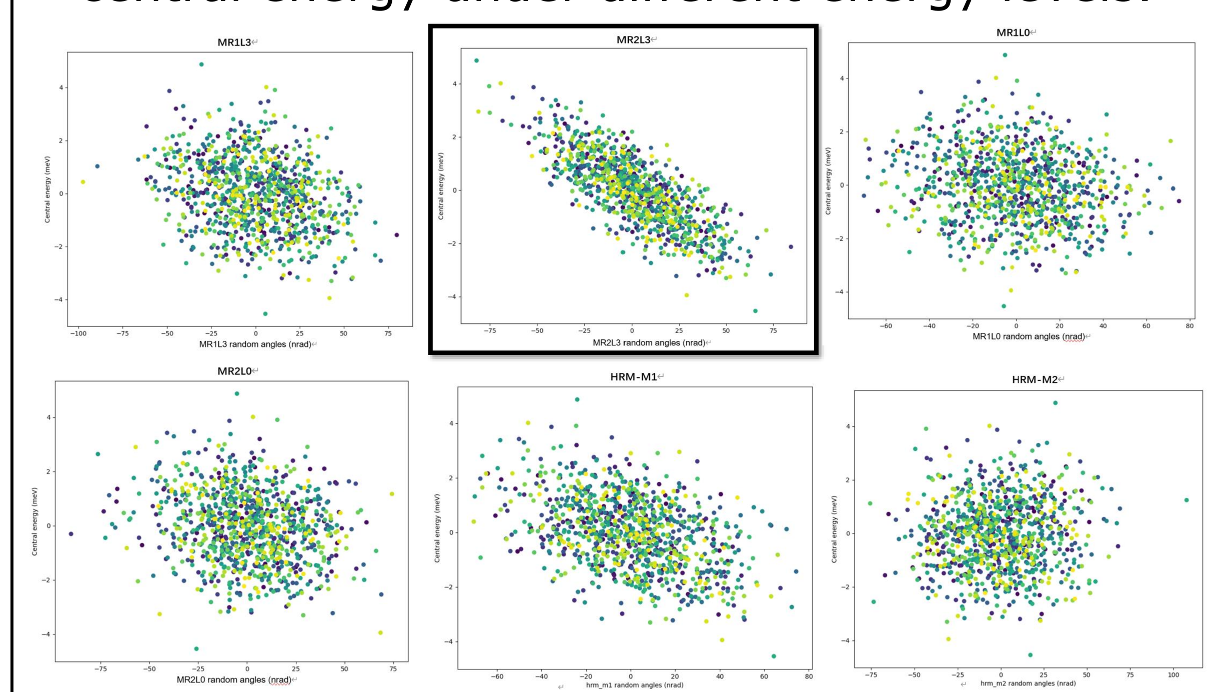
Fig.3: "Misalignment angles (nrad) vs. Central Energy Shifts (meV)" plots of the 8 different components in the simulated propagation under energy level 9500 eV. With the same range of angles, MR2L3 (first row, second column) has the greatest slope among these components, meaning that it is the most sensitive device in the configuration.

Devices E_0 (eV)	mr1l3	mr2l3	mr1l0	mr2l0	hrm_m1	hrm_m2	c1&c2
9000	-0.0147	-0.0422	-0.0085	-0.0091	-0.0249	0.0001	-0.0086
11215	-0.0198	-0.0573	0.006	0.004	-0.03	0	-0.0159
5500	-0.0101	-0.028	-0.0054	-0.0059	-0.0127	6.75e-06	-0.0075

Table 1: The slope of the "Misalignment angles vs. Central Energy Shifts" line of different components under 3 different energy levels. As shown above, MR2L3 has the greatest value however the energy changes, quantitatively confirming that it is the most sensitive device.

2. Randomly Distributed Alignments

- Now with our results in the linear case, we could forward the alignment tolerance testing to a more complex scenario: examining the relation between randomly distributed angles of the components and the resulting beam's central energy under different energy levels.



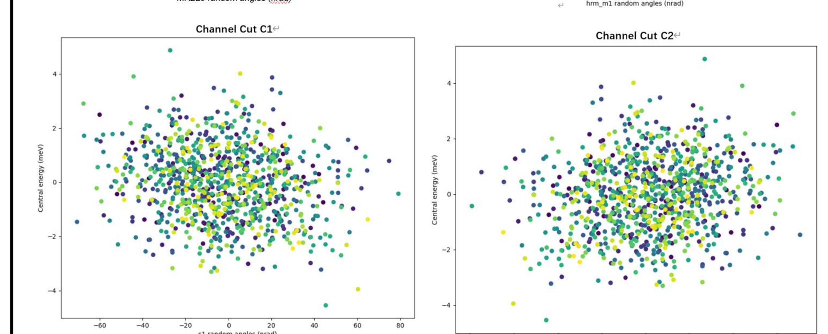


Fig.4 : "Random Misalignment angles(nrad) vs. Central Energy Shifts(meV)" plots of the 8 different components in the propagation under energy level 9500 eV. Again, only MR2L3 (first row, second column) has a strong correlation between the central energy shifts and randomly generated angles, indicating it is the most sensitive device.

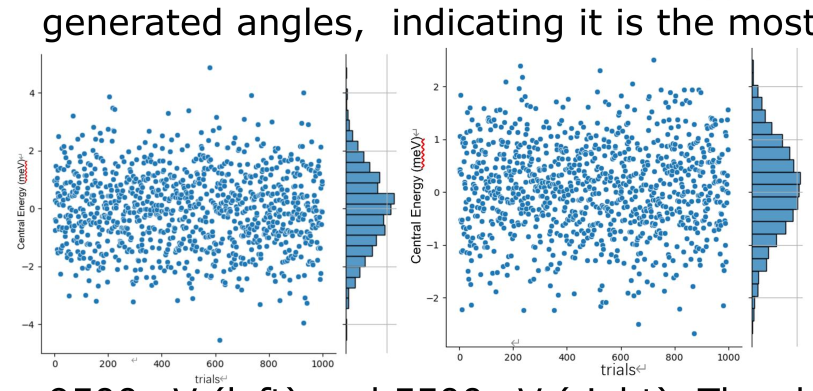


Fig.5 : "Distribution of the Central Energy Shifts" plots of the entire configuration under the energy levels of 9500 eV (left) and 5500 eV (right). The shape of the result is close to a Gaussian Distribution, which is what we expected.

3. Comparison with Diagnostic Spectrometer

- We will comparing our results above with the data from a diagnostic spectrometer inside 4f-HRM as a sanity check, since the value of central energy shifts cannot be obtained in real experiments. We need to convert the centroids providing by the spectrometer to central energy shifts and examine the results.

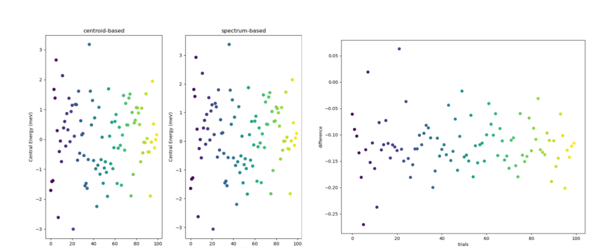


Fig.6 : Plots of the comparison between the different-methods-generated central energy shifts. The left figure shows the central energy shifts by converting the centroids measured by the spectrometer; the middle figure shows the central energy shifts measured by the computer simulation; and the right figure shows the difference between these two types of central energy shifts. As shown in the plot, the differences are small enough to be ignored (within ±0.5meV), indicating that our simulated results can be applied to reality.

II. Optimization of Heat Compensation

- The equipment's crystals are prone to deform under high-power beam and lose its required high-resolution capabilities [2].

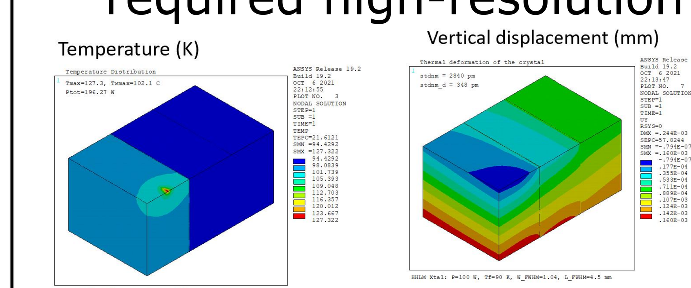


Fig.7: Crystals' Heat Deformation caused by the high temperature generated by high-power beam. [1]

- We choose to use Bayesian Optimization [3], which is an efficient method for global optimization of black-box functions, since our simulated beam-propagations are time-consuming to be evaluated.

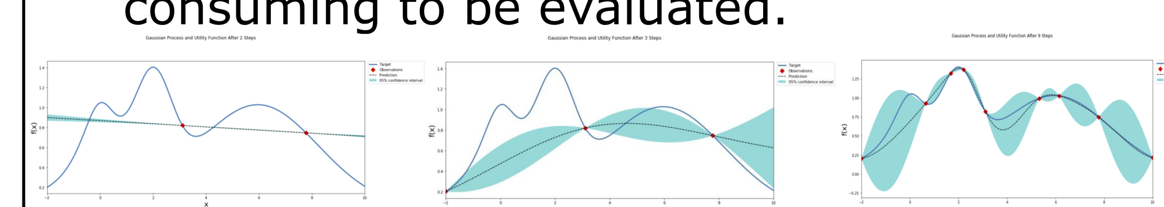


Fig.8: Processes of Bayesian Optimization [3]. The predicting curve will approach to the original function after each iteration.

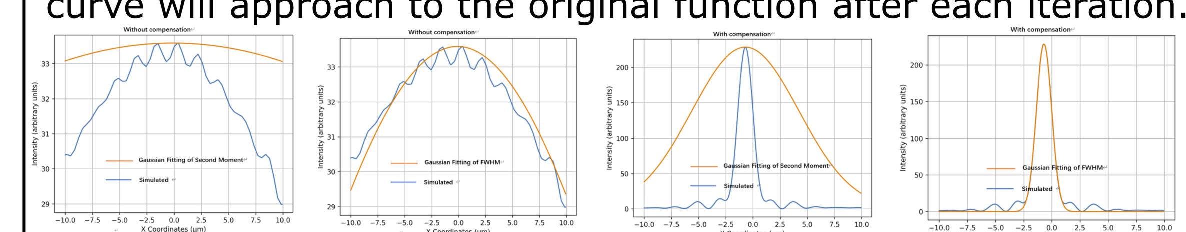


Fig.9 (above): Comparison of results with or without the existence of compensation, measuring the second moment of the x lineouts and FWHM

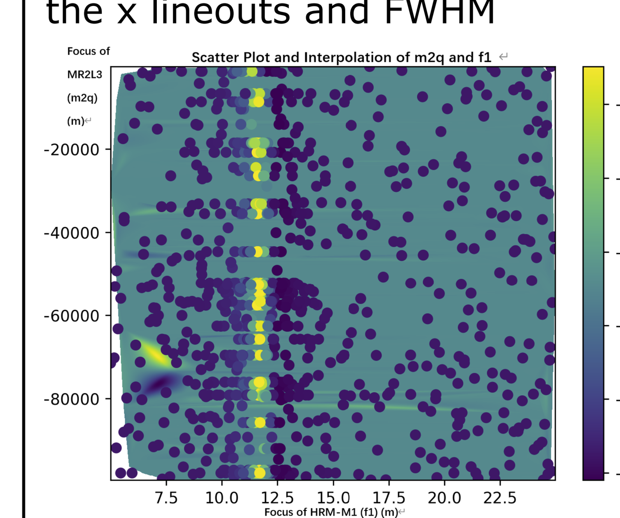


Fig.10 (left): The scatter plot shows the resulting second moments with a specific configuration of m2q (focus of MR2L3) and f1 (focus of HRM-M1). The interpolation of these two variables is the background of the figure. Plugging the optimal values, we have the resulting curve in the two plots on the right of Fig.9

Conclusions

Outcome

- With the linearly and randomly distributed angles, the relations between the misalignments and central energy shifts are examined and recorded
- MR2L3 is the most sensitive device among the components
- The crystals' heat deformation are successfully compensated with the m2q value of -20833.18 meters and the f1 value of 11.58 meters.

Further Work

- Misalignment data will be handed to engineering group for physical production.
- "p" value of MR2L3 and HRM-M1 would be added to optimization as parameters for further improvements.
- Add "phase shift" to the propagation for better fitting of the curve in Fig.9

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References

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