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ABSTRACT
The finite element method (FEA) was used for thermal mechanical behavior analysis of a monochromator subjected to high heat load for a beamline at the High Energy Photon Source (HEPS). Without using reflection mirror, high energy photons deposit directly on the first crystal of DCM (Double Crystal Monochromator) with power density up to 69W/mm². This paper introduces an indirect cooling structure with multi-channels cut inside the cooling blocks, which can effectively reduce the crystal deformation caused by high heat deposition. The effects of power and power density on crystal temperature and deformation are compared and its variation discipline with the distance between monochromator and light source (undulator) are studied. The research results have reference significance for thermal management of monochromators as well as other optical elements in HEPS.

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I. INTRODUCTION

The High Energy Photon Source (HEPS), a 6 GeV diffraction-limited ~60 pm rad storage-ring light source, is under construction in Beijing, China, and will be operational before 2025.

HEPS is designed for brighter and more intense light and there are 14 beam lines in design at present, its light will be widely used in physics, chemistry, biology, medicine, archeology, materials, science, microelectronics, environmental protection etc.

The thermal deformation caused by high brightness and high flux light is an important problem for optical components. The thermal deformation of the crystal induces rocking curve broadening, which leads to a loss of monochromatic flux. Furthermore, the shape change of the reflecting surface may deform the wave-front and thus have a negative impact on coherent and micro-focusing experiments. At present, cryogenic cooling with liquid nitrogen is mainly used to evacuate heat of silicon crystal either by direct cooling or indirect cooling. It is worth mentioning that the fabrication of directly cooled crystals is much more complicated, time-consuming and costly. Considering the complex manufacture of direct cooling process, indirect cooling is generally used when it can meet the requirements. Indirectly cooled silicon monochromator will be used in HEPS, to judge the whether the cooling structure meets the requirements, thermal deformation prediction and thermal management optimization are necessary. Usually, the first optical component in a synchrotron radiation beam-line is subjected to a high heat load form the X-ray source, monochromator is the first optical element in some HEPS beam lines. The beam footprint on crystal (X-ray beam illuminated area) is variable and typically much smaller than the crystal size because of the variable and large Bragg angle.

Numerous studies have been carried out to assess the performance of crystal with cryogenic cooling both by simulation and experimental testing. FEA simulations can determine the strain field in a heat-distorted crystal, and therefore the deformed shape of the crystal. L. Zhang et al. presented the details of the finite element modeling procedure used to calculate the thermal deformation generated by the X-ray power absorbed in silicon crystal. The reliability of FEA prediction has been verified by A. K. Freund et al., they found out good agreement between the calculated crystal rocking curve and the observed ones. Therefore based on the finite element method, the crystal temperature distribution and surface deformation analysis in HEPS is carried out in this paper. The results can
be used as reference for parameter selection and provides a basis for optimal heat management.

The heat load is attached on surface of crystal with different distributions. This paper discusses the effect of power and power density on crystal’s deformation. In addition, for purpose of reducing surface deformation of crystal, this paper studies the influence of distance from the monochromator to light source on crystal deformation, and compares the differences between two operating conditions (maximum power and maximum power density energy points). The study results have reference significance for the selection of optics position in the beam line.

II. FINITE ELEMENT MODELING

The maximum heat flux of 69 W/mm² in an undulator beamline would mainly cause local ball and crystal lattice thermal distortions, due to temperature gradient distribution of the crystal bulk. Indirect cooled method is adopted here, the crystal is clamped between two copper heat exchangers and the clamping pressure is set to be about 0.4 MPa. Liquid nitrogen flows through 16 rectangular channels inside the cooling block with a net surface area of as much as about 345 cm². According to Aleksandra Chumakov et al., that the crystal surface deviates from a flat plane by a certain slope error δ, which is proportional to the beam power P according to

\[ \delta \propto \Delta d \propto \alpha \Delta T \propto (a/k)P \]  

Where \( \alpha \) is the temperature expansion coefficient, \( k \) is the thermal conductivity, \( \Delta T \) is the temperature gradient and \( \Delta d \) is the variation of the lattice constant.

A. Geometry

An example of crystal geometry with its cooling structure is shown in Figure 1. It is useful to oversize the crystal height in order to increase the heat exchange surface area between cooper and silicon.

The dimensions of crystal is 60mm×24mm×40mm, which is based on existing published research experiences. Both of the length and height of the cooling blocks are larger than those of the crystal’s.

Small and dense cooling channels can greatly increase the heat transfer area, but at the same time the flow resistance increases. Therefore, a proper selection of channel structure is important for heat transfer efficiency as well as stability of cooling system.

B. Boundary conditions

From the view of direct causes of crystal deformation, there are three main methods for reducing deformation: 1) Reducing the thermal deformation quality coefficient of the crystal material (\( a/k \)); 2) Using an appropriate cooling method and cooling structure; 3) Increasing the footprint size on the crystal surface.

1. Material properties

Silicon has a coefficient of thermal expansion of zero at 125 K, which is an ideal deformation zone. In fact, at temperature below 125 K, the deformation of crystal is in a contracted state, and when temperature exceeds 125 K, it begins to translate to an expanded state. Research has shown that when this maximum temperature is near \( T=165 \) K, the thermal deformation of the crystal reaches a local minimum (but not zero deformation since the temperature in the crystal is not uniform). The expansion coefficient of the cooling material needs to be close to the expansion coefficient of silicon, otherwise it will cause extrusion deformation and oxygen-free copper is an excellent choice. The thermal conductivity and coefficient of thermal expansion of silicon versus temperature is shown in Figure 2.

2. Heat transfer settings

The thermal resistance of the interface between cooling block and silicon causes temperature step, thus directly affecting the temperature of crystal. When the amount of heat transfer is given, the temperature step value is inversely proportional to the heat transfer resistance. The magnitude of contact thermal resistance depends both on the smoothness of the contact surface and on the clamping pressure. In the example of this paper, the contact thermal resistance is set to be \( 10^4 \) W/mm² K. Heat transfer is driven by the temperature difference, and the presence of thermal resistance will weaken the process and the heat amount will drop. Using the thermoelectric analogy method:

\[ I = \frac{V}{R_e} \sim Q = \frac{\Delta T}{R_h} \]  

Where \( I \) representing current, \( V \) is voltage; \( Q, \Delta T \) and \( R \) represents heat transfer capacity, temperature difference and resistance respectively.

The convection heat transfer coefficient is applied to the inner surface of the rectangular passages, and its value is adjusted according to the actual calculated temperature. Both the ambient and initial temperature is given at 80 K (the evaporation temperature of liquid nitrogen at atmospheric pressure is 77.9 K). The essence of increasing the convection heat transfer coefficient is to reduce the temperature difference between the cooling medium and the cooling channel wall. When the temperature difference is relative small or the change of the temperature difference is not obvious as the heat transfer coefficient changes, it is considered that increasing the coolant flow is not helpful. For a synchrotron monochromator, the absorbed heat is constant, so the convective heat transfer coefficient is inversely
proportional to temperature difference. In formula (3) \( h \) and \( A \) is heat transfer coefficient and heat transfer area.

\[ Q = h \cdot A \cdot \Delta T \] (3)

3. Heat load

For monochromator, the energy points with the maximum total power and the maximum energy density must be thermally analyzed, since the surface deformation depends both on power and power density. Micro-focusing X-ray protein crystallography beamline in HEPS has the largest total power up to 160 W when the fundamental wave energy is 2.9 k eV. Due to the relative big Bragg angle of 23.292° at 5 k eV, the peak power density almost reaches 70 W/mm². Figure 3 shows the power density distribution at the distance of 35 meter away from the light source.

III. RESULTS

A. Temperature

During optical design, the heat deposited on surface of the monochromator can be weaken by applying diamond window and reflection mirror in prior line. On the other hand, the power density can be reduced by increasing the footprint area. The conclusions about the trade-offs between these two parameters can be used for design reference.

The temperature distributions after cooling under two cases are calculated and the temperature drop is mainly concentrated in the footprint and the small area of its surroundings. The results show that at the energy point of 5 k eV, the temperature range (the gap between the maximum temperature and the minimum temperature of crystal bulk) is less than that of 2.9 k eV's. The specific parameters of two operating conditions are given in Table 1 for specific analysis and comparison. Figure 4 shows the temperature distribution of two case after cooling.

By comparing the data in Table 1, it can be found that although the power density is large due to the small footprint size at 5 k eV, the required coolant flow rate the total temperature difference are less than those at 2.9 k eV, thus the following conclusions can be drawn:

1) The magnitude of the absorbed power has a greater effect on the temperature distribution of the crystal than the power density. Excessive power density may cause large local bump, but has relative small effect on total temperature distribution and
TABLE I. The specific parameters of two cases.

| Cases | Total Power (W) | Peak Power Density (W/mm$^2$) | Heat Transfer Coefficient (W/m$^2$ K) | Footprint (mm$^2$) | Total Temperature difference (K) |
|-------|----------------|------------------------------|--------------------------------------|-------------------|---------------------------------|
| 2.9 k eV | 160            | 62                          | 3500                                 | 3.3917×0.77     | 63.775                          |
| 5 k eV   | 102.4          | 69.3                        | 650                                  | 1.9473×0.77     | 56.76K                           |

cooling medium’s flow rate. Therefore, in order to reduce the cooling medium’s flow rate, which is fatal to the stability of the system, it is necessary to reduce the total absorbed power on the crystal, such as putting reflection mirror in front of the crystal.

2) Compared with the total power at 5 k eV, the power at 2.9 k eV increases by 36%, but the convection heat transfer coefficient increases several times, it seems that the increase of the convection heat transfer coefficient cannot bring significant cooling effect. The reason is that when the convection heat transfer coefficient increases to a certain extent, the temperature difference between the cooling surface and the coolant is getting closer, so the cooling effect of increasing convection heat transfer coefficient becomes less and less obvious. We know the temperature difference is the driving force of heat transfer.

3) The total temperature difference of the crystal (from the wall surface of the cooling channel to the center of the footprint) increases as the footprint area becomes larger.

B. Deformation

The surface shape and deformation data of both meridional direction and sagittal direction in the footprint under two energy conditions are calculated and presented in Figure 5. During the calculation, the acceptance angle of $4\sigma$ is chosen to receive more photons and $3\sigma$ of the footprint center is actually used. Therefore, attention is paid to the light in the actual use range and the slope error are all within $4\mu$rad. In practice, some quadric optics in the rear optical system will be used after monochromator to correct the shape. The corrected error needs to be controlled within $1\mu$rad, which is a well-recognized surface shape. By analyzing the deformation results, the following conclusions can be drawn:

1) When the crystal temperature is around 140 K, the deformation shape is still concave;

2) The deformation and slope error at 5 k eV are both greater than that at 2 k eV, this is due to its small footprint size and large power density which causes large temperature gradient at the footprint area. The temperature gradient are about 17 K/mm at 5 k eV and 11 K/mm along the incident direction in the footprint;

3) The deformation in the sagittal direction is less than meridional direction. By observing the deformation contour, the deformation difference between two directions increases with the increases of the footprint area. The reason is that the acceptance angle and power distribution of the incident beam are identical in meridional and sagittal directions. Smaller Bragg angle leads to larger length in footprint area, thus inducing larger deformation difference between two directions.
IV. HEAT MANAGEMENT OF MONOCHROMATOR

According to previous analysis, the power density has a greater influence on the deformation of footprint area than total power. When the acceptance angle of the light source is fixed, increasing the distance between monochromator and light source can increase the footprint area, thereby reducing the power density. Increasing the distance between monochromator and light source is one of the simple and practical ways to reduce power density in footprint area. This paper explores the scheme aiming at finding a better way to improve the surface deformation of crystal.

In this paper, the effect of distance between monochromator and light source on crystal deformation are studied at 2.9 k eV and 5 keV. The deformation of monochromator at 35 m to 60 m with increasing step of 5 m are calculated respectively. Table II and Table III separately show the power density and footprint size as a function of distance at two case.

Power density is inversely proportional to the square of the distance. Therefore, increasing the distance is more effective for reducing power density when the power density is larger. The deformation of monochromator at different distance is calculated, which provides a reference for the thermal management of the monochromator for the optical design.

Similarly, the temperature of crystal at each condition is very close by adjusting the flow rate (it is hard achieve the same temperature because a large amount of flow regulation tests are required) in order to compare the deformations.

A. Temperature

Figure 6 and Figure 7 represent the temperature field of footprint area at the energy points of 2.9 k eV as well as 5k eV. It can be seen from the temperature distribution contour that as the distance increases, the temperature range of the footprint area...
TABLE II. Value of footprint size and average power density as a function of distance @2.9 keV.

| Distance (m) | Total Power (W) | Footprint size (mm$^2$) | Average Power Density (W/mm$^2$) |
|-------------|----------------|-------------------------|-------------------------------|
| 35          | 160            | 2.6116                  | 61.26                         |
| 40          | -              | 3.4111                  | 46.91                         |
| 45          | -              | 4.3171                  | 37.06                         |
| 50          | -              | 5.3298                  | 30.02                         |
| 55          | -              | 6.4491                  | 24.81                         |
| 60          | -              | 7.6749                  | 20.85                         |

TABLE III. Value of footprint size and average power density as a function of distance @5 keV.

| Distance (m) | Total Power (W) | Footprint size (mm$^2$) | Peak Power Density (W/mm$^2$) |
|-------------|----------------|-------------------------|-------------------------------|
| 35          | 102.4          | 1.4994                  | 68.29                         |
| 40          | -              | 1.9584                  | 52.29                         |
| 45          | -              | 2.4786                  | 41.31                         |
| 50          | -              | 3.0601                  | 33.46                         |
| 55          | -              | 3.7027                  | 27.66                         |
| 60          | -              | 4.4065                  | 23.24                         |

gradually decreases, but the trend becomes less obvious with the increase of distance. Therefore, there exists a reasonable distance beyond which less effect will be brought by increasing the distance between monochromator and light source.

The following is a comparison of the crystal deformation under different working conditions. Combined with the flow rate of the cooling medium (characterized by the convection heat transfer coefficient), a relative optimal distance value can be found. Since the deformation trends of sagittal direction are in consistence with those of meridional direction, only the deformation data of the center line in meridional direction are used for comparative analysis.

B. Deformation

Observing Figure 8 and Figure 9 we can see, the increase in distance makes the shape of footprint area becomes more gradual,
FIG. 9. Slope error of footprint area at various distances (5 k eV, meridional direction).

which fully highlights the effect of increasing footprint size on reducing crystal’s deformation. At distance of 60 m, slope error of both 2.9 k eV and 5 k eV are around 2 μrad.

The root mean square (RMS) of deformation under each working condition is calculated for further analysis. For 2.9 k eV energy point, with distance increasing from 35 m to 60 m, the RMS value of the footprint area is reduced by 50.2% and the decreasing process is basically linear; For 5 k eV energy point, this parameter is reduced by 59.25% and the decreasing process becomes gentle as the distance increases. Variation of RMS can be clearly seen in Figure 10. By analyzing the variation of crystal deformation with the distance between monochromator and light source under two conditions, the following conclusions can be drawn:

1) For energy point with pretty large power density, increasing distance between monochromator and light source can effectively reduce the power density so that the deformation of crystal can be controlled with an acceptable range. It should be noted that the decreasing process becomes less obvious as the distance further increases. For the example in this paper, addition of distance during the practical design can be adjusted according to the crystal deformation demands;

2) For the energy point whose power density can be easily handled, increasing the distance has approximate linear effect on crystal deformation. Therefore, practical design can be comprehensively selected according to both crystal shape demand and the line station space.

V. CONCLUSION

Finite element analysis (FEA) was used to simulate thermal deformation of monochromator in HEPS. For Micro-focusing X-ray protein crystallography beamline, two energy points (maximum total power: 2.9 k eV and maximum power density point: 5 k eV) were thermally analyzed. By analyzing temperature distribution of the crystal and deformation of the footprint area, the different influences of power and power density on crystal temperature and deformation are obtained. For the currently calculated beamline, from the perspective of thermal management, the optimal distance is about 50 m, and the gain is no longer obvious after this distance. Of course the distance that the monochromator is placed must also be considered from view of optical design. The results also show that increasing the distance is more effective for energy point with a higher power density.

In addition, thermal management of monochromator in beamline is explored. Results show that the distance between monochromator and light source has different effects on crystal with different power densities. The research results can be used as a reference to control surface shape of crystal in the optical design.

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