DESY Summer Student Project 2010

Finite element analysis of the stress-relieving cuts in the diamond monochromators

Workgroup: European XFEL, WP-73

Author: Michal Borovský

Supervisors: Fan Yang, Harald Sinn

Contents

1 Introduction

The European X-ray free electron laser (XFEL), which is currently under construction and in the development phase, will be the one of the most advanced FEL research facilities in the world. It will produce the 27 000 ultrashort coherent X-ray flashes per second with the peak brilliance, which is a billion times higher than that of the best conventional X-ray sources at the moment. It is obvious that the 4^{th} generation light source of such a unique characteristics requires the technological equipment of very specific properties.

The crystal monochromators are one of the key parts used in the X-ray beam transport. Their main capability is to select desirable bandwidth from the polychromatic light source. This can be done by either Bragg reflection or Laue transmission. The silicon single crystals are the most common choice because they can be produced in large proportions without significant lattice defects and they can be cut into any shape practically. But the problem arises when we want to use them in XFEL due to enormous head load which is applied on it and this causes lattice deformations despite the use of the cooling medium. Therefore the diamond single crystals are planned to be used in XFEL instead of the silicon because they have a higher thermal conductivity and smaller thermal expansion at low temperatures.

Unfortunately, the process of synthesizing large diamond single crystals, which are optically perfect in the X-ray spectrum, has not been developed yet. Nowdays, we are able to create a single crystals only a few millimeters large by the means of High Pressure-High Temperature (HPHT) method. Such a small crystals have a small thermal capacity, therefore they have to be bonded to some heat sink medium with high thermal conductivity under low temperatures. The best material suitable for this is the Chemical Vapor Deposition (CVD) diamond.

The next step is to bond single crystal diamond to CVD diamond. The currently studied method is shown in the Fig. 1. At first the cut is made of the single crystal shape in the center of CVD disc by laser. Then we let

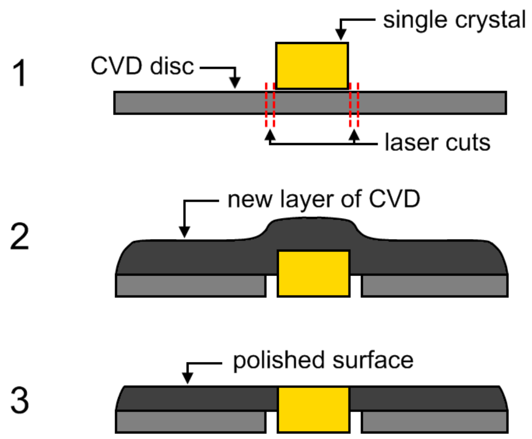


Figure 1: Process of bonding single crystal diamond to CVD diamond disc

it over-grow with a new layer of CVD and in the end the surface of new-created CVD is polished. This method provides a good heat sink due to direct bonding, but on the other hand the stress and bending of the single crystal are observed. The possible solution to relieve this stress is to make cuts in the CVD. The realization of this idea is presented in the Fig. 2.

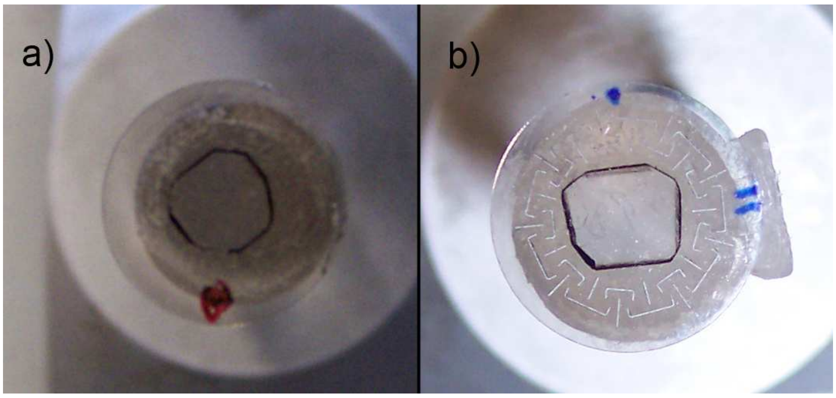


Figure 2: Technical realization of the stress-relieve cuts. a) sample "15_1" without cuts, b) sample "13_2" with cuts.

The goal of our work is to simulate the stress on the models both with or without cuts and observe the deformations of the single crystal part and compare the obtained results between each other.

2 Method

For the numerical simulations, we used finite element analysis (FEA) software ANSYS 11.0 Academic Version. In ANSYS the FEA has steps as shown in Tab.1.

PRE-PROCESSING	• create the geometrical model of the studied object • discretize the object into a finite number of elements connected together with so called nodal points (NP) • define the elements' material properties (e.g. modulus of elasticity, density, Poisson's ratio, thermal expansion coefficient,...) • specify the supports (boundary conditions) • specify the loads (forces, thermal expansion, deflections,...)
ANALYSIS PHASE	• formulate simultaneous equilibrium equations to each degree of freedom at each NP representing the total structure's stiffness • solve these equations for the displacements at each NP • uses NP displacements to solve for stress within each element
POST-PROCESSING	• make sense out of the large amount of data generated in the analysis phase

Table 1: FEA in steps

Our first step was to learn some basics of working with ANSYS Workbench, which is the software framework where FEA activities are preformed. After that we were capable of creating 3D-model of studied monochromator with or without cuts in Design Modeler as you can see in Fig. 3.

The model has following dimensions. The CVD disc is 12 mm in diameter and 0.4 mm thick. The single crystal is represented by the square cuboid of length 5 mm and height 0.4 mm with filleted corners to avoid computational singularities. To describe the model we need also to define material properites and boundary conditions. We didn't specify material properties separately for

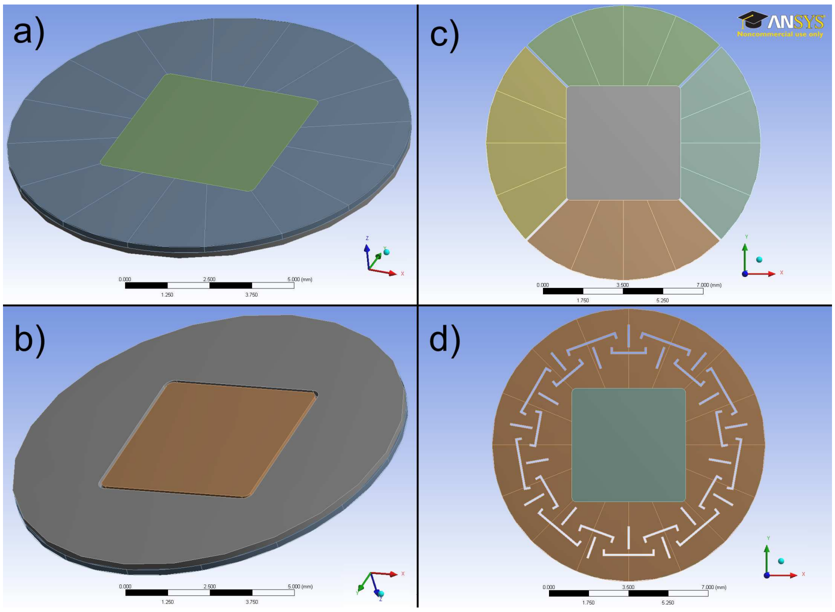


Figure 3: Geometry of diamond monochromator. a) without cuts from front side, b) and back side, c) with simple cuts d) with cuts suggested by Diamonds Materials.

the single crystal and for the CVD, because they vary very slightly. For the boundary condition, we fixed the bottom surface of single crystal diamond.

Maybe the hardest part was to choose suitable load, that would describe the real stress developed in the single crystal part during the bonding procedure. The diffraction topography, which was done on the beamline E2 during the Exercise week by D. Novikov (group leader), L. Samoylova, M. Khenkin, R. Lane, R. Al-Khuzheyri and M. Boroský, revealed, that the crystal is bent and its surface is deformed. Furthermore, the white beam interferometer at ESRF showed that the surface of single crystal is concave and the CVD dics bends convex, see Fig. 4.

The first assumption of the loading condition is to apply bending moments on the top surface of the CVD, that forms the CVD into desirable shape. The second loading assumption is to apply in plane pressure, that acts on the side surfaces of new layer of the CVD. In the case of cuts in the CVD the pressure was applied also on vertical surfaces of cuts. The third model is applied with

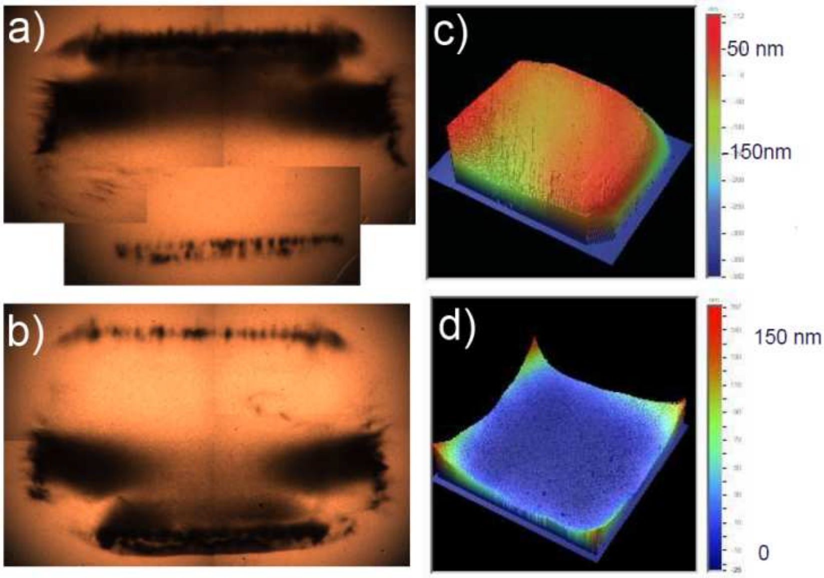


Figure 4: White beam topograms of the sample "13_2": a) left tale of rocking curve, b) right tale of rocking curve. Interferometer measurements: c) of the single crystal diamond, d) of the CVD.

temperature gradient between the top surface and the other surfaces of the new CVD layer. In the static thermal-structural analysis this gradient causes a thermal contraction. These three models with different loading conditions are shown in Fig. 5.

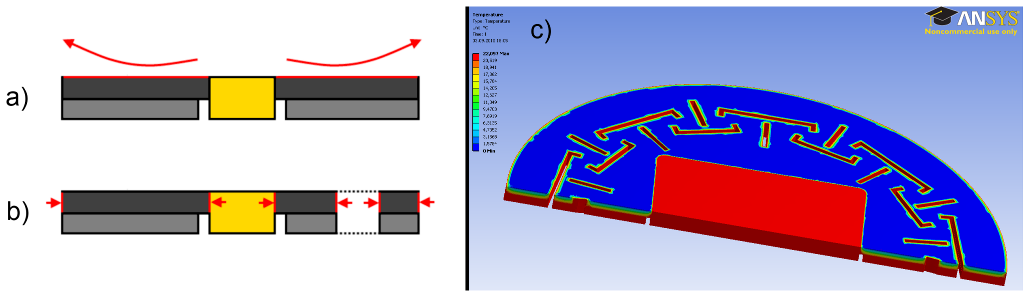


Figure 5: Models with different types of the specified load: a) the moment, b) the pressure, c) the thermal gradient.

The magnitude of applied loads was determined like this. The reference model was without any cuts with the moment of 1 N/mm. The reference parameter, that helped us to set the other loads, was the displacement in z-axis direction in the middle of top surface of single crystal, that in the case of moment model was approx. 10^{-9}. According to that we took the 14 MPa as a value for the pressure and the temperature gradient was from 0 to 22 $°C$, where 0 $°C$ is the temperature of top surface of new CVD.

3 Results

In the interpretation of our data we focused mainly on the displacement in the z-direction on the surface of single crystal, because this kind of parameter directly affects Bragg or Laue diffraction, which is dependent of the interplanary distance of the crystallographic planes. At first we will analyze how the different types of loads affects the flatness of the surface of our model. Obtained results are presented on the Figure 6. The values of the displacement were taken from the middle cross-section of the monochromator along the x-axis. The zero value refers to the center of the single crystal.

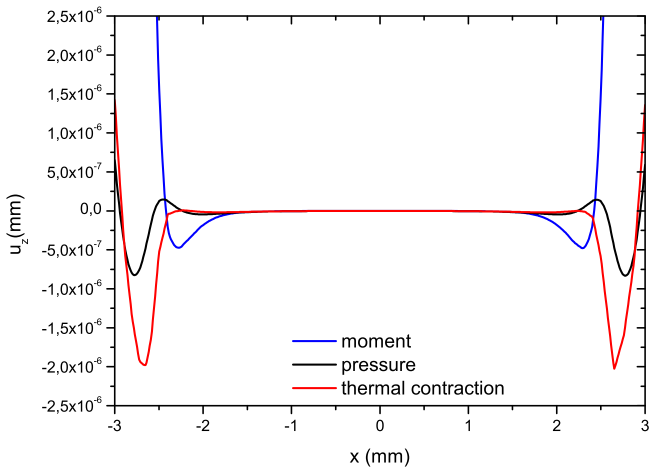


Figure 6: Vertical deformation along the diameter for the model without cuts.

As you can see the moment model shows, that the single crystal forms a simple concave bend and CVD is bend convex, which correspond with observation of real samples. Although, the two other simulations contains one more additional effect, which is the small hill formed on the edges of the single crystal. The possible evidence of its existence can be observed in topograms. On the Fig. 7 you can see the stress distribution.

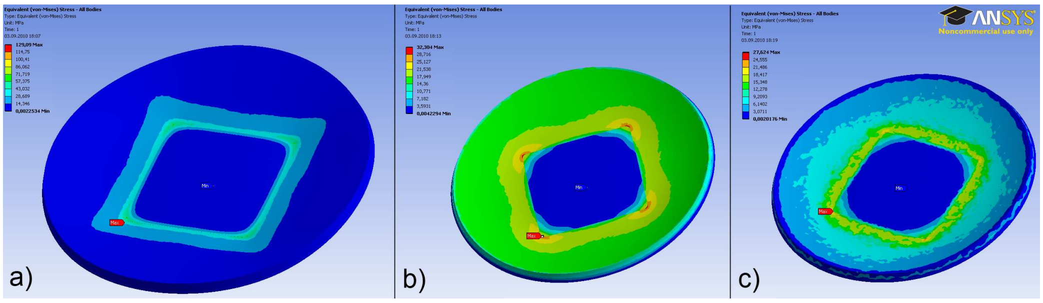


Figure 7: Equivalent stress distribuition in monochromator for: a) the moment, b) the pressure, c) the thermal contraction.

The second part of results is the investigation of the behavior of the single crystal, when stress-relieving cuts are included in the model. At first, lets have a look on the moment simulation. The deformation of the surface of the single crystal is shown in the Fig. 8.

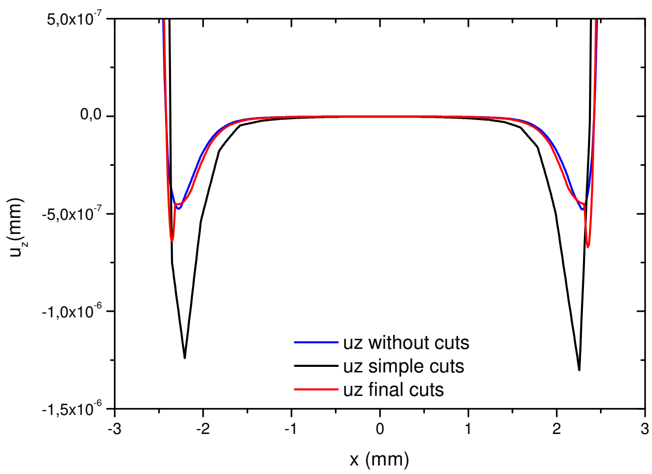


Figure 8: z-component of the displacement's dependency on x-axis position of cross-section for the moment model.

The presence of the cuts in the model with applied moment led to more bend surface of the single crystal. However, the case with the final cuts made by Diamond Materials has almost the same level of the deformation as a case without cuts. We can mention that this model is fairly inaccurate due to the rough approximation of the real deformation, where we didn't pay an attention to cause of the problem but to the final effect.

The results of the simulation with pressure acting on the new layer of the CVD diamond are presented on the Figure 9. When we compare the model without cuts with the model with the simple diagonal cuts, the first thing, which is noticeable, is the evidently smaller bend. Furthermore, the "hill" effect almost vanished in this case. The model with final cuts is also less strained, although in the smaller range. The reasonable explanation for this is, that the stress has its maxima in the corners of the single crystal in the non-cut model (see Fig. 7) and this is the exact place, where the diagonal cuts are made. We also know, that the pressure acting on the object in one direction causes the longitudinal contraction and transverse dilatation of the object. In the model with diagonal cuts there is an extra pressure that acts on the side of the CVD, whose transverse effect partially cancels the original contraction.

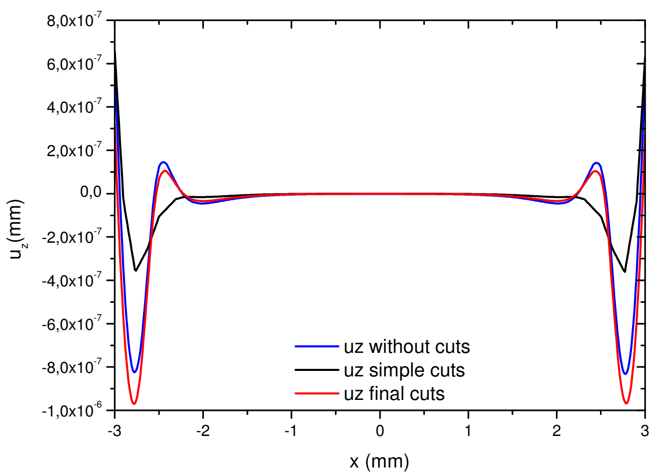
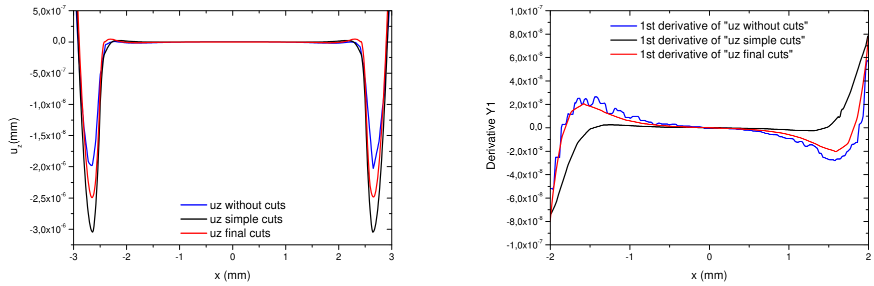


Figure 9: z-component of the displacement's dependency on x-axis position of cross-section for the pressure model.



(a) u_z (b) $\frac{du_z}{dx}$

Figure 10: z-component of the displacement as a function of x-axis position of cross-section for the thermal expansion model and its first derivative.

The third simulation is dealing with the thermal contraction of the CVD. The z-axis directional displacement is plotted in the Fig.10(a). The differences in the deformation between these models are very subtle. Therefore we have to look on the first derivative to determine the inclination in the center part of the single crystal (see Fig. 10(b)). As you can see the most flat surface in the middle of the crystal has the model with simple diagonal cuts.

To sum up, we compared the vertical deformation in the center of the top surface of the single crystal for every model, see Tab. 2.

	WITHOUT CUTS	SIMPLE CUTS	FINAL CUTS
MOMENT	$-9.4053.10^{-10}$	$-2.1123.10^{-9}$	$-1.0182.10^{-9}$
PRESSURE	$-9.8784.10^{-10}$	$-3.5352.10^{-10}$	$-7.4250.10^{-10}$
TH. CONTRACTION	$-1.01030.10^{-9}$	$-1.9291.10^{-10}$	$-5.5400.10^{-10}$

Table 2: z-component of the dis model and different types of load in kPa.

In the end lets see how these cuts affect the stress. In the Table 3 are values for the equivalent stress in the center of the single crystal. As you can see the on the pressure and thermal compression data the cuts really bring the relief in the stress. It is very clear that the most effective way is to cut CVD next to the corners of the single crystal where is the biggest stress. For the illustration, how is the stress distributed in the models, see Fig. 11.

	WITHOUT CUTS	SIMPLE CUTS	FINAL CUTS
MOMENT	9.958	20.659	11.483
PRESSURE	10.688	3.448	8.025
TH. CONTRACTION	8.520	2.075	5.991

Table 3: Values of the equivalent stress for different model and different types of load in kPa.

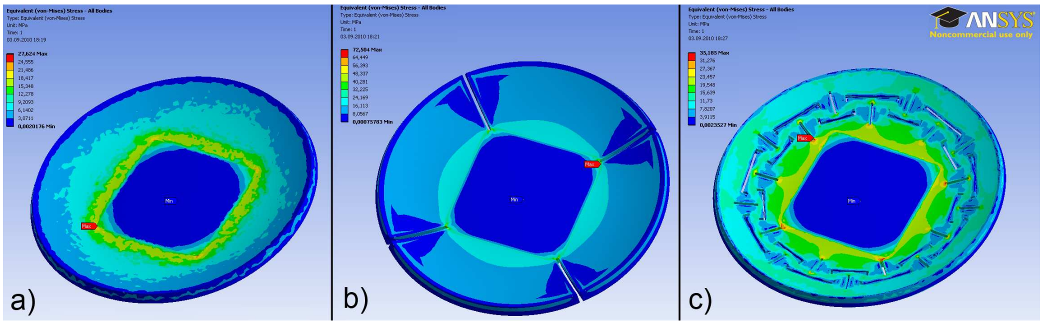


Figure 11: Equivalent stress distribution in the thermal compression model: a) without cuts, b) with simple cuts, c) with final cuts.

4 Conclusions

We have proven on the finite element analysis simulations the stress relieving effects of the cuts. However, the bending of the single crystal is still the remaining problem. The same information was obtained by the diffraction topography of the sample "13_2", so our findings correspond with the real sample. We know that the flatness of the surface is essential in proper function of the monochromator, therefore the further investigation of the bending problem has to be done.