Computer simulation of heat transfer in zone plate optics exposed to X-ray FEL radiation

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ABSTRACT

Zone plates are circular diffraction gratings that can provide diffraction-limited nano-focusing of x-ray radiation. When designing zone plates for X-ray Free Electron Laser (XFEL) sources special attention has to be made concerning the high intensity of the sources. Absorption of x-rays in the zone material can lead to significant temperature increases in a single pulse and potentially destroy the zone plate. The zone plate might also be damaged as a result of temperature build up and/or temperature fluctuations on longer time scales. In this work we simulate the heat transfer in a zone plate on a substrate as it is exposed to XFEL radiation. This is done in a Finite Element Method model where each new x-ray pulse is treated as an instantaneous heat source and the temperature evolution between pulses is calculated by solving the heat equation. We use this model to simulate different zone plate and substrate designs and source parameters. Results for both the 8 keV source at LCLS and the 12.4 keV source at the European XFEL are presented. We simulate zone plates made of high Z metals such as gold, tungsten and iridium as well as zone plates made of low Z materials such as diamond. In the case of metal zone plates we investigate the influence of substrate material by comparing silicon and diamond substrates. We also study the effect of different cooling temperatures and cooling schemes. The results give valuable indications on the temperature behavior to expect and can serve as a basis for future experimental investigations of zone plates exposed to XFEL radiation.

Keywords: X-ray optics, Zone plate, XFEL, Heat transfer

1. INTRODUCTION

Hard X-ray Free Electron lasers (XFEL) are novel sources of X-rays with extremely short pulses and unprecedented peak brilliance. These sources will enable new and exciting science in a variety of fields. For many of the envisaged applications it is important to focus the large beam down to focal spot sizes as small as 100 nm or even less. One possibility is to use diffractive zone plate optics, i.e. circular diffraction gratings with decreasing grating period. Zone plates are high quality optics that are used at present synchrotron sources, providing diffraction-limited focal spots as small as 10 nm[1-3]. As any other optics used at an XFEL source zone plates will have to face the problem of handling the high pulse intensities as well as the sometimes high average power. The zone plate has to be radiation hard to survive the integrated dose and it also has to be thermally stable enough to survive the temperature fluctuations from each pulse and any average temperature increase. As a first step to evaluate the thermal stability of zone plates in an XFEL beam we developed a Finite Element Method (FEM) model and simulated the temperature behavior of a metal zone plate on a diamond substrate[4]. It was found that it should be possible to keep the temperature below the melting temperature for the experimental conditions at the European XFEL.

In the present work we expand the simulations to include the conditions at LCLS. Apart from a metal zone plate on a diamond substrate we also simulate the temperature in a pure diamond zone plate. We consider in more detail how the cooling temperature and the heat transfer to the cooling holder influence the average temperature increase. In our first publication it was recognized that the monochromaticity of the radiation will limit the possible diameter of a zone plate to sizes much smaller than the beam size. For that reason a second case with a larger zone plate in combination with a

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monochromator was investigated in Reference 4. Another solution is to prefocus the XFEL beam to a size that better matches the zone plate size and we have therefore calculated the single pulse temperature increase for some selected materials at different beam sizes. The results of the expanded simulations give new insights into the limiting factors for the thermal management problem of using zone plates at XFEL sources.

2. BEAM PARAMETERS AND ZONE PLATE DESIGN

We have investigated two XFEL sources, the LCLS in Stanford and the European XFEL under construction in Hamburg. Table 1 summarizes the most relevant source parameters. The main difference between the two sources is the repetition rate and the wavelength. The more complex pulse structure of the European XFEL will produce a heat load of 9000 W within a pulse train. This can be compared to the continuous heat load of 0.24 W at LCLS. When comparing the single pulse heat load the situation is roughly the same at the two sources, with 2 mJ energy in a 750 μm – 1000 μm large beam.

Table 1. Beam parameters for the two free electron lasers considered in this paper.

	LCLS	European XFEL (SASE1)
Photon energy [Wavelength]	8 keV [0.15 nm]	12.4 keV [0.1 nm]
Pulse energy	2 mJ	2 mJ
Repetition rate	120 Hz	Trains of 2700 pulses in 0.6 ms
Beam size at lens position	750 μm (FWHM)	982 μm (FWHM)
E/ΔE	500	1000

When constructing a zone plate, one of the most important parameters is the zone material. For maximum diffraction efficiency the zone material should ideally produce a phase shift of π without absorbing any radiation. For the hard x-ray radiation produced at the considered sources, this can be achieved by using a low Z material such as diamond or silicon. Unfortunately, for π phase shift the zones need a thickness in the order of 10 μm which becomes a problem when high diffraction efficiency should be combined with high resolution. The resolution, or focal spot size, of a zone plate is approximately equal to the width of the outermost zone of the zone plate. If we require a resolution of 100 nm the aspect ratio of the outermost zone for π phase shift has to be as large as 100:1 which is extremely difficult to fabricate with today's nanofabrication techniques. An alternative solution is to use a high Z element, such as gold, platinum, tantalum, tungsten or iridium, which interacts more strongly with the X-rays and produce a π phase shift already at a thickness of 1.5 μm – 2 μm. The drawback of this is that the zone material also absorbs a significant part of the radiation. Figure 1 shows a comparison of the diffraction efficiency for tungsten, diamond and silicon. The diffraction efficiency for the other metals listed above is close to tungsten.

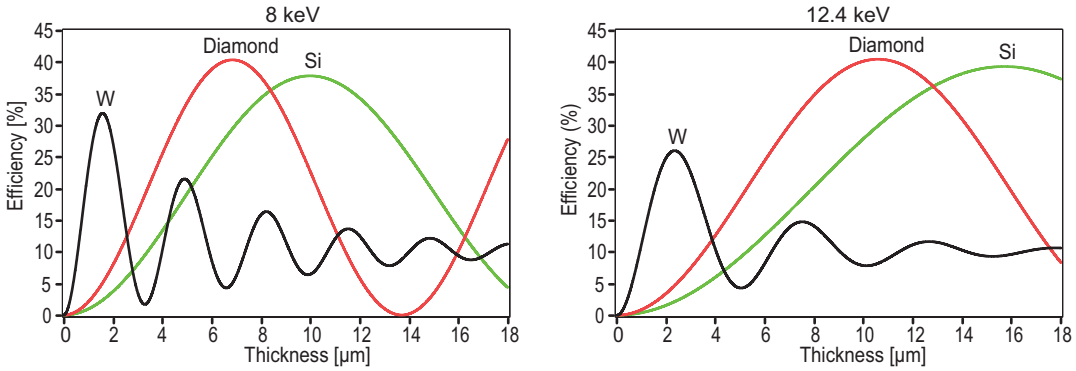

Figure 1. Diffraction efficiency of a zone plate in first order as a function of zone thickness at 8 keV and 12.4 keV

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In the present paper we consider both a low Z material zone plate made of diamond and a high Z material made of tungsten (Table 2). The reason for choosing tungsten is somewhat arbitrary since the relevant thermal properties are similar for the metals mentioned above and simulation results are very similar[4]. The zone plates are assumed to have an outermost zone width of 100 nm and to be fabricated on a round 10 mm diameter and 100 μm thick CVD diamond substrate for efficient cooling. Because of chromatic aberrations the number of zones in the zone plate cannot be larger than the monochromaticity (E/ΔE) of the beam. This limits the diameter of the zone plate to 400 μm for the European XFEL and 200 μm for the LCLS. The thickness of the tungsten zone plate is 1 μm. For the thermal simulations of a diamond zone plate it is enough to consider just the diamond substrate with nothing on top since they are equal from a heat management perspective. This is easily seen when considering that a diamond zone plate is fabricated by etching the pattern directly in a thick diamond substrate. The cooling of the zone plates is applied on both sides of the substrate with the exception for the 2 mm diameter central part where the beam passes through. Figure 2 shows the geometry for a 400 μm large tungsten zone plate. The effect of different cooling temperatures and heat transfer coefficients between holder and substrate is investigated in Section 4.3.

Table 2. Parameters of the tungsten and diamond zone plates.

	Tungsten (LCLS/European XFEL)	Diamond (LCLS/European XFEL)
Diameter	200 μm / 400μm	200 μm / 400μm
Outermost zone width	100 nm	100 nm
Number of zones	500 / 1000	500 / 1000
Zone thickness	1 μm	-†
Substrate material	Diamond	Diamond
Substrate thickness	100 μm	100 μm
Substrate diameter	10 mm	10 mm

3. SIMULATION METHOD

The simulation is based on the FEM software COMSOL. The model uses the transient heat equation where the heating from an XFEL pulse is implemented as an instantaneous temperature increase calculated from the absorbed energy distribution. This approximation is assumed to be valid as long as the absorbed energy is low enough to avoid the damage processes taking place on the ultra short time scale during and shortly after the pulse. The solver steps forward in time, increases the temperature at each new pulse and calculates the heat flow towards the cooled edges in-between pulses. In this way it is possible to simulate both the 120 Hz continuous operation at LCLS and a full pulse train of 2700 pulses at the European XFEL. An alternative for the full pulse structure is to simulate the average intensity, either at steady state for LCLS or transiently within a pulse train of the European XFEL. This greatly reduces the computational time and produces the same average temperature behavior, except for the rapid temperature spikes at each pulse, as can be seen in Figure 4 and 5.

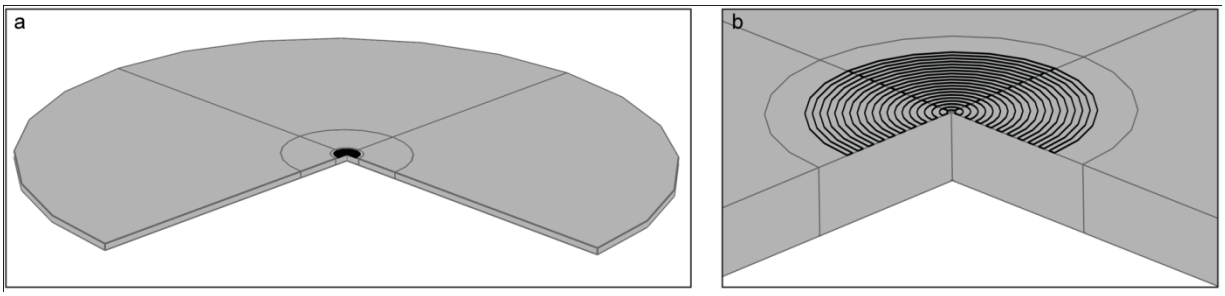

Figure 2. (a) 400 μm diameter and 1 μm thick tungsten zone plate on a 10 mm diameter and 100 μm thick diamond substrate (b) Closer look of the same geometry.

† The thickness of the diamond zones is not relevant for the thermal simulations since the problem is essentially equivalent to that of only a diamond substrate.

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The geometry for a tungsten zone plate on a diamond substrate is shown in Figure 2. The problem is circularly symmetric so it is possible to use a 2D mode which speeds up the calculations. It is also possible to replace the very fine structure of the zone plate with a courser one. This is possible since the heat flow in the zones is only in the vertical direction, towards the substrate. The interface between the metal zone plate and the dielectric substrate is assumed to have a thermal boundary conductivity of 40 MW/m^2K[4-6]. The cooling is applied on both of the substrate surfaces, except for the central part below the radius 1 mm. The simulations uses temperature dependent material parameters and the values for tungsten is from the materials library included in COMSOL whereas the values for CVD diamond is taken from Reference 7.

4. RESULTS

4.1 Single pulse

Already a single XFEL pulse can be potentially devastating, especially for a metal zone plate. The absorbed dose is determined by the x-ray absorption length of the material, the pulse energy and the size of the beam. Figure 3 shows the temperature increase in a 2 mJ pulse for different beam sizes. Tungsten has the shortest absorption length (3.1 µm for 8 keV and 2.4 µm for 12.4 keV) and is heated by several 100 K already for moderate beam sizes around 1000 µm. Diamond on the other hand has a much longer absorption length (651 µm for 8 keV and 2466 µm for 12.4 keV) and experiences only small temperature increases in the order of 1 K at a beam size of 1000 µm. Silicon is somewhere in between the two with an absorption length of 69 µm for 8 keV and 252 µm for 12.4 keV.

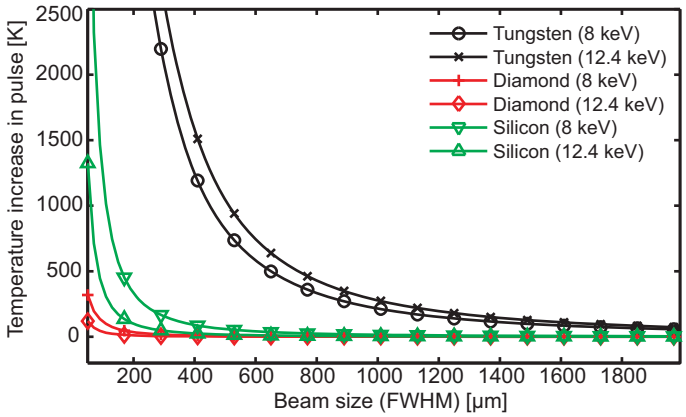

Figure 3. Calculated temperature increase in a 2 mJ XFEL pulse for different zone plate materials as a function of beam size. The temperature in the zone plate before the pulse was 300 K.

When comparing the size of the zone plate, 200 µm diameter for LCLS and 400 µm diameter for XFEL, it is clear that the overall efficiency would benefit from a smaller beam size. The absorbed dose, and temperature, in a metal zone plate quickly increases to catastrophic levels below a beam size of about 500 µm but the silicon and especially the diamond show potential for surviving a much smaller beam. Another possibility is to increase the monochromaticity of the beam, for instance with a monochromator, and use a larger zone plate. The increased monochromaticity comes at the price of a greatly reduced intensity. A reduction in intensity, although negative from an experimental point of view, is of great benefit for the zone plates. For example, the single pulse temperature increase in a metal zone plate reduces from 300 K to around 20 K – 30 K.

4.2 Many pulses at LCLS

The temperature in the hottest point of a tungsten zone plate is shown in Figure 4. The temperature increase in each pulse is 320 K but the heat quickly diffuses down into the substrate where it eventually is conducted away through the cooled surfaces and the result is a low average temperature of about 312 K for a moderate heat transfer coefficient of 20 W/m^2K at the cooled surfaces. The figure also shows the average temperature calculated from a continuous average intensity

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(solid black), as described in Section 3 and the agreement is good. It should also be noted that for the LCLS case it is still satisfactory to use a silicon substrate, with only somewhat increased average temperature. As is described in Section 4.3 this is not possible for the European XFEL case.

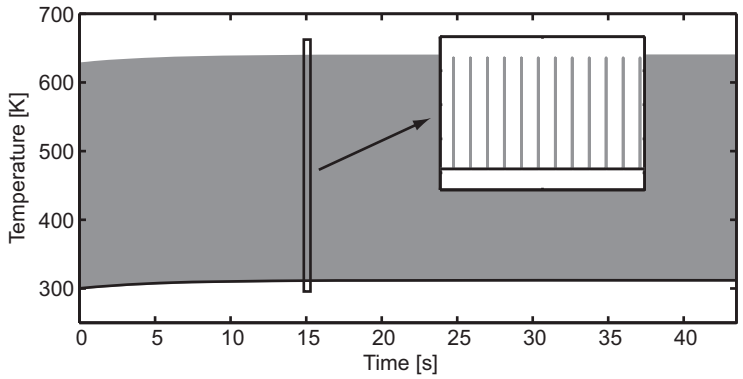

Figure 4. Temperature in the center of a 200 μm large and 1 μm thick tungsten zone plate on a diamond substrate in the LCLS beam. The complete solution including the rapid temperature fluctuations (gray) is compared to the solution obtained from the average intensity (black). The substrate is cooled with a heat transfer coefficient of 20 W/m^2K at a temperature of 300 K.

4.3 SASE1 pulse train at European XFEL

When the source parameters are changed to those of the SASE1 undulator at the European XFEL the main difference is that that the repetition rate is increased from 120 pulses per second to 2700 pulses in 0.6 ms. The resulting temperature during a pulse train is shown in Figure 5. The temperature increase in each pulse is comparable at 277 K but the average temperature at the end of the pulse train is as high as 1280 K. If the substrate is changed to silicon the temperature reaches several thousand Kelvin long before the end of the pulse train. This is mainly a result of the higher absorption in silicon. For this reason we only consider diamond substrates in the European XFEL simulations.

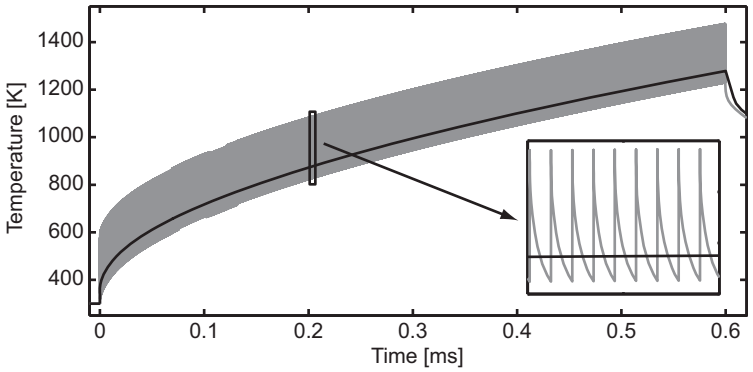

Figure 5. Temperature in the center of a 400 μm large and 1 um thick tungsten zone plate on a diamond substrate during a pulse train of 2700 pulses at the European XFEL. The complete solution including the rapid temperature fluctuations (gray) is compared to the solution obtained from the average intensity (black). The substrate is cooled with a heat transfer coefficient of 0.04 MW/m^2K at a temperature of 300 K.

In order to determine the influence of the cooling temperature and the heat transfer coefficient h between diamond and a cooled copper holder we have simulated the temperature during a pulse train for two different temperatures, 77 K and 300 K, and three different values of h. The values chosen for h are the two extreme cases where h = 0 MW/m^2K and h = ∞ plus a value of h = 0.04 MW/m^2K for diamond and copper with GaIn as an interstitial material [8]. The two extremes

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correspond to a thermally insulated substrate and one where the cooled surface is kept at a constant temperature. The results are shown in Figure 6. The perhaps most interesting thing to notice when comparing the different results is that the temperature evolution is almost independent of h, except for the extreme case of $h = \infty$ at 77 K which is not achievable in a real system. This means that during the pulse train, heat from the zone plate is taken up and stored in the large thermal bulk of the diamond substrate, but is only slowly transferred to the holder. After the pulse train, the only requirement on the cooling is that it is efficient enough to cool the substrate down to ambient temperature before the next pulse train, i.e. in 0.1 s. This is easily achieved with $h = 0.04$ MW/m^{2}K. Looking at the temperature curves one might ask why the $h = 0$ MW/m^{2}K curve also is seen to decrease after the pulse train. The reason is that it takes some time for the whole substrate to reach a homogeneous temperature, which is above the initial temperature but also below the peak temperature in the center of the zone plate, the point for which the temperature is plotted here.

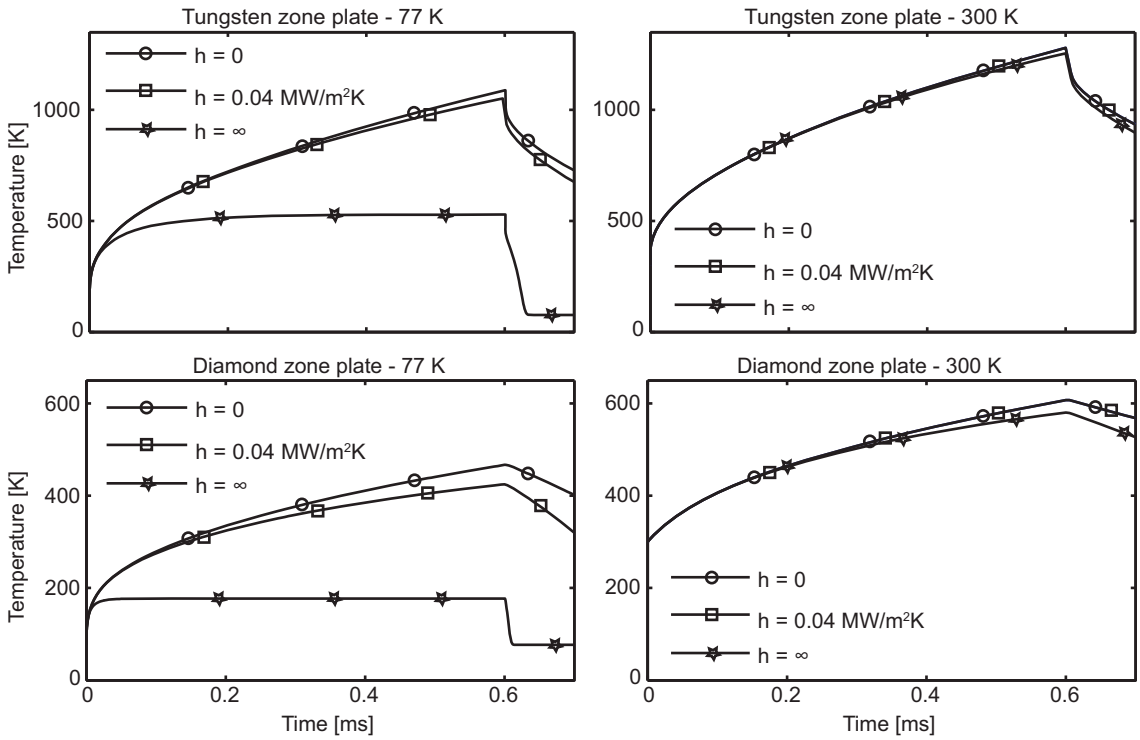

Figure 6. Influence of cooling temperature and heat transfer coefficient on the temperature during a pulse train of 2700 pulses at the European XFEL for a tungsten zone plate on a diamond substrate and a pure diamond zone plate. The temperature is the average temperature in the center of the zone plate.

Another interesting thing to note is that the maximum average temperature for the tungsten zone plate is only 2 times higher than that of diamond when the difference in absorption coefficient is a factor of 1000. To explain this, we consider the geometry and estimate how much of the incident radiation is absorbed in the two cases. The diamond is 100 μm thick and as such absorbs 4 % of the radiation. This can be compared to the absorption in 1 μm of tungsten, which is 34 %. Taking into account that an actual zone plate only has half of the area covered by tungsten, the absorbed fraction is reduced to 17 %. Finally one has to take into account that only about 10 % of the beam is within the area of the zone plate. All in all, the zone plate only absorbs 1.7 % of the radiation which should be compared to the 4 % absorbed in the diamond, meaning that the tungsten zone plate (including substrate) absorbs 5.5 % and the diamond zone plate 4 %. Comparing these numbers the original question might be reversed: Why is the difference in temperature as large as 2 times? The reason is that the radiation absorbed in the zone plate is confined to the center of the substrate, far away from the cooler edges, whereas the radiation absorbed in the diamond is spread out over a larger area.

One should also note that the effectiveness of the cooling to a large extent depends on the geometry of the system. One improvement is to apply the cooling closer to the heat source, but this is problematic since the beam has to have a free

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passage through the holder. Another improvement is to gradually increase the substrate thickness outside of the zone plate to create a very large thermal bulk and contact area to the cooling. The average heat problem for at zone plate is essentially the same as that for a diamond monochromator and any cooling scheme used for a monochromator could in principle also be used for a zone plate.

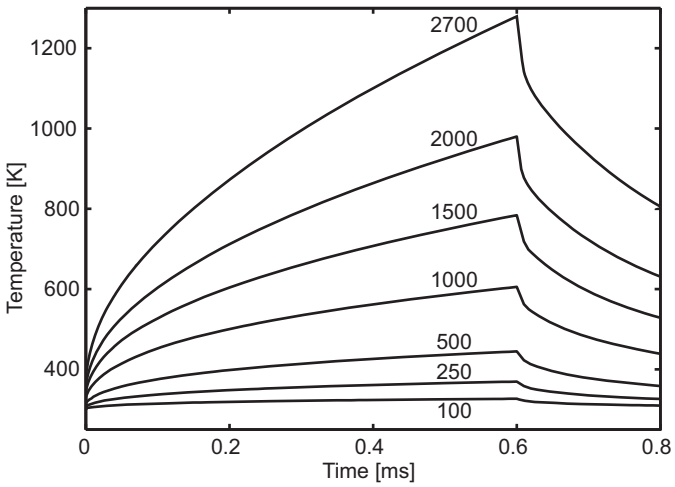

Figure 7. Average temperature in the center of a tungsten zone plate on a diamond substrate during a pulse train with varying number of pulses at the European XFEL. Starting temperature was 300 K and $h = 0.04$ MW/m^{2}K.

The results in Figure 5 and Figure 6 are a worst case scenario where the pulse train contains the maximum number of pulses, 2700. It is quite possible that an individual experiment does not need all of these pulses and in that case the number of pulses in the pulse train could be reduced, with reduced heat load as a clear benefit. We have therefore simulated the temperature in a tungsten zone plate for different number of pulses in the pulse train and Figure 7 shows the resulting average temperatures. As expected, the temperature increase during the pulse train is approximately proportional to the number of pulses in the pulse train. Although the temperature remains well below the melting point of tungsten (3695 K) for all cases there are other effects that probably will limit the acceptable average temperature. Among these are the graphitization of CVD diamond occurring at temperatures around 1800 K[7,9], possible phase changes in the tungsten at temperatures around 1000 K or even lower[10,11] and distortions to the zone plate pattern due to thermal expansion[12] . One also has to remember the rapid temperature fluctuations not visible in the average temperature simulations. The magnitude of the fluctuations is around 300 K and might possibly destroy the zone plate in a single pulse or over time as a result of fatigue.

5. CONCLUSIONS

The temperature behavior for a tungsten as well as a diamond zone plate on a diamond substrate was simulated using FEM software. This was done for the source parameters of both LCLS and European XFEL. The temperature in the zone plate remained below the zone plate melting temperature for all cases. It was found that for the LCLS the low repetition rate makes it possible to use a silicon substrate. For the higher repetition rate at the European XFEL it is necessary to have a diamond substrate and even though the temperature was kept below the melting point it was found to be as high as 1300 K where other thermal damage mechanisms such as graphitization in the substrate[9] and phase changes in tungsten[10,11] become important. When looking at a single pulse it is clear that the metal zone plates will have to withstand substantial temperature fluctuations in the order of 300 K. As expected for the diamond zone plate, the temperature fluctuations was found to be much lower in the order of 1 K. Nonetheless will the diamond zone plate be heated to 600 K at the European XFEL.

The thermal simulations alone cannot answer the questions if a specific zone plate will survive at LCLS or at the European XFEL. It can be shown that the zone plates should not melt but it is still possible that the thermally induced stress and strain will damage the zone plate. This needs to be investigated experimentally. Another problem that should

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not be overlooked is that of radiation damage. The available experimental data is sparse but seems to suggest that metal nanostructures as well as diamond substrates should be reasonably radiation hard[13-15]. It is also likely that the radiation hardness of the fabricated zone plate and substrate system is dependent on the fabrication process. There is therefore a clear need for more experiments in this area.

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