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ANALYTICAL THERMAL ANALYSIS OF THIN DIAMOND IN HIGH-INTENSITY HIGH-REPETITION-RATE APPLICATIONS*

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Abstract

Thin diamond plates are used in monochromator for X-ray Free-Electron Laser (XFEL) self-seeding scheme. To function properly, they must endure high-intensity and high-repetition-rate XFEL pulses without crossing thresholds set by various adverse effects, such as thermal strain-induced diffraction distortion and graphitization. In this work, a theoretical model is developed, and an analytical solution is derived to elucidate potential thermal runaway under edge cooling condition. It is shown that the crystal edge cooling can effectively mitigate the issue to a certain extent. The analytical solution can be used as an efficient tool for XFEL operation parameter setup.

MANUSCRIPTS

X-ray free-electron laser (XFEL) can generate high peak-power pulses with atomic and femtosecond scale resolution, impacting cutting-edge scientific research [1, 2]. Thin diamond layers are used in spectrometer and monochromator for XFEL self-seeding [3, 4, 5]. When an X-Ray pulse passes through a thin diamond layer, a part of its energy is deposited into the diamond lattice. This process thermalizes the crystal lattice causing temperature buildup within the crystal [6]. In high-repetition rate applications, such temperature buildup may reach a thermal runaway condition, alongside with considerable lattice deformation and local permanent damage, such as local graphitization on the surface and internally at the grain boundary of a diamond plate [7, 8, 9]. Graphitization happens when the absorbed energy is greater than the activation energy of the crystal [10].

In the present paper, an analytical steady-state solution for continuous-wave (CW) laser input is derived to address potential thermal issues in thin diamond. The temperature-dependent thermal properties of diamond, i.e., thermal conductivity [11] and specific heat capacity [12], valid for temperature in the range from 100 K to 3000 K, are used in the calculation. The objective of this study is to provide a quick estimation tool for determining operational guideline based on thin-diamond material properties and cooling condition under focused laser heating at high repetition rates. From the steady-state solution, by setting the central temperature $T_0^*\rightarrow\infty$, the (definite) thermal runaway condition can be defined. A relaxed thermal runaway condition can also be defined by setting T_0^* equal to a finite value, for instance, graphitization temperature, to address a particular effect of concern. The relationships between dimensionless terms of cooling edge distance to laser waist size ratio R/a, edge cooling temperature T_R, and critical (allowed) laser heating power fI are discussed. It shows that the critical heating power fI is higher with smaller R/a, and lower T_R. However, when it comes to design of an edge cooling system, there are limits such as the size of the working area and the size of the cooling device.

Problem Formulation

Consider a train of X-Ray pulses impinging perpendicularly at the center of a circular, thin diamond crystal at repetition rate f, as illustrated in Fig. 1. The circumferential sink temperature is held constant via a cooling system. The pulses are assumed to be Gaussian, and extremely short compared to all other time scales under consideration. The heat is deposited instantaneously while a laser pulse passes through the crystal. The problem is axisymmetric with radial axis r set from the center. The temperature field is assumed to be uniform in the through-thickness direction. The deposited energy is dissipated by conduction inside the plate only; any radiative heat transfer is assumed to be negligible.

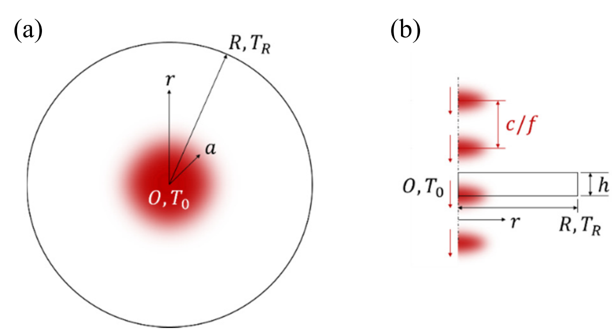

Figure 1: Schematic show of high repetition rate laser heating in a thin crystal: (a) top view and (b) side view. The cylindrical coordinate system is established for reference.

The flux of laser heat deposition from the top surface is expressed as,

$$i(r,t)= i_0 e^{-2(r/a)^2}\delta(t-n/f) \quad (1)$$

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where a is the transverse waist-size, i_0 is the central (peak) intensity, δ is the Dirac delta function, t is the time, and integer n indicates the nth laser pulse. Under the assumption of cooling edge distance $R \gg a$, the deposited energy per pulse I, is approximated as,

$$I \approx \frac{1}{2}\pi a^2 i_0 \tag{2}$$

The one-dimensional heat conduction equations inside diamond are given by,

$$j = \kappa \frac{\partial T}{\partial r} \tag{3}$$

$$\frac{1}{r}\frac{\partial (rj)}{\partial r} - \frac{i}{h} = \rho c_p \frac{\partial T}{\partial t} \tag{4}$$

where T is the temperature, j is the heat flux in the radial direction, κ is the thermal conductivity, c_p is the specific heat, ρ is the mass density, and h is the thickness.

Coefficients κ and c_p are taken from [11, 12] (which may also be found in [13, 14]), which are highly temperature dependent. Especially, for the range of temperature from 0 K to about 100 K, κ increases from zero to its maximal magnitude. It then decreases continuously for temperatures greater than about 100 K. Except temperatures before and near the peak, its variation may be roughly approximated by a power law,

$$\kappa = \alpha T^{\beta} \tag{5}$$

where α and β are fitting constants, regarded as material constants, different for diamond in different grades. ρ is assumed to be independent of temperature.

The boundary condition is set by,

$$T(r=R) = T_R \tag{6}$$

In the limiting case of high repetition rate and low individual pulse energy, the laser heating process may be well described by approximating the discrete laser pulses as a continuous wave. An analytical steady-state solution is derived under the continuous wave condition below.

By averaging the pulse energy by pulse interval, the source flux replacing Eq. (1) is given by,

$$i(r,t) = \frac{2fI}{\pi a^2}\, e^{-2(r/a)^2} \tag{7}$$

In the steady state, the total incoming heat flux, $\int_0^r 2\pi r' i(r',t) dr'$, through the top surface over an area πr^2 must be conducted away with a total outgoing flux, $2\pi rhj$, through the cylindrical side surface of an area $2\pi rh$ for the sake of energy conservation. By setting them equal, substituting Eq. (1), and integrating, the circumferential heat flux is derived as,

$$j = \frac{a^2 f i_0}{4hr}\left[1 - e^{-2(r/a)^2}\right] \tag{8}$$

The above equation can be directly derived by setting the time derivative term on the right-hand side to be equal to zero and integrating from Eq. (4) as well.

By substituting Eq. (5) and (8) into Eq. (3) and integrating, one obtains,

$$\frac{T_0}{T_R} = \left[1 - \frac{(\beta-1)fI}{4\pi h \alpha T_R^{1-\beta}} Ein\left(\sqrt{2}R/a\right)\right]^{1/1-\beta} \tag{9}$$

where T_0 is the temperature at $r = 0$, and special function $Ein(\sqrt{2}R/a) \equiv 2\int_0^R \frac{1-e^{-2(r/a)^2}}{r} dr$. κ is curve-fitted to the experimental data for diamond given in Wei & Kuo [11], $\alpha = 23.9\times10^6$ and $\beta = 1.63$ by unit W/mK, Since $\beta > 1$, central temperature T_0 would become unbounded under certain conditions, raising concern in practice. also T_0 can be taken to indicate the severity of laser heating. It is also taken to derive a runaway condition by setting it equal to a threshold, T_0^*. The threshold, T_0^*, may be set to be infinite, or finite such as at graphitization temperature and according to an X-ray diffraction quality requirement.

Results & Discussion

By using above κ values of α and β, setting $h = 110\ \mu m$ of a thin diamond crystal, steady-state runaway conditions are evaluated for various values of T_R, T_0^*, and R/a. Some selected results are presented in Figs. 2-6. Figure 2 shows the variation of steady-state central temperature T_0 as a function of laser input power fI for various edge cooling temperatures from 100 K to 300 K and fixed crystal size to laser spot size ratio $R/a = 50$. Fig. 3 shows the critical power fI as a function of R/a for $T_0^* = \infty$. It gives the perspective of viewing the variation of critical power with varying cooling edge distance but a fixed laser spot size. It may be useful in different practical stages of device design and its use, respectively. Similarly, Figs. 4-6 show critical power fI as a function of R/a for various target tolerable temperatures with edge cooling temperatures T_R=100, 150, 200, 250 and 300 K, respectively.

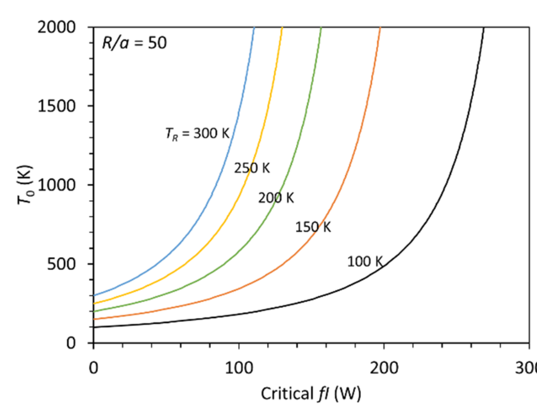

Figure 2: Variation of steady-state central temperature as a function of laser heating power for fixed R/a =50 and various T_R=100, 150, 200, 250 and 300 K.

As seen from Fig. 2, steady-state central temperature T_0 increases relatively slowly with increasing laser input

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power at small power magnitudes. It then increases rapidly at higher power magnitudes, and eventually approaches to infinity at a critical power, at each one of the cooling temperatures. At the critical power, the definite thermal runaway condition is reached.

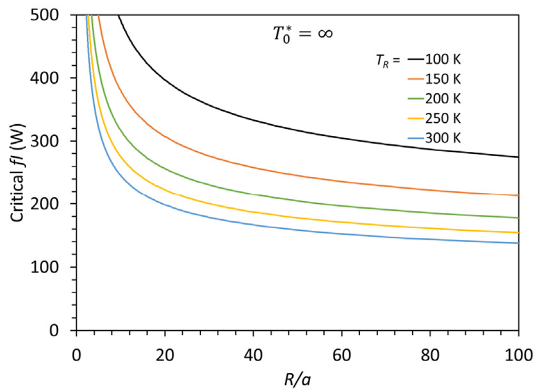

Figure 3: Variation of critical laser heating power at definite runaway condition (T_0^*=∞) as a function of R/a for various T_R=100, 150, 200, 250 and 300 K.

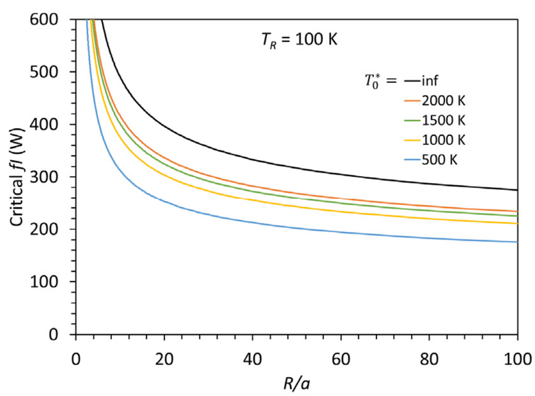

Figure 4: Variation of critical laser heating power at various runaway conditions (T_0^*=∞, 2000, 1500, 1000, 500 K) as a function of R/a for T_R=100 K.

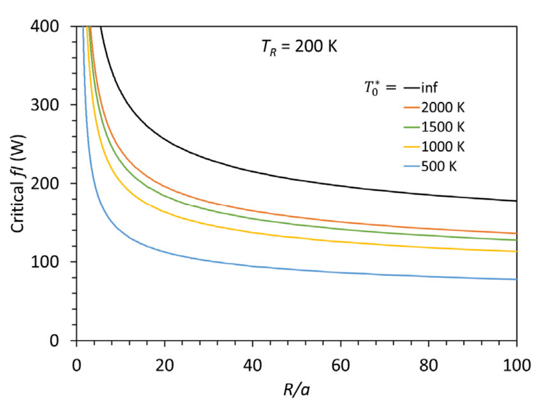

Figure 5: Variation of critical laser heating power at various runaway conditions (T_0^*=∞, 2000, 1500, 1000, 500 K) as a function of R/a for T_R=200 K.

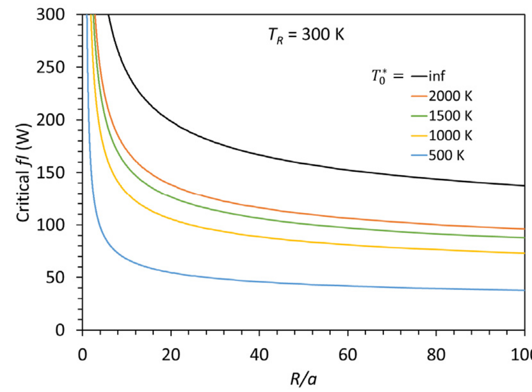

Figure 6: Variation of critical laser heating power at various runaway conditions (T_0^*=∞, 2000, 1500, 1000, 500 K) as a function of R/a for T_R=300 K.

Lowering edge cooling temperature improves the critical power *fI*. However, it cannot eliminate the thermal runaway, as shown in all Figs. 2-6. The critical runaway conditions are sensitive to the cooling temperature and cooling edge distance when R/a ratio is small, i.e., when the cooling edge is close to the laser spot, as shown in Figs. 3, 4, 5, and 6. For a given laser spot size a, moving cooling edge closer to the laser does not help very much critical power *fI* for large ratios of R/a. Depending on cooling edge temperature, when R/a is in the range of $10-20\ \mu m$, the improvement rises abruptly. Practically, this strategy of imposing heat sink this close may work for large spot sizes, for instance, $a>100\ \mu m$. However, for small spot sizes, for instance, $10-20\ \mu m$, it can be challenging.

Setting lower target runaway temperature, the critical power *fI* would be lower. The reduction in critical *fI* is more significant at higher cooling edge temperature. These results as shown in Figs. 3-6 can help estimate the effect semi-quantitatively for different lab settings.

CONCLUSION

Thermal analysis of thin diamond crystal under high-repetition-rate high-intensity laser heating is carried out to address the potential thermal issue, analytically. The steady-state solution for CW laser heating is derived. It can be utilized as an efficient estimation tool for future design and optimization calculations. The results in a few selected cases are plotted and discussed for definite thermal runaway condition by setting $T_0^* \rightarrow \infty$. The solution can also be used for estimation of relaxed thermal runaway conditions by setting T_0^* to a finite temperature, required by optical performance or at graphitization temperature. Although diamond is a thermally superior material, thermal fatigue may also be worth attention, while pushing the limit under such extreme laser heating. These results can provide a meaningful guideline in designing the optical devices and its edge cooling system for high-intensity high-repetition-rate XFEL applications. It can also be used as operational parameter setup guideline to the end users.

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