Some thermal formulas useful for XPCS

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This document derives a simple solution of the heat equation for a circular heat source incident on a disk conductively cooled on its edge. I also give some estimates of the thermal gradient produced and the spatial FWHM of the thermal bump, a result not nearly as easily available. A formula for the temperature profile is also derived. The thermal profile for a few sample is also calculated for a typical XPCS set up.

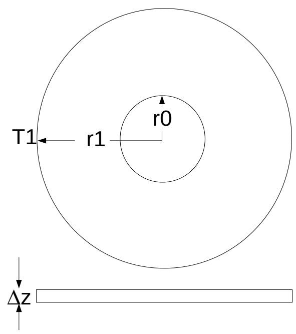

FIG. 1. The thermal geometry.

The thermal load on X-ray optics and on absorbing samples becomes an important consideration in experiments performed at state of the art synchrotron radiation sources. The optical elements and sample can absorb a large amount of heat given the high incident heat load on their surface, which is typically on the order of 100 Wmm^{-2}, which is bound to increase as improvements to the source are made in the years to come. Here we give a simple solution to the heat equation with a cylindrical geometry which can be used to estimate the temperature gradients in a given optical component like an X-ray filter, made with a thin absorbing foil like graphite. We will assume the cooling is done on the outside edge of a disk of radius r_1 and thickness Δz (see Fig. 1). The cylindrical symmetry is chosen for its simplicity. It is also a geometry which has been used previously in X-ray Photon Correlation Spectroscopy experiments experiments (XPCS) [1] to mount a colloidal sample for example [2], thus this solution will help in evaluating gradients on a sample. Furthermore, it will also provides a numerical estimate of the spatial extent of the hot area on the sample through the half width at half maximum (HWHM) of the temperature peak profile $T(r)$.

An X-ray beam illuminates the sample within a circle of radius r_0. We assume that a circular target is held on a circular mount with radius $r_1 > r_0$ at a constant temperature $T(r_1) = T_1$. This is the only fixed temperature boundary condition. We assume that some fraction of the incident power is absorbed in the sample **uniformly** over Δz. We define ϕ as the absorbed power per unit area. This approximation will be valid when the thickness of the sample is much smaller than the X-ray absorption length. If Δz is much larger than the absorption length, then our calculation will be an underestimate of the surface temperature rize, and the temperature depth profile will be non-uniform. The solution must satisfy the steady state heat equation

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = -\frac{q}{\kappa}, \tag{1}$$

where the absorbed power density $q = \phi/\Delta z$ (in Wcm^{-3}), and κ is the thermal conductivity (in Wcm^{-1}K^{-1}).

A solution can be found easily using Gauss theorem solving $\int_S \mathbf{J} \cdot \mathbf{dS} = -\int_V q dv$, where $\mathbf{J} = -\kappa \nabla T$, S and V are respectively the surface and volume element of the cylindrical enclosed region, and $\mathbf{J}$ is the heat current. We find

$$\frac{\partial T}{\partial r} = \begin{cases} -\frac{\phi r}{2\kappa \Delta z} & \text{for } r < r_0, \\ -\frac{\phi r_0^2}{2\kappa\Delta z}(\frac{1}{r}) & \text{for } r_0 < r < r_1, \end{cases} \tag{2}$$

One can easily integrate Eq. 2 to find the temperature

$$T(r) = \begin{cases} T_1 + \frac{\phi r_0^2}{2\kappa\Delta z}\ln(\frac{r_1}{r}), & \text{for } r > r_0, \\ T_1 + \frac{\phi r_0^2}{2\kappa\Delta z}\{\ln(\frac{r_1}{r_0}) + \frac{1}{2} - \frac{r^2}{2r_0^2}\}, & \text{for } r < r_0. \end{cases} \tag{3}$$

By inspection, the solution matches the boundary conditions, and satisfies Eq. 1.

The maximum temperature difference between the center and the edge is

$$T(0) - T(r_1) = \Delta T_{max} = \frac{\phi r_0^2}{2\kappa\Delta z}\{\ln(\frac{r_1}{r_0}) + \frac{1}{2}\}. \tag{4}$$

The temperature rise ΔT_{max} depends on the absorbed power on the illuminated area $P = \phi\pi r_0^2$. It is inversely proportional to the conductivity κ, and thickness Δz. The logarithmic term tells us that the farther the heat sink is from the heated area, the larger the temperature rise will be. This value of ΔT_{max} is very similar to the one normally found in standard heat transfer text, apart from a factor 1/2 within the brackets, which is due to the different boundary conditions considered here. Standard texts [3] consider the temperature of the inside circle of radius r_0 to be fixed at temperature T_0. In our problem, we consider a constant flux ϕ over the inside circle, which is closer to the experimental condition of a material subjected to a synchrotron beam.

From Eq. 3, it is also easy to show that the half width at half maximum (HWHM) of this temperature profile is

$$r_{HW} = \begin{cases} r_0\sqrt{\ln(\frac{r_1}{r_0}) + 1/2} & \text{for } r_0 < r_1 < \sqrt{e}\, r_0, \\ \\ \sqrt{\frac{r_1 r_0}{\sqrt{e}}} & \text{for } r_1 > \sqrt{e}\, r_0. \end{cases} \quad (5)$$

It is interesting to notice that r_{HW} depends only on the geometry of the experiment, and not on the thermal properties of the material. The gradient in Eq. 2 though depends on the thermal properties and heat flow. If $r_1/r_0 < \sqrt{e}$, the HWHM radius is smaller than r_0, whereas if $r_1/r_0 > \sqrt{e}$, this radius is larger than r_0. For most experimental setup, $r_1 >> r_0$, thus the HWHM will be much larger than r_0.

For XPCS experiments near a critical point, we are also interested in the change of temperature within the illuminated beam since the X-rays only probe this region of the material. We thus want to minimize the temperature rise

$$\begin{aligned} \Delta T_{beam} &= T(0) - T(r_0) = \phi r_0^2/(4\kappa\Delta z) \\ &= P/(4\pi\kappa\Delta z) \approx P_0/(4\pi\kappa\delta). \end{aligned} \quad (6)$$

This temperature rise is in practice always smaller than ΔT_{max}. Interestingly enough, this temperature change is independent of how we cool the sample in this cylindrical geometry. It depends only on the power P absorbed by the sample in the illuminated volume, the heat conductivity, and the thickness of the material.

For a monochromatic beam, the aborbed power can be written as $P = P_0(1 - \exp(-\Delta z/\delta(E)))$, where $P_0 = \pi I_0 r_0^2$ is the incident power, I_0 is the incident power density, and δ is the X-ray penetration length at this energy E. If the thickness Δz is much smaller than δ, then we can substitute for P in all the previously derived equation $P \approx P_0\Delta z/\delta$. Then the thickness dependence disappears in Eq. (6). It is interesting to note that in a transmission experiment, if the sample thickness is much smaller than the absorption length, the thermal rize is dependent on the incident power, and the product $\delta\kappa$, but independent of Δz. We can also rewrite Eq. (4) as

$$\Delta T_{max} \approx \frac{P_0}{2\pi\kappa\delta}\{\ln(\frac{r_1}{r_0}) + \frac{1}{2}\}. \quad (7)$$

A useful example is shown in Table I for several materials. For this example, the undulator gap is set at 16.5 mm, for a fundamental energy of 7.15 keV. The beam area is set to a square of side equal to the horizontal transverse coherence length $l_h = 5.9\mu$m. The undulator spectrum is filtered by a double bounce fixed angle (8.75 mrad) Pt coated mirrors set up providing a coherent flux in the square opening of 8.6×10^{10}ph/s/100mA with an average energy $<E> = 6974$ eV and a bandwidth of 2.6 %. The power in this small beam is $P_0 = 0.172$ mW. If we assume circular symmetry for simplicity, the radius of a circle with an area equal to l_h^2 is $r_0 = l_h/\sqrt{\pi} = 3.33\mu$m. We set a typical cooling radius of $r_1 = 1$ mm, and the thickness $\Delta z \ll \delta$.

TABLE I. Thermal rise of several materials that could be investigated in the future at the APS for a 5.9 μm×5.9 μm "pink beam" at 7 keV.

material	δ (mm)	κ (mW mm^{-1} K^{-1})	ΔT_{max} (K)	ΔT_{beam} (mK)
n-Hexane/Nitrobenzene	1.51	0.123[a]	0.915	73.7
Water	0.661	0.66	0.386	31.4

[a]For pure n-hexane at 300 K. [5]

Table I shows calculations of Eq. (6) and (7). For all these samples, the radius $r_{HW} = 142\mu$m, thus the thermal bump's radius is much larger than the beam radius r_0. For the mixture n-hexane and nitrobenzene, ΔT_{max} is nearly 1 K, a substantial offset from the temperature bath T_1. The sample cell geometry could be improved by making the cooling radius much smaller than 1 mm. The geometric factor $\ln(r_1/r_0) + 1/2$ is equal to 6.2 for a $r_1 = 1$ mm. It can be reduced to 3.9 with $r_1 = 0.1$ mm, a reduction in thermal rize of 37 %. With a "pink beam", a temperature offset between T_1 and T(0) will be inevitable unless one reduces the incident flux with filters or by using a monochromatic beam.

The more significant thermal change is $\Delta T_{beam} =$ 73.7 mK for the mixture of n-hexane/nitrobenzene. This will affect our ability to approach the critical temperature closer than about 75 mK, thus the gain in scattering will be limited, and our model structure factor will have to be weighted for thermal gradient effects.

For comparison, in our latest experiment at the APS, the flux at 13 keV was 7.7×10^{10} ph/s/$(100\mu\text{m})^2$, for a total incident power of 0.16 mW. For a cooling radius of 1 mm, and $r_0 = 56.4$ μm, a measured absorption length of 9.5 mm, $\Delta T_{max} = 0.073$ K, and $\Delta T_{beam} = 10.9$ mK. Both effects were small in our experiment, and would be much smaller in a XPCS experiment with a monochromatic beam.

In conclusion, this document reports several helpful relationships to estimate thermal gradients in a XPCS experiment. Care in the selection of materials with a large thermal conductivity and with a large X-ray penetration depth would reduce thermal gradients. Reducing the heat load by adequate monochromation, as well as minimizing the distance between the beam's footprint and the heat bath are also important factor to consider.

ACKNOWLEDGMENTS

This small write up was developped while making several thermal estimates for X-ray filters to be used on the MHATT-CAT insertion device beam line. This work develops in more details some of the ideas written by Gene Ice [4] in a MHATT-CAT report on the requirements for X-ray filters.

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[1] For a review of the field, see S.B. Dierker, NSLS Newsletter, July 1995, and references within. This document is available in hypertext at `http://www.nsls.bnl.gov/Intro/Newslet/Jul95/speckle.html`.

[2] S.B. Dierker *et al.*, Phys. Rev. Lett. **75**, 449 (1995).

[3] A Physicist's Desk Reference, American Institute of Physics, New York, 1989. See also H.S. Carslaw and J.C. Jaeger, Conduction of Heat in Solids, Oxford University Press, London, 1959.

[4] Gene Ice, Private Communication (1996).

[5] Y.S. Touloukian, P.E. Liley, and S.C. Saxena, Thermal Conductivity Nonmetallic Liquids and Gases, in Thermophysical Propoerties of matter The TPRC Data Series, Volume 3, IFI/Plenum, NY 1970.