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Evaluation of the fused silica thermal conductivity by comparing infrared thermometry measurements with two-dimensional simulations

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A self-consistent approach is proposed to determine the temperature dependent thermal conductivity $k(T)$ of fused silica, for a range of temperatures up to material evaporation using a CO$_2$ laser irradiation. Calculation of the temperature of silica using a two-dimensional axi-symmetric code was linked step by step as the laser power was increased with experimental measurements using infrared thermography. We show that previously reported $k(T)$ does not reproduce the temporal profile as well as our adaptive fit which shows that $k(T)$ evolves with slope discontinuities at the annealing temperature and the softening temperature. © 2012 American Institute of Physics. [http://dx.doi.org/10.1063/1.4764904]

Fused silica is the most commonly used material in laser studies, and CO$_2$ laser-processing is often governed by heat transport in this material. The knowledge of its thermal physical properties at temperatures where material is removed or evaporated is crucial. The thermal analysis of the laser-material interaction under CO$_2$ laser irradiation has been widely investigated with both experiments and simulations. Nevertheless, some aspects are still subject to considerable uncertainty. For example, the behavior of $k$, the thermal conductivity of silica, at temperature $T > 1000$ K, is not settled, with experiments reporting quite different values for it.

An experimental and analytical method to measure the $T$ dependence of $k$ has recently been investigated. These authors found good agreement with measurements where radiation losses were carefully eliminated in the experiment. In contrast, disagreement was observed with measurements in which radiation losses were not prevented and were shown to be the dominant transport mechanism. Therefore they conclude that $k(T)$ increases as $\sim T^3$ at small $T$ but reaches a constant value at high $T$. On the basis of simplicity, it has been proposed that the $T$ dependence of $k$ should be ignored and that a fixed value be used. We note that by using a linear $T$ dependence of $k$ that fits data on fused silica given by glass manufacturers, some analyses found good agreement between calculated stresses and experimentally observed residual stresses.

In this letter we propose an original method to determine the thermal conductivity. We perform a calculation of the temperature of a CO$_2$ laser-irradiated silica sample using a two-dimensional (2D) code developed at Commissariat à l’Energie Atomique, and we link it with previously available experimental measurements of the silica surface using infrared (IR) thermography. By comparing simulation and experimental data step-by-step as we increase the maximum of temperature reached at the end of the irradiation (by increasing the CO$_2$ laser power), we estimate the parameterized thermal conductivity. More precisely, we assume that at high $T$, $k(T)$ is a piecewise linear function, whose slope changes discontinuously at two temperatures, the annealing temperature $T_A$, and the softening temperature $T_S$. These temperatures correspond to the beginning and the end of the region of anomalous behavior of the thermal expansion coefficient, respectively, as shown by Brückner in Figure 8(a) of Ref. 10.

The values we used (for silica Suprasil 312, Type II), $T_A = 1395$ K and $T_S = 1875$ K, were supplied by the manufacturer (Heraeus). Although this is at best a crude approximation, we obtain a reasonable fit to the data, and our results are compatible with some earlier determinations of $k(T)$.

The samples considered in this paper were cylinders of glass Suprasil 312 from Heraeus, with a diameter of 50 mm and a thickness of 3 mm. To measure the temperature at their surface during CO$_2$ laser heating, IR thermography has been used, with the same operating condition as reported by Robin and co-workers.11 Our CO$_2$ laser operates at 10.6 $\mu$m and presents a quasi-Gaussian shape with beam diameter of 700 $\mu$m at $1/e^2$. For the study presented here the laser pulse duration was fixed at 1 s, and its power, which is constant throughout the pulse, was varied between 3 W and 9 W on the sample’s front surface. For each irradiation, a 2D surface temperature cartography as a function of time was recorded.

For our calculations, we use a specific lagrangian numerical code, where the irradiated target material is meshed in a 2D axi-symmetric geometry. We have chosen a mesh consisting of quadrangular cells. The laser energy deposition is obtained using a ray-tracing method. The axial laser beam is represented by 100 individual rays, where each ray is characterized by its position, its angle of incidence, and the energy it carries. In the target, the ray travels through the mesh and is refracted at each mesh interface. The energy reflected at the target surface is evaluated by means of the Fresnel relation. The energy that a ray deposits in each mesh cell obeys a Beer-Lambert attenuation law. Heat transfer is managed by the heat diffusion relation depending on the temperature gradient following Fourier’s law and the...
temperature dependant heat capacity and thermal conductivity. In our 2D axi-symmetric geometry, each mesh gives energy and receives energy from its four nearest neighbors. Then, the implicit resolution of the diffusion equation consists in solving a linear system associated with a pentadiagonal matrix of $N \times N$ dimension, where $N$ is the total number of cells which constitute the target. The linear system is solved using a Gauss-Seidel iterative method.

Since the density of the target does not vary appreciably during the laser irradiation, the physical data needed to model the interaction of a CO$_2$ laser beam with a silica sample are:

(i) Temperature dependent real and imaginary index of refraction of the silica at standard density for the CO$_2$ laser wavelength;\(^1\)

(ii) Temperature dependent heat capacity of the silica at standard density;\(^2\)

(iii) Temperature dependent thermal conductivity of the silica at standard density which is discussed in this article.

The others parameters used in the simulations are a target profile cylinder of 2.8 mm radius and 2.8 mm length. Such values permit us to avoid finite-size effects and perturbations caused by the sample limits for a 1 s laser irradiation. The radial dimension of the silica target is described with 60 sections whose axial dimension varies from 3.5 $\mu$m (near the axis) to 190 $\mu$m (at 2.8 mm from the axis). The longitudinal dimension of the target is described with 60 sections whose length varies from 3.5 $\mu$m (near the surface) to 190 $\mu$m (at a depth of 2.8 mm). The silica target is located behind the laser focal waist and the 100 rays which constitute the gaussian beam have incidence angles varying from $0^\circ$ (on the axis) to $4^\circ$ at 700 $\mu$m from the axis. At the level of the target’s surface, the distance between two neighboring rays varies from 4.5 $\mu$m (near the axis) to 11 $\mu$m (at 700 $\mu$m from the axis). Each ray contains the appropriate energy to describe a global Gaussian spatial profile. The laser beam, at the level of the target surface, is then gaussian with an 1/e$^2$ diameter of 700 $\mu$m. The simulation includes black body radiative losses at the sample’s surface, but these represent only 1%–2% of the incident energy. This agrees with the results of a detailed study that has recently appeared.\(^4\) The code itself was benchmarked by comparing the results of a simulation in which the thermal diffusivity and optical indices are assumed to be constant with an exact calculation using Green propagators. The thermal diffusivity $D(T)$ is defined by $D(T) = k(T)/\rho C_v(T)$, where $\rho$ is the density and $C_v(T)$ is the specific heat. The results agreed at approximately the 1% level for temperature values. From our calculation we obtain a 3D-map corresponding to temperature values in the irradiated area for any desired time during the interaction, as shown in Fig. 1 for the end of the laser pulse.

For laser energy increasing from 3 W to 6.5 W we recorded the temperature as a function of space and time. The very fast cooling of silica following the CO$_2$ laser shut down is also well reproduced by simulation, regardless of the laser power. For temperatures $>700$ K, the conductivity is chosen to be a piecewise linear function, with slope discontinuities at two particular temperatures, $T_A$ and $T_S$, as mentioned above. The data show that the temperature rises rapidly during the first 50 ms of irradiation and subsequently increases less rapidly. This rupture is strongly dependent on the thermal conductivity. The temperature is presented as a function of time at three different radial positions for each power level. We observe very good agreement even at 150 $\mu$m off-axis from the center of irradiation, while the temperature remains below $\sim 2000$ K.

Since several different thermal conductivities have been published, we show a comparison with our resulting thermal conductivity in Fig. 3(a). In it are displayed several experimental determinations of the thermal conductivity; some early measurements are represented by dashed curves (light green,\(^3\) dark green,\(^3\) and orange curves\(^4\)), while more recent laser based data are shown as individual points (lozenges with error bars\(^5\) and a square, which represents an average power. Whenever a significant disagreement was observed, we performed a new simulation with a modified value of $k(T)$ that differs only at the highest temperature reached. When satisfactory agreement is found we iterate the procedure with a slightly greater energy. Proceeding in this way we reach the maximum temperature available, with a $k(T)$ that fits reasonably well our large collection of data. The resulting thermal conductivity that we deduce in this way is shown in Fig. 2(a). Comparisons of calculations using this form with experimental data at 4.8 W, 5.3 W, and 5.8 W are shown in Figs. 2(b)–2(d), respectively. For temperatures $>700$ K, the conductivity is chosen to be a piecewise linear function, with slope discontinuities at two particular temperatures, $T_A$ and $T_S$, as mentioned above. The data show that the temperature rises rapidly during the first 50 ms of irradiation and subsequently increases less rapidly. This rupture is strongly dependent on the thermal conductivity. The temperature is presented as a function of time at three different radial positions for each power level. We observe very good agreement even at 150 $\mu$m off-axis from the center of irradiation, while the temperature remains below $\sim 2000$ K.

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For laser energy increasing from 3 W to 6.5 W we recorded the temperature as a function of space and time, using the IR camera set-up. The laser stationary power was turned on at $t = 0$ and turned off at $t = 1$ s. We then perform calculations with our code using the thermal conductivity data furnished by the manufacturer.\(^7\) We then begin a step-by-step procedure of comparing data with the smallest
value\textsuperscript{(16)}. These latter display such a large scatter that we see no simple way to parameterize them. There is also a set of data points supplied by the manufacturer, on which we base a simple linear parameterization (blue line)\textsuperscript{8} and our proposed piecewise linear estimation (red).

Additionally, for these thermal conductivities that can be parameterized, heat diffusion simulations were performed with a laser power of 5.3 W, which corresponds experimentally to the highest power without matter ejection. The resulting on-axis temporal profiles of temperature are compared with experiment in Fig. 3(b). These results are fairly easy to interpret. The green curves show a conductivity which is less than ours in the range of 700 K–1800 K and, therefore, predict a greater temperature increase than our model. In contrast, the blue and orange curves attain high conductivities at high temperature and thus evacuate the heat more rapidly than our model does, thereby failing to reach high temperatures in the sample. Some large discrepancies are observed even 100 ms after the laser turn on. At the end of the irradiation, the closest calculation using the Wray upper data displays a difference comparable to the experimental uncertainty. Moreover, these authors conclude their article by claiming: “The inflections in the thermal conductivity vs temperature curves are probably due to inaccuracies in measuring the slopes of the power vs wire temperature curves.”

As above for \(k(T)\), we show in Fig. 4 a comparison of our resulting thermal diffusivity \(D(T)\) with data from early measurements.\textsuperscript{17} These are bounded by dark and light green lozenges that correspond to upper and lower values, respectively, and dashed curves indicate a fit we made. Our indirect
determination of $D(T)$ has a lowest value for a temperature of 500 K, then increases with the temperature until the annealing point, in good agreement with the directly measured points. We also show a recent determination carried out using an IR thermal detection setup similar to ours. Although our results are generally about 10% greater than these recent measurements, there is only one value of temperature (1300 K) where a significant difference is apparent. We conclude that our indirect determination is consistent with this collection of measured points.

In conclusion, we have developed a 2D code and linked it with experimental measurements of the silica surface using IR thermography. By comparing simulation and experiment step by step as we increase the CO2 laser power, we performed an original method to determine the thermal conductivity. A very good correspondence between measured and calculated temperature is obtained both in time and in space, simply using a piecewise linear function for the thermal conductivity dependence in temperature. Our approach shows that $k(T)$ evolves with slope discontinuities at the annealing temperature and the softening temperature. These slope discontinuities, which occur at temperatures where the thermal expansion coefficients display anomalous behavior, might be further investigated by experiments that measure the residual stress in the silica after CO2 laser heating.