Modelling of CO_2 Laser Polishing of Glass

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Problem posed by Alain Cournoyer, INO

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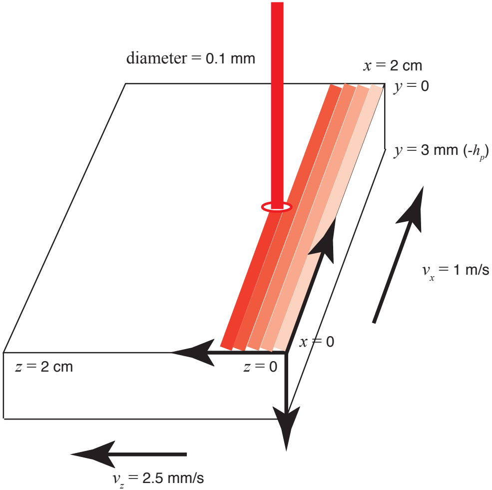
Outline

Problem background



The laser polishing process.

Problem background

A workpiece of dimensions about 2cm $\times$ 2cm (a few mm depth) is to be polished using a laser. Assume the workpiece is silicon (glass).

The polishing process

The laser rapidly heats the glass until it reaches the melting temperature. The molten silicon then flows so that bumps are evened out. In this way the surface roughness on the glass may be reduced, or removed.

Note

In ideal operation, no glass is vapourised. To machine by vapourization, see the other INO problem!

Objectives

The main aims of the investigation to consider:

1. What kind (length scale) of non-uniformities might be smoothed out by the process?
2. What are the main features of the heat transfer problem and how does the laser heat the material?
3. Can we propose a predictive model for the smoothing of non-uniformities?
4. When might we expect cracking to occur and can we predict this?

Note

The dynamic viscosity μ of the glass is a strong function of temperature T.

Identifying the dominant processes

Competing mechanisms: surface tension, viscosity, gravity. We consider a bump to be smoothed of height h and length L.

What is doing the spreading?

Surface tension (worst case): $h \sim 1\mu$m, $L \sim 100\mu$m

$$\frac{\gamma h}{L^3} \sim 3 \times 10^5 \text{ N m}^{-3}, \quad \text{bump over long distance}$$

Gravity: $\rho g \sim 10^4$ N m^{-3}.

Conclusion

Viscosity balances surface tension — gravity never important. The timescale τ for a bump of height h and length L to smooth out satisfies

$$\frac{\gamma h}{L^3} \sim \frac{\mu L}{\tau h^2}.$$

Identifying the dominant processes

Observation ($h \sim 1\mu$m, $L \sim 1\mu$m)

Only heat up the volume of a bump:
The diffusion time is $\frac{h^2 \rho c_p}{k} \sim 4 \times 10^{-7}$s.
The time it takes for the bump to flow is $\frac{\mu L^4}{\gamma h^3} \sim 3 \times 10^{-1}$s which is way too long.

Conclusion

What should be done and actually is done is to heat up a much deeper layer so that more of the fluid is mobile and it takes longer for the heat to diffuse away.

Identifying the dominant processes

For the thermal diffusion replace h with the penetration depth $h_p \sim 50\mu$m and consider flowing a bump of height $h \sim 1\mu$m over $L \sim 1\mu$m. Heating a relatively deep patch to smooth out the bumps.

Interesting and realistic bumps ($h \sim 1\mu$m, $L \sim 1\mu$m)

Time for viscous flow over distance L: Time for heat to diffuse over a height h:

$$\tau_{\text{diffuse}} = \frac{h_p^2 \rho c_p}{k} \sim 1 \times 10^{-3} s,$$

$$\tau_{\text{viscous}} = \frac{\mu L^4}{\gamma h^3} \sim 3 \times 10^{-1} s.$$

One can now expect reasonable smoothing with a number of passes over the workpiece.

Problem statement

The problem was separated into three interrelated subproblems:

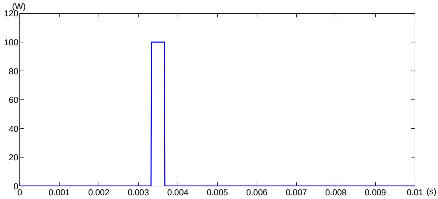
1. **Thermal problem** characterized by a rapid volumetric heating by the laser which reduces the viscosity of the glass and allows any defects to be smoothed away under the action of surface tension.
2. **Flow problem** modelled assuming a thin viscous incompressible fluid (lubrication theory) where the viscosity is suitably reduced through heating.
3. **Cracking mechanism** that considers both the thermal stress generated in either the heating and cooling of the material and compensates for a variable viscosity.

Volumetric laser heating

Let **v** be the convection velocity and let k be the thermal conductivity. The temperature T satisfies,

$$\rho c_p \left(\underbrace{\frac{\partial T}{\partial t}}_{1} + \underbrace{\mathbf{v} \cdot \nabla T}_{2} \right) = \underbrace{k \left(\frac{\partial^2 T}{\partial^2 x} + \frac{\partial^2 T}{\partial^2 y} + \frac{\partial^2 T}{\partial^2 z} \right)}_{3} + \underbrace{\Phi(t)}_{4}, \qquad (1a)$$

$$\Phi(t) = \frac{\alpha(T)\beta}{\pi d^2/4} I_0(t) e^{-\alpha(T)y}. \qquad (1b)$$



A typical short duration heating pulse of $I_0(t) = 100$ watts for 10^{-4}s.

Heat balances

$$\rho c_p \left(\underbrace{\frac{\partial T}{\partial t}}_{1} + \underbrace{\mathbf{v} \cdot \nabla T}_{2} \right) = \underbrace{k \left(\frac{\partial^2 T}{\partial^2 x} + \frac{\partial^2 T}{\partial^2 y} + \frac{\partial^2 T}{\partial^2 z} \right)}_{3} + \underbrace{\Phi(t)}_{4}.$$

- A very rapid heating phase implies that 1 balances 4.
- No source for the cooling phase so 1 balances 3.
- For heat diffusion the temperature varies predominantly with respect to the depth (y) so that only $\partial^2 T / \partial y^2$ dominates 3.
- Diffusion dominates convection on these time and space scales so that 2 can be ignored to first order.

Heating/Cooling problems

Heating ($0 < t < t_1$)

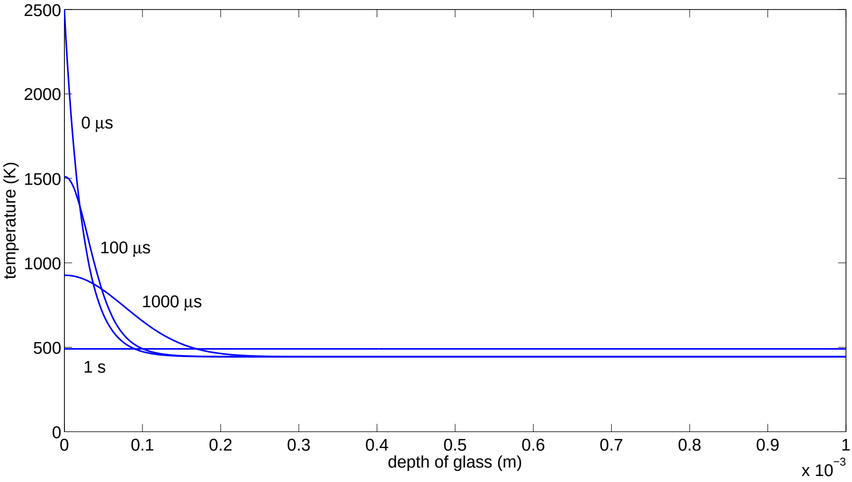
$$\begin{cases} \rho c_p \dfrac{\partial T_a}{\partial t} = \dfrac{\alpha(T_a)\beta}{\pi d^2/4} I_0(t) e^{\alpha(T_a)y}, \\ T_a(0,y) = T_0(y). \end{cases} \tag{2}$$

Cooling ($t > t_1$)

$$\begin{cases} \rho c_p \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial^2 y}, & -h_p < y < 0, \\ k \frac{\partial T}{\partial y} = \sigma_{\mathrm{rad}}(T^4 - T_{\mathrm{b}}^4), & y = 0, \\ k \frac{\partial T}{\partial y} = 0, & y = -h_p, \\ T(t_1, y) = T_a(t_1, y), & -h_p < y < 0. \end{cases} \tag{3}$$

The viscosity can be determined as a function of position and time.

Results (thermal)

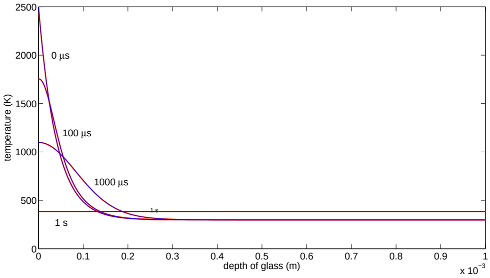


Temperature rise as a function of depth into the workpiece for various times.

Boundary condition at the surface

Radiative versus no flux

Comparison of the numerical solution for the temperature with the radiative and the no flux surface condition shows no appreciable difference over the spatial domain.



Comparison of the temperature rise for a radiative and a no flux boundary condition at the surface $y = 0$.

Governing equations

We start with the incompressible Navier-Stokes with variable viscosity

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{1}{\rho} \nabla p + \nabla \cdot \sigma + \mathbf{g}, \tag{4a}$$

$$\nabla \cdot \mathbf{v} = 0 \tag{4b}$$

where $\sigma = \mu[\nabla \mathbf{v} + (\nabla \mathbf{v})^T]$, $\mathbf{v}$ is the velocity, μ the viscosity, ρ the density, and p the pressure.

- Vertical: $h_p \sim 10^{-5}$ m (heated layer thickness near the surface);
- Horizontal: $L \sim 10^{-4}$ m (size of the laser beam).

Surface and other boundary conditions

At the top free-surface $y = h(t, x, z)$, we have the usual kinematic and dynamic conditions $\mathbf{v} = \langle \mathbf{u}, v \rangle$

$$
\begin{aligned}
\frac{\partial h}{\partial t} + \mathbf{u} \cdot \nabla_{xz} h - v &= 0, & y &= h, & \text{(5a)}\\
p - \sigma \cdot \mathbf{n} &= p_a - \gamma \kappa, & y &= h, & \text{(5b)}\\
\sigma \cdot \tau &= 0, & y &= h, & \text{(5c)}\\
\mathbf{v} &= 0 & y &= -h_p, & \text{(5d)}
\end{aligned}
$$

where $\mathbf{u}$ and v are the horizontal and vertical directions, p_a the atmospheric pressure, γ the surface tension coefficient, κ the surface curvature, $\mathbf{n}$ and τ the unit normal and tangential vector.

- Simplification 1: ignore z direction for now (easily included);
- Simplification 2: small h (10^{-6} m).

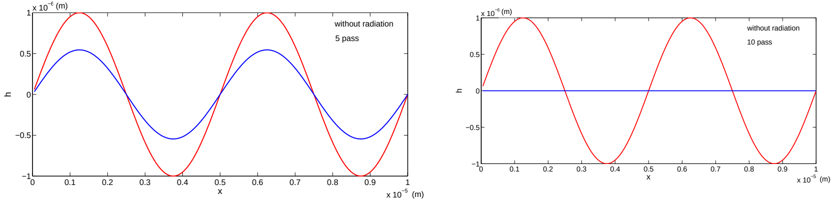
One-dimensional thin film equation

We arrived at an integral equation

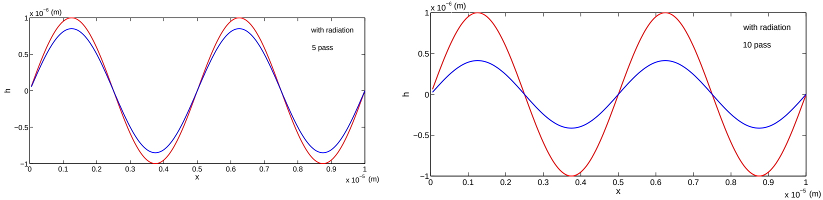
$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial x}\left(\int_{-\infty}^{h} \frac{\gamma(y-h)^2}{2\mu} dy \frac{\partial^3 h}{\partial x^3}\right) = 0. \tag{6}$$

Note that in general we have to solve the equation numerically or use Watson's lemma to estimate the integral.

Smoothing a bump over multiple heating passes



(5 passes, No flux) (10 passes, No flux)

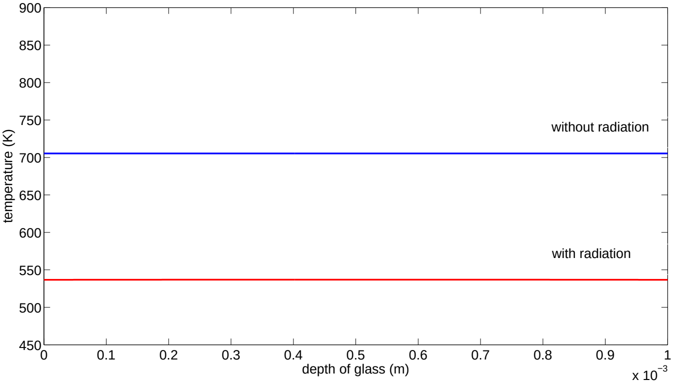


(5 passes, Radiation) (10 passes, Radiation)

Evolution of the surface roughness.

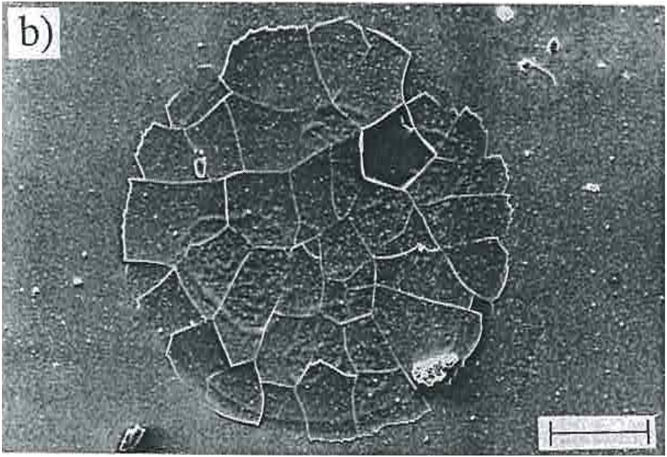
Residual heating of the material

After 10 passes there is some residual heat left in the material. The amount depends on if the no flux or the radiation boundary condition is used.

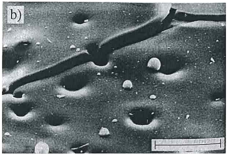


Cracking of the workpiece

If the thermal regime is to severe in some way then there may be cracking ("crazing") This will render the workpiece useless.



Cracking of the workpiece



Observations

1. When cracking does happen, the whole of the workpiece is normally affected.
2. The length of the "crazy paving" cracks is typically 100μm.
3. The crack depth is maybe 10μm.
4. Experiments seem to show that the cracking does not occur during heating ("boiling water on a freezing windscreen") but occurs later during cooling ("windscreen cracks in Rex's car when it gets cold in Calgary").

Mechanisms

Competition

- Thermoelasticity (elastic expansion when heated)
- Viscosity (acts to dissipate the extra stress by flowing)

Note

- When T is very large, the thermoelastic stress is high, but the viscosity is low enough for flow and stress dissipation
- When T is very small, the material is solid and there is no flow - but there is also no significant thermoelastic stress.

Suggestion

There is a "in between" regime where cooling cracking can happen. We should consider thermoviscoelasticity.

Simplest model: Ignore viscosity (thermoelastic)

1−D thermoelastic

Contraction of material during cooling is given by $\alpha(T - T_{\mathrm{ref}})$.
($\alpha =$ coefficient of linear thermal expansion).
This generates stress $\sigma = \alpha E(T - T_{\mathrm{ref}})$.

Result: if α is large then there could be cracks.
Limitation: no flow effects included.

Next simplest model: Maxwell kludge (viscoelastic)

Simple physics model in the literature (Allcock et al., 95)

Add viscous effects kludge: 1−D Maxwell model where

$$\epsilon = u_x = \frac{\sigma}{E} + \frac{1}{\mu}\int^t \sigma\, dt \sim \frac{\sigma}{E} + \frac{\sigma t}{\mu} \tag{7}$$

where $t =$ relaxation time (Note: u is displacement). Then just do thermoelasticity, but with

$$E = E_{\text{eff}} = \frac{1}{\frac{1}{E} + \frac{t}{\mu}}. \tag{8}$$

"relaxation time scale decreases E to E_{eff} to allow for viscosity".
Maxwell version seems inconsistent in 1−D — (no time for details).

Our model A: Voight (thermoviscoelastic)

Voight model

In one dimension we have

$$\sigma_x = 0, \qquad \sigma = E(u_x - \alpha(T - T_{\mathrm{ref}})) + \mu u_{xt} \tag{9}$$

where in general $\mu = \mu(T(x,t))$.

Heating problem

First do $\mu =$ constant. Flow is over $0 \leq x \leq 1$ for $t > 0$. Assume material is confined so that always $u(0,t) = u(1,t) = 0$. We have:

$$t = 0: \qquad T(0,x) = 0, (T_{\mathrm{ref}} = 0, u(0,x) = 0), \tag{10a}$$

$$t > 0: \qquad T(t,x) = (1 - e^{-qt})x(1-x). \tag{10b}$$

Our model A: Voight (cont)

Solve equation for u etc. - we find that

$$u(x,t) = \alpha E \left(\frac{x^2}{2} - \frac{x^3}{3} - \frac{x}{6} \right) g(t;\mu,E,q) \tag{11a}$$

$$g(t;\mu,E,q) = \left[\frac{1}{\mu} \left(1 - e^{-\mu t/E} \right) - \frac{1}{\mu - qE} \left(e^{-\mu t/E} - e^{-qt} \right) \right] \tag{11b}$$

which gives $\sigma(t) = -\frac{\alpha}{6}$. This does not depend on μ, but does give a non-zero value as $t \to \infty$ ("locked-in stress")

Note

If μ is a function just of t then the same conclusion holds, but in general if μ is a function of temperature (in particular x) this can affect the final stress state.

Our model B: Maxwell (thermoviscoelastic)

We extend the Maxwell model in space one-dimension (between $0 \leq z \leq 1$)

$$\frac{\sigma}{E} + \int_0^t \frac{\sigma}{\mu} ds = \alpha(T - T_{ref}) - u_z, \tag{12a}$$

$$\sigma_z = 0, \tag{12b}$$

where σ is the stress and u_z strain rate. We assume that $u = 0$ at $z = 0$ and 1 and initially $T = T_{ref}$. Our model is more general than the one in Allcock et al. (1995) as

- T could depend on z and t; and
- μ could depend on z and t (as a function of temperature).

Simplification of the Maxwell model

From $\sigma_z = 0$, we can immediately conclude that $\sigma = \sigma(t)$. Integrate the first equation in z and apply $u = 0$ at $z = 0$ and 1 to obtain

$$\frac{\sigma}{E} + \int_0^t \frac{\sigma}{\bar{\mu}(t)} ds = \alpha \overline{T}, \tag{13}$$

where

$$\frac{1}{\bar{\mu}(t)} = \int_0^1 \frac{1}{\mu(t,z)} dz, \quad \overline{T}(t) = \int_0^1 (T(t,z) - T_{ref}) dz. \tag{14}$$

Equivalently, we have

$$\dot{\sigma} + \frac{E}{\bar{\mu}(t)} \sigma = \alpha E \dot{\overline{T}}(t). \tag{15}$$

- This is an ODE we can solve numerically in general; and
- It is exactly the same form when the temperature and viscosity in Allcock et al (1995) are integrated as the space average.

Solution of the Maxwell model

We consider a simple case where $\bar{\mu}$ is constant. We find the solution

$$\sigma = \alpha E \int_0^t \dot{\overline{T}} e^{E/\bar{\mu}(s-t)} ds. \tag{16}$$

Special case: $\overline{T} = (e^{-t/p} - 1)$.

- Elastic $\bar{\mu} = 0$: $\sigma = \alpha E(e^{-t/p} - 1)$;
- Viscoelastic

$$\sigma(t) = \frac{\alpha E}{1 - \frac{pE}{\bar{\mu}}} \left(e^{-t/p} - e^{-\frac{Et}{\bar{\mu}}} \right). \tag{17}$$

Remark

When $p \ll \bar{\mu}/E$ (rapid cooling), viscoelasticity has a small impact. However, if $pE/\bar{\mu} \gg 1$ (slow cooling), the viscoelastic effect is significant.

What have we learned?

1. What kind (length scale) of non-uniformities might be smoothed out by the process?

Defects on the size of 1μm can be completely removed after about ten passes if there are no radiative losses. This is made possible by heating a significant depth of the material $h_p = 50\mu$m. There is a residual heating affect that is accumulative. After five passes the temperature rise is about 500K (less if there are radiative losses).

What have we learned?

2. What are the main features of the heat transfer problem and how does the laser heat the material?

The defect removal is consistent with a rapid heating phase over the penetration depth and a relatively long cooling time over this depth. Heat flux is essentially dissipated into the workpiece and in comparison very little heat escapes through the surface.

What have we learned?

3. Can we propose a predictive model for the smoothing of non-uniformities?

A predictive model using lubrication theory and a simplified model for the volumetric heating has been effective at reproducing the smoothing out of the defects through a coupling of a reduction of the viscosity and the reducing surface tension. Heating a sufficient volume of the material is crucial to having this mechanism work.

What have we learned?

4. When might we expect cracking to occur and can we predict this?

Cracking is suspected to be a result of an excessive rate of cooling of the material (Allcock, 1995). Using a Voight model we show that the formation of excess stress is related to spatial variations in the viscosity. Preliminary analysis of a thermoviscoelastic Maxwell model indicates that it is possible to generate large stresses that could cause cracking if the material is hot enough to generate significant thermal stress yet not so hot as to have that stress dissipate through the flow of the material due to the reduced viscosity.

Thank-you!