Thermodynamics of optomechanical materials

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Abstract

1 Introduction

2 Cooling due to gas molecules only

Let us assume that a bead of surface area A and volume V is optically trapped using laser light of wavelength λ and intensity I Wm^{-2} in a vacuum chamber using intensity gradient in atmospheric condition. Subsequent to trapping, trapped bead is gradually taken to different levels of vacuum depending on applications. Assuming that the trapped bead has a complex refractive index ($n = \eta + i\kappa$), the amount of heat generated inside the bead can be expressed as Eq. (1), where C_{abs} is the absorption cross section of the bead.

$$H_G = C_{abs} I \tag{1}$$

Heat generated due to the absorption of light will raise the temperature of the bead to $T_1 = T_0 + \Delta T$, where T_0 is the atmospheric/room temperature. Actual temperature of the trapped bead depends on it's ability of absorbing light as well as on it's capability of dissipation. Among the dissipation mechanisms, black body radiation and heat loss due to collisions with the gas molecules are relevant. Heat loss (H_D) due to the latter process can be calculated using the kinetic theory of gases. In this regard, let us assume that, under the atmospheric condition, there are N_0 gas molecules per cubic meter and the atmospheric pressure is P_0. As the pressure inside the chamber goes down, the number of gas molecules per cubic meter reduces. At a given pressure $P < P_0$, the number of remaining gas molecules (N) inside the chamber can be found by combining equations (2) and (3), where k_B is the Boltzmann constant [1]. In the derivation, it has been assumed that the temperature inside the chamber is T_0, even though the temperature of the bead is $T_1 > T_0$.

$$P_0 = N_0 k_B T_0 \tag{2}$$

$$P = N k_B T_0 \tag{3}$$

$$N = N_0 \frac{P}{P_0} \tag{4}$$

Now, assuming that the trapped bead is tightly held (**not sure**

what impact it's movement will have on the number of collisions. Since oscillation is on the scale of nanometers, I guess this assumption is not necessary), the number of collisions (N_c) that the bead gets in a second at pressure P can be derived as follows. Elaborately, if the average velocity of the gas molecules is v_0, then the molecules between 0 and v_0 meters from the bead are capable of hitting the bead. The number of molecules within this distance is v_0NA [1]. Among these molecules, on the average, half will head towards the bead while the other half will move away from the bead. Consequently, the number of collisions that the bead will receive in a second can be expressed as Eq. (5).

$$N_c = \frac{1}{2} v_0 N A \tag{5}$$

Substituting N from Eq. (4), and given that v_0 can be expressed as $\sqrt{3k_BT_0/M}$, above can be reformulated as -

$$N_c = \frac{1}{2} N_0 A \frac{P}{P_0} \sqrt{\frac{3k_BT_0}{M}} \tag{6}$$

, where M is the molecular mass.

Assuming that the gas molecules are diatomic and the impinging gas molecules are in room temperature while that of the emerging gas molecules is the same as that of the bead, the amount of the heat energy (H_D) taken away the by colliding gases can written as Eq. (7).

$$
\begin{aligned}
H_D &= N_C * (3k_B\Delta T) \\
&= \frac{1}{2}N_0 A\frac{P}{P_0}\sqrt{\frac{3k_BT_0}{M}} * (3k_B\Delta T) \\
&= \frac{N_0}{P_0}\sqrt{\frac{27T_0k_B^3}{4M}}\Delta TAP
\end{aligned} \tag{7}
$$

Now the actual amount of heat that is left over to raise the temperature of the bead in the amount of time Δt can be found by subtracting H_D from H_G.

$$
\begin{aligned}
\Delta H &= (H_G - H_D)\Delta t \\
&= (C_{abs}I - \frac{N_0}{P_0}\sqrt{\frac{27T_0k_B^3}{4M}}\Delta TAP)\Delta t
\end{aligned} \tag{8}
$$

Provided that ΔH can be expressed as $VC_v\Delta T$, where C_v is the volumetric heat capacity of the trapped bead, in the limit $\Delta t \to 0$, Eq. (8) can be reformulated as Eq. (9).

$$
\begin{aligned}
VC_v\Delta T &= (C_{abs}I - \frac{N_0}{P_0}\sqrt{\frac{27T_0k_B^3}{4M}}\Delta TAP)\Delta t \\
VC_v\frac{d}{dt}T &= (C_{abs}I - \frac{N_0}{P_0}\sqrt{\frac{27T_0k_B^3}{4M}}APT) \\
\frac{d}{dt}T &= \frac{1}{VC_v}(C_{abs}I - \frac{APN_0}{P_0}\sqrt{\frac{27T_0k_B^3}{4M}}T)
\end{aligned} \tag{9}
$$

Eq. (9) is a first order linear differential equation (similar to $Y^{'} =$

$aY + b$). The solution ($Y(t) = C\exp(at) + \frac{b}{a}$) of the above equation is -

$$T = \frac{C_{abs}IP_0}{APN_0}\sqrt{\frac{4M}{27T_0k_B^3}} + C\exp\left(-\frac{APN_0}{VC_vP_0}\sqrt{\frac{27T_0k_B^3}{4M}}t\right) \tag{10}$$

After applying the initial condition $T(0) = 0$, one can find -

$$T = \frac{C_{abs}IP_0}{APN_0}\sqrt{\frac{4M}{27T_0k_B^3}}[1 - \exp\left(-\frac{APN_0}{VC_vP_0}\sqrt{\frac{27T_0k_B^3}{4M}}t\right)] \tag{11}$$

3 Some results and observations

For a sphere of radius $R << \lambda$, C_{abs} can be calculated using Rayleigh approximation [2] and is given by Eq. (12), where $k = 2\pi/\lambda$ and $\epsilon = n^2$.

$$\begin{aligned} C_{abs} &= \pi R^2 * 4kR\Im[\frac{n^2-1}{n^2+2}] \\ &= 3kV\Im[\frac{\epsilon-1}{\epsilon+2}] \end{aligned} \tag{12}$$

On substitution of C_{abs} in Eq. (11) one gets-

$$T = \frac{3VkIP_0}{APN_0}Im[\frac{\epsilon-1}{\epsilon+2}]\sqrt{\frac{4M}{27T_0k_B^3}}[1 - \exp\left(-\frac{APN_0}{VC_vP_0}\sqrt{\frac{27T_0k_B^3}{4M}}t\right)] \tag{13}$$

From Eq. (13) one can see that T is inversely proportional to P. This signifies that, for a given set of parameters A, V, I, and λ, as the pressure decreases temperature of the bead will increase as has been found experimentally [3]. Further, T is also proportional to the ratio of V and A. Elaborately, as the size of a bead shrinks, the ratio between V and A decreases and a consequence of this is that larger beads will have higher T_1 compared to smaller beads. Or a larger bead will melt at a higher pressure compared to a smaller bead under the same experimental conditions. This has also been experimentally verified in [3]. From Eq. (13), it can also be said that asymmetric beads, which have lower volume to surface ratios, will be more resilient to low pressure compared to their spherical counterparts (**this is good for our diamond experiment, in which beads are mostly asymmetric**). The ratio between A and V also plays roles in how quickly a bead will approach T_1 under a given circumstance. It is obvious that smaller beads will do it quickly compared to larger particles. In regards to T_1, for a given size bead, it can also be observed that beads with higher C_v will require more time to reach T_1 than beads with smaller C_v as expected.

Fig. 1 shows data corresponding to $R = 50$ nm gold and silica spheres at different pressures and $I = 145\ GW/m^2$ (300 **mW at the focus, typical trapping power**). Refractive indices of gold [4] and silica [5] at $\lambda = 1064$ nm are $\epsilon = 0.258 + i6.965$ and $\epsilon = 1.5 + i10^{-7}$, respectively. From this figure it can be seen that at about $P \approx 20$ mB

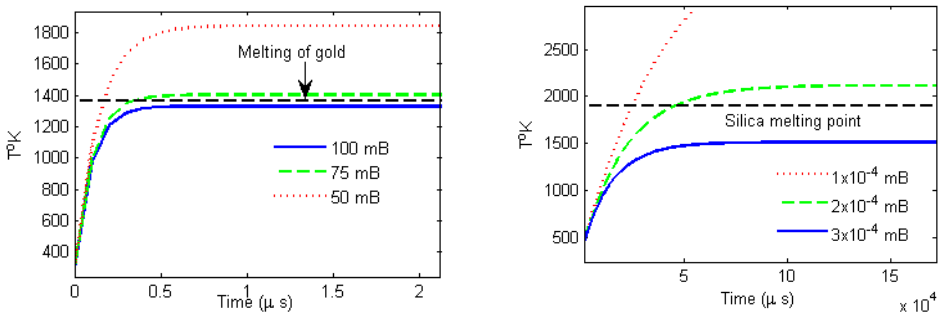

Figure 1: T vs t for $I = 145\ GW/m^2$ (a) for a 50 nm gold sphere, and (b) for a 50 nm silica sphere at different pressure.

and $P \approx 10^{-4}$ mB, gold and silica respectively melt. From this figure it can also be observed that the ultimate temperature for a given set of parameters is reached on the scale of a second or less. In the limit $t \to \infty$, the exponential term from Eq. (13) can be dropped. After this simplification one can write -

$$T = \frac{3VkIP_0}{APN_0} Im[\frac{\epsilon - 1}{\epsilon + 2}] \sqrt{\frac{4M}{27T_0 k_B^3}} \tag{14}$$

Exploiting Eq. (14), Fig. 2 (a) shows various pressures that can be reached before beads melt for three different radii of silica beads for a constant laser intensity of $I = 145\ GW/m^2$ (typical trapping power in our set-up). It can be seen that as the bead size increases, lowest pressures that can be sustained without melting the beads increases as well. This has been confirmed in [3]. In contrast, Fig. 2 (b) demonstrates effects of laser intensity on the lowest pressure that can be reached before a 50 nm silica bead melts. From Fig. 2 (b) one can

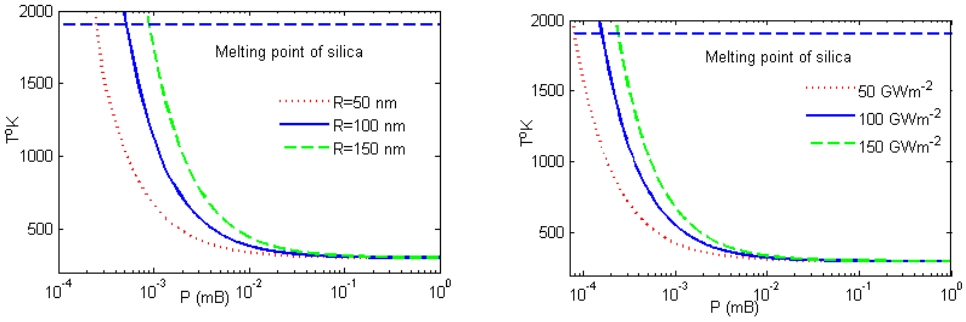

Figure 2: (a) T vs P for silica spheres at different radii for $I = 145\ GW/m^2$ and (b) T vs P for a $R = 50$ nm silica sphere at three different laser intensities.

see that for $I = 50\ GW/m^2$ our model predicts $P \approx 1.43 \times 10^{-5}$ mB at which $R = 50$ nm silica beads are expected to melt. Further, as the trapping power increases, melting pressure rises accordingly. Again, this is in qualitative agreement with Millen et al. [3].

To compare the performance of our model, Table 1 shows some data from the literature along with the prediction based on the model developed here. Since some of the beads used in the literature do not fulfill the Rayleigh approximation, one needs to use Mie theory [2] to find absorption cross sections. In the limit $t \to \infty$ and using full Mie theory, Table 1 shows predicted melting pressures as per Eq. (11) for different silica beads. In case of $R = 70$ nm [6] and $R = 1500$ nm [7] (**diameters -** 140 **nm and** 3 μ**m respectively**) spheres, the lowest reported pressures are 9×10^{-6} mB and 1.3×10^{-3} mB, respectively (with feedback reported lowest pressures are - 2.56×10^{-6} mB [6] and

Table 1: Some results on silica from literature

Radius (nm)	Laser Intensity (GWm^{-2})	Minimum pressure reported without melting (mB)	Melting pressure according to Eq. (13) (mB)
70	48.00	9×10^{-6} [6]	1.00×10^{-4}
1250	13.00	1.0 [3]	1×10^{-3}
1500	76.86	1.3×10^{-3} [7]	1×10^{-2}

5.2×10^{-5} mB [7]). From the table one can see that the agreement between the predictions of the model and data from the literature is very good.

4 Blackbody plus gas cooling

Cooling due to blackbody radiation is given Eq. (16) [8]

$$\frac{dE_{bb}}{dt} = \frac{72\zeta(5)}{\pi^2}\frac{V}{c^3\hbar^4}\Im[\frac{\epsilon_{bb}-1}{\epsilon_{bb}+2}](k_B T_I)^5 \tag{15}$$

where $\zeta(5)$ is the Reimann zeta function ($\zeta(5) \approx 1.4$), V is the bead's volume, ϵ_{bb} is the dielectric constant of the bead over the blackbody radiation spectrum (approximation), T is the bead's internal temperature. T can be expressed as $T_I = T_0 + \Delta T$, where T_0 is the room temperature and ΔT is the temperature increment over the room temperature due to absorption of light.

Cooling due to the gas molecules can be expressed as [8]

$$\frac{dE_g}{dt} = -\alpha_g \sqrt{\frac{2}{3\pi}} \pi R^2 P v_{rms} \frac{\gamma_{sh}+1}{\gamma_{sh}-1} (\frac{T_I}{T_0} - 1), \tag{16}$$

where α_g the accommodation coefficient, R is the radius of the particle, P is the pressure in pascal, v_{rms} is the rms speed of gas molecules at pressure P, γ_{sh} is the specific heat ratio of the gases, T_I is the internal temperature of the levitated particle and T_0 is the atmospheric temperature.

Overall temperature reached by a trapped particle can be expressed as Eq. (17).

$$\begin{aligned}
C_v V(T_I - T_0) &= P_{abs} - E_g - E_{bb} \\
&= P_{abs} + \alpha_g \sqrt{\frac{2}{3\pi}} \pi R^2 P v_{rms} \frac{\gamma_{sh}+1}{\gamma_{sh}-1} (\frac{T_I}{T_0} - 1) - \frac{72\zeta(5)}{\pi^2} \frac{V}{c^3\hbar^4} \Im[\frac{\epsilon_{bb}-1}{\epsilon_{bb}+2}] k_B^5 (T_I^5 - T_0^5) \\
&= C_{abs} I + \alpha_g \sqrt{\frac{2}{3\pi}} \pi R^2 P v_{rms} \frac{\gamma_{sh}+1}{\gamma_{sh}-1} (\frac{T_I}{T_0} - 1) - \frac{72\zeta(5)}{\pi^2} \frac{V}{c^3\hbar^4} \Im[\frac{\epsilon_{bb}-1}{\epsilon_{bb}+2}] k_B^5 (T_I^5 - T_0^5) \\
&= 3kV \Im[\frac{\epsilon-1}{\epsilon+2}] I + \alpha_g \sqrt{\frac{2}{3\pi}} \pi R^2 P v_{rms} \frac{\gamma_{sh}+1}{\gamma_{sh}-1} (\frac{T_I}{T_0} - 1) - \frac{72\zeta(5)}{\pi^2} \frac{V}{c^3\hbar^4} \Im[\frac{\epsilon_{bb}-1}{\epsilon_{bb}+2}] k_B^5 (T_I^5 - T_0^5)
\end{aligned} \tag{17}$$

Fig. 5 shows data corresponding to Eq. (17). From left to right this figure shows the effect of the size of beads for R = 50 nm, R = 150 nm and R = 250 nm while top to bottom demonstrates the effect of refractive index for $\sqrt{\epsilon} = 1.5 + i1 \times 10^{-9}$, $\sqrt{\epsilon} = 1.5 + i1 \times 10^{-8}$ and $\sqrt{\epsilon} = 1.5 + i1 \times 10^{-7}$. I was fixed to $\approx 232\ GWm^{-2}$ (e^{-2} intensity corresponding to our minimum trapping power of 150 mW at the focus with NA=0.80). In all of this figures blue solid lines represent cooling due to gas molecules alone while dashed red lines show the effect of blackbody plus

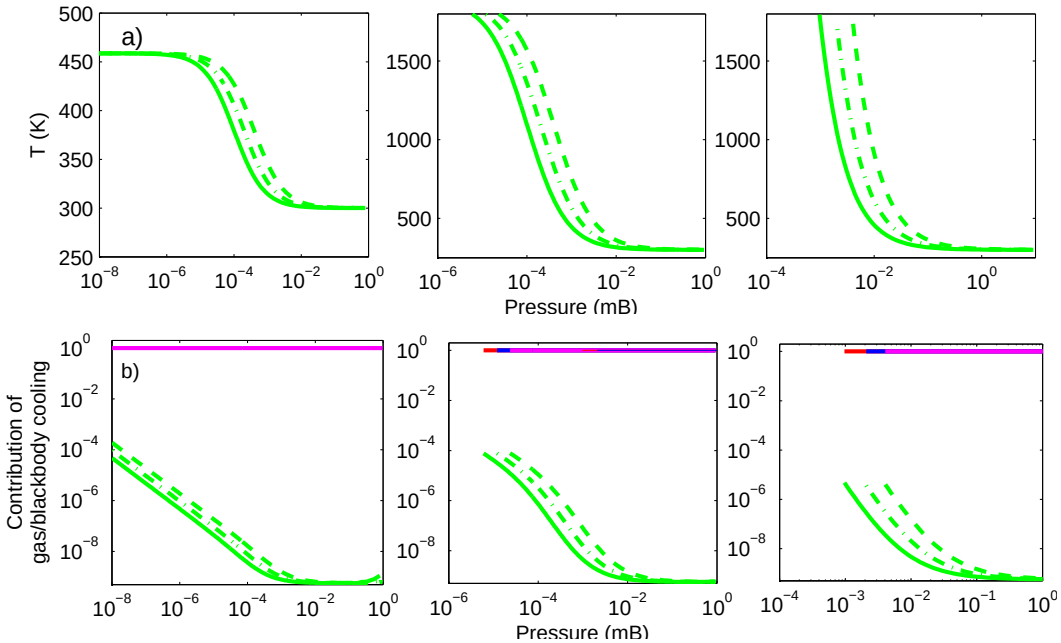

Figure 3: a) Effect of size and refractive index on the steady state temperature of silica nanoparticles- solid lines correspond $R = 50$ nm while dash-dot and dash lines represent $R = 100$ nm and $R = 200$ nm, respectively. From left to right refractive index increases starting from $\sqrt{\epsilon} = 1.5 + i1 \times 10^{-10}$, then $\sqrt{\epsilon} = 1.5 + i1 \times 10^{-9}$ and lastly $\sqrt{\epsilon} = 1.5 + i1 \times 10^{-8}$. b) Contribution of blackbody and gas(solid lines) cooling in the total heat dissipated by the particles considered in a).

gas cooling. As the size of a bead increases probably we see some effect of volume; meaning blackbody cooling is proportional to volume. It can also be interpreted as, I suppose, a nanoeffect. That is as we reduce the size of a bead surface area to volume ratio increases and hence gas cooling becomes more efficient.

It can also be observed that for smaller beads difference between gas cooling and cooling due gas and blackbody is smaller.

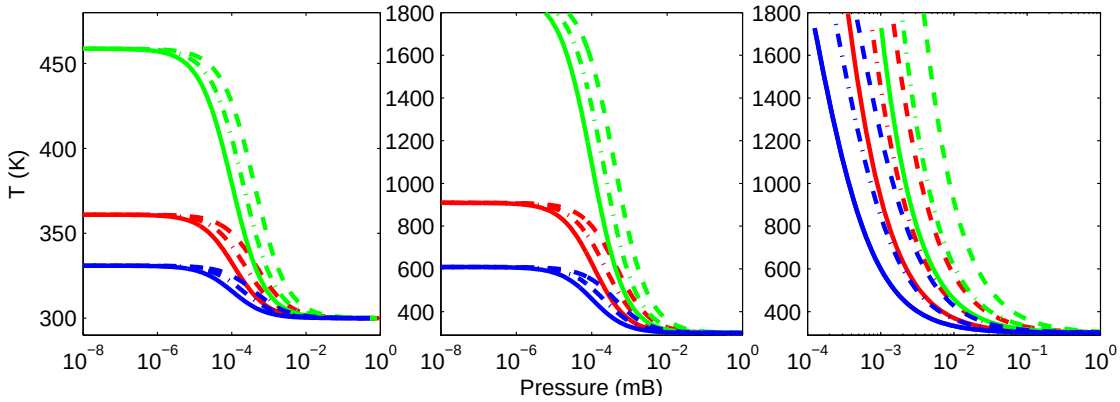

Figure 4: Effects of materials on the overall temperature reached as a function of pressure for a given trapping laser power - blue silicon, red diamond and green silica. Respective solid lines represent $R = 50$ nm while dash-dot and dash lines correspond $R = 100$ nm and $R = 200$ nm, respectively. From left to right imaginary components of the respective materials are $\sqrt{\epsilon} = 10^{-10}$, $\sqrt{\epsilon} = 10^{-9}$ and $\sqrt{\epsilon} = 10^{-8}$. Real components of the refractive indices of silicon, diamond and silica are 4.5, 2.5 and 1.5 at $\lambda = 1064$ nm, respectively.

5 Impact of materials

6 Determination of the imaginary part of the refractive index

Assuming that the size of a levitated particle is known and a levitated particle reaches its melting temperature $T_m = T + T_0$ at pressure P and assuming that cooling due to the blackbody radiation is much smaller than gas cooling, from Eq. (14) one can write-

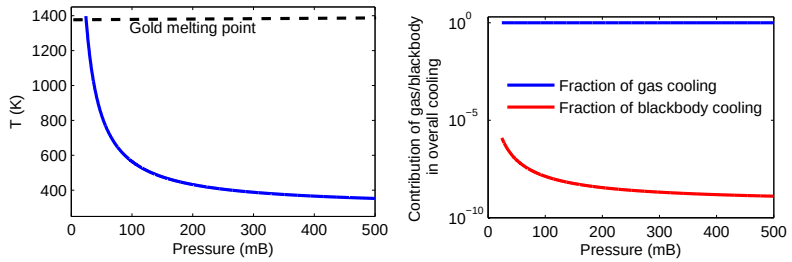

Figure 5: $\sqrt{\epsilon} = 0.1715 + i * 7.1058$, $R = 33$ nm, NA=0.80, Power=$180 * 0.87$ mW, $C_v = 2.492 \times 10^6$

$$Im[\frac{\epsilon - 1}{\epsilon + 2}] \quad = \quad \frac{AN_0PT}{3kIP_0V}\sqrt{\frac{27T_0k_B^3}{4M}} \tag{18}$$

7 Effects of shape and size

8 Effects of materials

9 Conclusions

References

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