Effects and side effects of plasmonic photothermal therapy in brain tissue

Yue He, Kristoffer Laugesen, Dana Kamp, Salik A. Sultan, Lene B. Oddershede, and Liselotte Jauffred
The Niels Bohr Institute, University of Copenhagen, Copenhagen, DK-2100, Denmark

Additional text

Derivation of heat transfer equations

Following the train of thought from Ref.[1] we obtained the expressions from an investigation of the energy balance of the system:

$$\sum_i m_i C_{p,i} \frac{dT}{dt} = \sum_j Q_j \tag{1}$$

where the left side is the sum of products of masses, m_i, and the corresponding heat capacity, $C_{p,i}$, of the different components, T is the temperature and t is time. The right hand side is the sum of energy terms, Q_j. Eq. (1) is valid when the time it takes for the system to reach thermal equilibrium within the cuvette is less than the time needed to obtain thermal equilibrium with the surroundings. The source term Q_1 is the heat dissipated by electron-phonon relaxation of plasmons on the nanoparticle surface at the laser wavelength, λ:

$$Q_1 = P(1 - 10^{-A_\lambda})\eta, \tag{2}$$

where η is the photothermal transduction efficiency, i.e., the efficiency to convert the incident absorbance, A_λ, of laser light to heat. A_λ is given by Beer-Lambert's law and is often referred to as the optical density. Q_0 is the heat dissipated in the cuvette and the media containing the nanoparticles. The terms Q_1 and Q_0 add heat to the system and are counteracted by energy terms describing exchanges with the surroundings. The first term is energy conducted to air, sample holder etc.:

$$Q_{cond} \propto \Delta T, \tag{3}$$

where $\Delta T = T - T_{amb}$ and T_{amb} is the ambient temperature. Furthermore, there is thermal radiation, Q_{rad}, given by Stefan-Boltzmann's law:

$$Q_{rad} \propto T^4 - T_{amb}^4 \tag{4}$$

For large T, i.e., $T > T_{amb}$, $Q_{rad}/\Delta T$ varies little respect to ΔT. For ΔT less than 10° K we can approximate $Q_{rad}/\Delta T$ with a constant value as the variation is less than 5%.[1] As a result,

$$Q_{ext} = Q_{cond} + Q_{rad} \propto \Delta T \tag{5}$$

and, thus, is written as:

$$Q_{ext} = hA(T - T_{amb}), \tag{6}$$

where h is a heat-transfer coefficient and A is the surface area for radiative heat transfer. Thus, eq. (1) is simplified to:

$$\sum_i m_i C_{p,i} \frac{dT}{dt} = Q_1 + Q_0 - Q_{ext} \tag{7}$$

We define the system's characteristic time constant to be

$$\tau := \frac{\sum_i m_i C_{p,i}}{hA} \tag{8}$$

To extract τ we focus on thermal equilibrium with the surroundings via conductive and radiative heat transfer, i.e. after laser is turned off. In this case $Q_1 = Q_0 = 0$ and eq. (7) reduces to

$$\sum_i m_i C_{p,i} \frac{dT}{dt} = -Q_{ext} \tag{9}$$

We define the dimensionless driving force to be

$$\theta := \frac{T_{amb} - T}{T_{amb} - T_{ss}}, \tag{10}$$

where T_{ss} is the maximum temperature reached or the steady-state temperature. Then, we substitute τ and θ into eq. (9) and get

$$\frac{d\theta}{dt} = -\frac{\theta}{\tau} \tag{11}$$

and integrate

$$\int \frac{1}{\theta} d\theta = -\frac{1}{\tau} \int dt \tag{12}$$

Using the initial condition that $\theta = 1$ when $t = 0$, i.e., when irradiation ceases, we get

$$\log \theta = -\frac{t}{\tau} \tag{13}$$

such that

$$\theta = e^{t/\tau} \tag{14}$$

By substituting θ we find the expression given in Eq. (2) in the main article:

$$\Delta T = \Delta T_{ss} e^{-t/\tau}. \tag{15}$$

When the laser is irradiating the system, heat is added ($Q_0 + Q_1 > 0$) and we use the initial condition that $\theta = 0$ when $t = 0$ we find

$$\theta = 1 - e^{t/\tau} \tag{16}$$

By substituting θ we get Eq. (1) in the main article:

$$\Delta T = \Delta T_{ss}(1 - e^{-t/\tau}) \tag{17}$$

References

1 D. K. Roper, W. Ahn, and M. Hoepfner, "Microscale Heat Transfer Transduced by Surface Plasmon Resonant Gold Nanoparticles," *Journal of Physical Chemistry C* **111**, 3636–3641 (2007).