

# Laser induced Coulomb explosion of gold nanoparticles : potential role for nanophotolysis of Breast cancer

M.G.B ASHIQ, NOORDDIN IBRAHIM, M.A.SAEED, M.SHAHID  
 Department of Physics, Universiti Teknologi Malaysia (UTM)

Gold nano-particles are the most capable competitors for nano-photolysis since they are strong absorbers, photostable, nontoxic, easily conjugated to antibodies and have flexible optical properties. High intensity femto-second laser pulse matter interaction has let slipped a new host of phenomena with remarkable potential applications especially in nano-photolysis. This article explores the laser-induced explosion of gold nano-particles in selective nano-photolysis of cancer tumor. A simulation study has been carried out to probe the conduct of nano-bullets on the basis of Coulomb explosion principle. The approach described here has some potential for determining the optimal temporal and spatial confinement of laser parameters with the use of spherical nano-particles in therapeutics of cancer modalities especially in breast cancer.

(Received January 9, 2012 accepted January, 29, 2012)

*Keywords:* Nano-photolysis; Short pulse laser; Nano-bullets; Cancer;

## 1. Introduction

Among other inorganic NP-systems, gold nanostructures play a vital role in cancer therapeutics because they can enhance the damage induced by radiation and anticancer drugs and can produce heat on exposure to laser. Hence provide the possibility of destruction of cancer cells through thermal ablation [1, 2]. Hence, gold nanostructures are being used as a therapeutic agent in radiation therapy, chemotherapy, photothermal therapy, and photodynamic therapy. These new opportunities allow innovations leading to effective therapy in the fight against cancer [3].

Interactions between intense ultra short high laser fields and clusters have received a great attention over the last few years [4-7]. Nano-photolysis with short pulse laser and nano-particles has recently demonstrated a great potential for selective killing of cancer tumor with slightest risk. [8]. Coulomb explosion (CE) is a mechanism of particular importance for many applications of laser-matter interaction, from laser ablation and micromachining to particle acceleration. CE is a dominant process of ion acceleration from a cluster irradiated by an intense laser pulse in the regime of cluster ionization [9–12]. In this regime, the laser pulse is intense enough to remove all electrons from the cluster before ions motion sets in. Ions acceleration then results from direct Coulomb repulsion between the cluster ions. Researchers have used laser-induced explosion of absorbing nano-particles in selective nanophotothermolysis of cancer. This is realized through fast overheating of a strongly absorbing target during a short laser pulse [13]. The resulting explosion of nano-particles may be accompanied by optical plasma and shock waves with supersonic expansion and particle fragmentation with fragments of high kinetic energy. These nanobullets can contribute to the killing of cancer

cells without damage the healthy tissues. During the irradiations some effects have been taken in [14-18],

- I. Decrease of gold nanoparticles and fragmentation.
- II. Appearance of yellow color around the tumor.
- III. Bubble formation
- IV. Bubble disappearance

On the basis of these findings the concept of nanobullets has been recently introduced. These nanobullets move from explosion zone with high kinetic energy, strike the tumor and damage it.

In present research, a simulation study has been carried out to probe the conduct of nano-bullets on the basis of coulomb explosion scenario. Different parameters such as nano-bullets energy, the energy distribution function and the laser parameters have been determined in therapeutics of cancer modalities.

## 2. Material and method

Consider a laser pulse of energy  $E$  smacks the gold nano-target of size  $r$  where

$$E = A e^{-i(\omega t - kz)} \quad (1)$$

This laser field accompanied optical plasma, shock waves with supersonic expansion and particle fragmentation due to electrostatic interaction with fragments of high kinetic energy. The nano-bullets move from explosion zone with high kinetic energy, strike the tumor and damage it, as revealed in Figure 1. The energy distribution function will be of the form

$$f = \frac{1125}{64 n_0 \pi^2 r^2 E^2 e^2 Z^2} \quad (2)$$

Where  $n_o$  is the particle density in side cluster,  $r$  is the cluster size,  $e$  is electrostatic charge,  $E$  is electrostatic field intensity and  $Z$  is atomic number of the target.

The absorption depth of target is

$$d = 1/\alpha \ln(F/F_t) \quad (3)$$

Where  $\alpha$  is the absorption coefficient and is the threshold fluence.

If enough energy is delivered to a cluster in a sufficiently short pulse, all the electrons may be removed “to infinity” before the ions have a chance to move significantly. In this extreme case, analysis of the subsequent ion motion becomes a simple electrostatic problem. The resulting ion kinetic energy spectrum is determined by the radial distribution of the cluster ions, with a sharp cutoff at the maximum energy for ions on the cluster surface:

$$E_{max} = \frac{4r^2 e^2 q^2 n_i}{3\epsilon_0} \quad (4)$$

Consequently electrons move out of the cluster forming an electron cloud and results in an ion kinetic energy distribution which rapidly rises from zero at the low-energy side corresponding to ions near the cluster centers, which are not accelerated much.

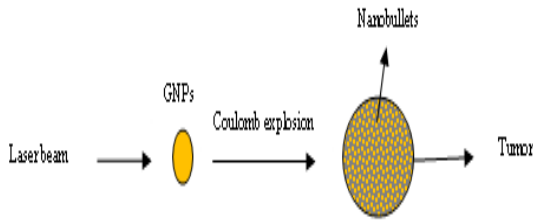


Fig. 1. A Schematic Diagram of Nanophotolysis of cancer tumor

### 3. Results

#### 3.1 Effect of laser fluence

Figure 2 shows the effect of laser fluence on the gold nanostructure. Results show that for small values of laser fluence, absorption depth was high, after that the effect was slightly less. Initially enough energy was delivered to a cluster in a sufficiently short pulse; all the electrons may be removed to infinity. The electrostatic forces became dominant over cohesive forces of the nanoparticles. Due to these electrostatic forces, coulomb explosion took part. This grounds the accelerating ions. This indicated that cell damage increased with increased numbers of laser pulses at relatively low energy, while at higher laser energy the most significant damage occurred during initial laser pulses; the cell damage did not change significantly during further increases in the number of pulses. This finding could be explained by the fact that high laser energy during just few pulses may destroy particles and further pulses interact with few or no particles.

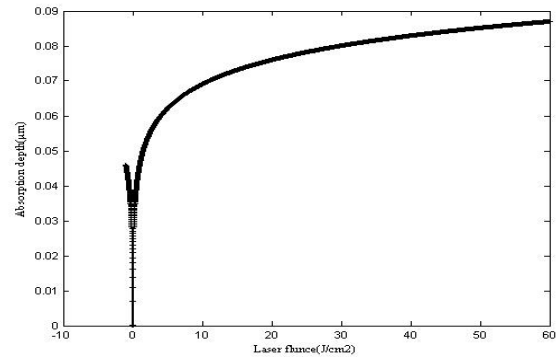


Fig. 2. A curve of laser fluence as a function of absorption depth

#### 3.2 Dynamics of nano-Bullets

Fig.3 enlightens the number of ions produced due to coulomb explosion set-up. Initially number of ions increased slowly because inter-atomic(cohesive) forces were dominant. As coulomb repulsion increased, it reduced the effect of inter-atomic forces consequently, more ions produced. The energy distribution function of these ions is shown in Figure 4. For small cluster size 1.5 nm to 3.5 nm energy distribution was maximum. For large cluster size energy decreased rapidly. The results depicted that almost no effect was found for cluster size  $r < 1.5$ -nm and a maximum effect for 1.5nm to 3.5 nm size, with reduced effects for further increases in cluster size up to 50 nm. This finding could be explained by an increased number of smaller particles and reduced distances between them, easily allowing the generation of bubbles from several closely located particles and plasma phases, negligible heat conduction, and the absence of liquid phase.

Outcomes of Figure 5 present the information about demeanor of electrons. During interaction, fraction of the kinetic energy of the incoming electrons is transferred to the tumor by scattering, excitation, and ionization or radiation loss. Maximum energy loss was found to be at 80 MeV. After that energy loss decreased exponentially with increase in energy of electrons. Because of the strong interaction with the absorber tumor, electrons experience immediate energy loss and the intensity drops rapidly. This limits the range of the electron beam in the tumor.

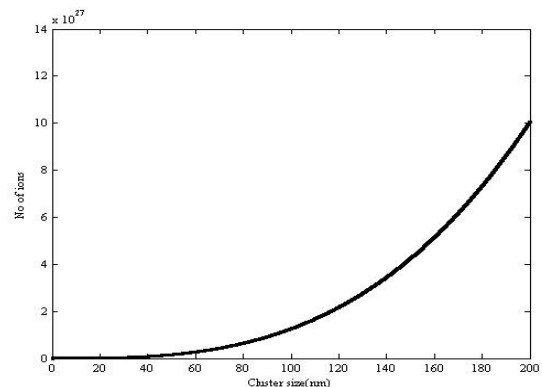


Fig. 3. A graph of number of ions Vs cluster size

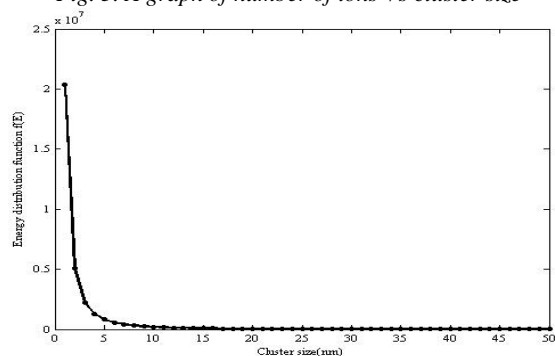


Fig. 4. A graph of energy distribution function of ions Vs cluster size

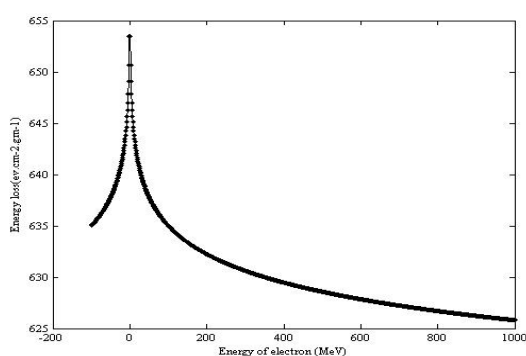


Fig. 5. Electron energy loss diagram.

#### 4. Conclusion

We have deemed over a new mechanism for selective laser killing of abnormal cells by laser Coulomb explosion of nano-particles (nano-bullets) delivered to the cells. Additionally, the effective therapeutic effect

for cancer cell killing is achieved owing to nonlinear phenomena that accompany the Coulomb explosion of the nano-particles, with generation of explosion yields with high kinetic energy. The approach described here has some potential for determining the optimal temporal and spatial confinement of laser parameters with the use of nano-particles. Investigations of laser ablation depicted that short-pulse lasers are very promising and inviting for nano-photolysis of cancer tumor.

#### Acknowledgements

The authors gratefully acknowledge the university teknologi Malaysia for their financial support through IDF.

#### References

- [1] S.D. Brown, P. Nativo, J.-A. Smith, D. Stirling, P.R. Edwards, B. Venugopal, D.J. Flint, J.A. Plumb, D. Graham, N.J. Wheate, *J. Am. Chem. Soc.* **132**, 4678 (2010).
- [2] Chithrani, B.D.; Jelveh, S.; Jalali, F.; Van Prooijen, M.; Allen, C.; Bristow, R.G.; Hill, R.P.; Jaffray, D.A. Gold nanoparticles as a radiation sensitizer in cancer therapy. *Radiat. Res.* 2010.
- [3] Muhammad Shahid, Noriah bidin, Yacoob mat daud, Gul bhar ashiq. Numerical study of laser induced ionized species in breast cancer tumor. *Journal of intense pulsed lasers and applications in advanced physics* **1**(2), 35
- [4] N. Boucerredj, Bricheni, k. Beggas, Coulomb explosion of Arn clusters irradiated by intense femtosecond laser fields. *journal of intense pulsed lasers and applications in advanced physics* **1**(4), 79 (2011).
- [5] U. Saalman, Ch. Siedschlag, J. M. Rost, *J. Phys. B, At. Mol. Opt. Phys* **39**, R39 (2006).
- [6] T. Döppner, T. Diederich, A. Przystawik, N. X. Truong, T. Fenel, J. Tiggesbäumker, K. H. Meiwes-Broer, *Phys. Chem.* **9**, 4639 (2007).
- [7] T. Raitza, H. Reinholz, G. Röpke, L. Morosov, E. Suraud, *Contrib. Plasma Phys.* **49**, (7-8), 496 (2009).
- [8] Salomeh Jelveh 1,2 and Devika B. Chithrani 2,3. Gold Nanostructures as a Platform for Combinational Therapy in Future Cancer Therapeutics. *Cancers*, **3**, 1081 (2011).
- [9] K. Nishihara, H. Amitani, M. Murakami, S. V. Bulanov, T. Zh. Esirkepov, *Nucl. Inst. Meth. and Meth.* **A 464**, 98(2001).
- [10] S. Sakabe, S. Shimizu, M. Hashida et al., *Phys. Rev. A* **69**, 23203 (2004).
- [11] I. Last and J. Jortner, *J. Chem. Phys.* **121**, 3030 (2004).
- [12] V. F. Kovalev and V. Yu. Bychenkov, *JETP* **101**, 212 (2005).
- [13] Carsten Momma, Boris N. Chichkov, Stefan Nolte, Ferdinand von Alvensleben, Andreas Tünnemann, Herbert Welling, Bernd Wellegehausen. Short-pulse laser ablation of solid targets. *Optics Communications* **129**, 134-142(1996)
- [14] Renat.R.Letfullin, Charles Joenathan, Thomas F George, Vladimir P Zharov. Laser-induced explosion of gold nanoparticles: potential role for nanophotothermolysis of cancer. *Nanomedicine* **1**(4), 473–480. (2006)
- [15] Zharov VP, Galitovsky V, Viegas M: Photothermal detection of local thermal effects during selective nanophotothermolysis. *Appl. Phys. Lett.* **83**, 4897–4899 (2003).
- [16] Brendan Francis Murphy, Dynamics of Noble Gas Cluster Expansion Driven by Intense Pulses of Extreme Ultraviolet Light. Ph.D Thesis. The University of Texas at Austin, 2009.
- [17] Zharov VP, Galitovsky V, Viegas M: Photothermal guidance of selective photothermolysis with nanoparticles. *Proc. SPIE* **5319**, 291–300 (2004).
- [18] Zharov VP, Galitovskaya EN, Jonson C, Kelly T: Synergistic enhancement of selective nanophotothermolysis with gold nanoclusters: potential for cancer therapy. *Lasers Surg. Med.* **37**, 219–226 (2005).

\*Corresponding author: bluefiber08@gmail.com