Femtosecond Laser Surface Texturing of Materials for Various Applications

Nforneh Benjamen

April 2013

Femtosecond Laser Surface Texturing of Materials for Various Applications

By

Nforneh Benjamen

A Thesis

Submitted to the African University of Science and Technology

Abuja-Nigeria

In partial fulfillment of the requirements for the

Award of Master of Science in Theoretical Physics

Supervisors: Prof. Wole Soboyejo and Dr. O. Akin-Ojo

April 2013

Femtosecond Laser Surface Texturing of Materials for Various Applications

A thesis approved by

Supervisor: ----------

Prof. Wole Soboyejo

Member----------

Dr. Omololu Akin-Ojo

Member----------

Prof. Chabi Orou

Femtosecond Laser Surface Texturing of Materials for Various Applications

Abstract

Femtosecond lasers represent an electromagnetic field with field intensities approaching and even exceeding atomic binding field. When irradiated on a target, the material responses change from linear to nonlinear within a very short time. In most situations nonlinear absorption dominates and can be used in micromachining of materials. In this work, analytical formulae are outlined relating laser and target parameters. This permits prediction of ablation conditions of materials. Ions are pulled out of a target due to charge separation caused by escaping electrons in the ablation layer which have acquired sufficient laser energy. In most cases the escaping electrons have energies equal or greater than the sum of the work function and the binding energy of the lattice. Additionally, the mechanisms of femtosecond laser melting, spallation and phase explosion of a titanium target are investigated using cascade simulations where the radiation event is modeled using molecular dynamics (MD) simulation combine with two temperature model (TTM). The model accounts for the electron heat conduction in the metal target and provide an adequate representation of the fast heating and cooling of the surface regions of the target. It uses the well-known TTM to represent heat transfer through and between electronic and atomic subsystems. The ablation yield is established for different laser fluences and the temperature evolution of the system identified. We conclude with a chapter that looks at two applications of femtosecond laser textured surfaces precisely in the photo-optics industry and in medicine.

Dedication

This work is dedicated to my father Neba Ngwa Victor Ndankwa and my mother Sirri Christina all of blessed memory. They gave me the best in life. May their souls rest in peace.

I equally dedicate this work to all the people who have supported me in one way or the other.

Table of content

List of figures

Acknowledgment

I would start by thanking God for giving me the strength to go through this work. Life is empty and meaningless without people. This work wouldn't have been possible if not for the ultimate sacrifices of some great people and African University of Science and Technology. My being alive is thanks to my parents and I would very much want to thank them for making me who I am. I would also want to thank my brother, Ngwamula'a Cletus, for his constant support and love.

The desire to work on this topic was ignited by Prof. Malik M Maaza and Prof. Wole Soboyejo to whom I owe much respect. My supervisors, Prof. Wole and Dr. Akin-Ojo have always been receptive to and supportive of my ideas, allowing me the opportunity to direct the course of my research. I would very specially want to thank sincerely Dr. Omololu Akin-Ojo for his insightful criticisms and constant support to this work and my life even when I least expected it. He was at the backbone of the simulation and equally read through my draft and made pertinent remarks.

I would also like to thanks my folks in class for the many sleepless nights we spent together trying to get things right; They and a host of others made my stay in Nigeria memorable especially Bennie Cornah and Padi Asare. It is impossible to list all the people who have been supportive in one way or the other as the list is endless. To crown it all, I would like to appreciate the constant support, love, and care form my friend Ngwa Pius and my sister Fube Bless (Quine).

Chapter 1

1.1 Background and Introduction

Modification of surface properties over multiple length scale plays an important role in optimizing a material's performance for a given application. A materials susceptibility to wear and surface damage can be reduced by altering its surface chemistry, morphology, and crystal structure. Also, one can consider the optical properties as well as the frictional, adhesive, and wetting forces acting at a materials interface as being strongly influenced by the size and shape of the micro and nano-scale features present.

It has been established that the interaction of laser light with a material can lead to permanent changes in the material's properties not easily achievable through other means. Laser irradiation induces changes to the local chemistry, the local crystal structure, and the local morphology, all of which affect how the material behaves in a given application.

This concept of texturing a material's surface has a wide range of applications ranging from light trapping devices[9,10] to biomedical applications such as implants[1,6,7]. However a variety of techniques have been utilized to texture a material's surface such as etching [13], lithographic techniques combined with isotropic etching [14], mechanical scribing [15] and solution based pattern deposition [16]. In contrast, laser texturing is a non-contact technique which can be utilized on materials. Laser is a monochromatic light source. One fundamental advantage of lasers as a tool for material processing is the ability to precisely control where in the material and what rate of

energy is deposited. When the material absorbs the laser energy, particles from the material surface can be removed and this is known as laser ablation.

Many people have worked on laser material interactions predicting various mechanisms responsible for the breakdown of the target. Zhigilei *et. al*, Perez *et. al*, and a host of others, [2-5], have all identified melting and resolidification as the chief cause of material breakdown when irradiated by a laser. Soboyejo *et. al*, Jianbo *et. al*, Mwenifumbo *et. al*, and Anil *et. al* [1, 6-8] have all shown that micro/nano-scale features created on material surfaces when irradiated by ultra-short laser pulses enhances cell proliferation. With all these advances, laser-material interactions still remains a complex topic as it embodies various branches of physics and is not without shortcomings as there are many challenges encountered when a laser is used to modify the morphology of a substance. Some of the shortcomings range from changes in the material's properties to the interaction time (longevity) of the laser pulse with the material.

1.2 Unresolved issues

Significant work has been done in the field of laser-material interactions, [2-5]. However, most of the work focused on explaining the basic physical principles responsible for the material breakdown associated with laser-material interactions. Moreover, the current understanding of material breakdown associated with laser-material interactions is less well understood. This will therefore be explored in the current work.

The main issue here is the ability to precisely deposit a large amount of energy into a material over a short time scale and in a spatially confined region near the surface. This

allows control of local surface properties relative to bulk and relative to other regions on the surface. However, more importantly the effect of this incident energy, the interaction time scale and other laser parameters can lead to material responses and changes that span multiple length scales. Another challenge is that when the laser pulse falls on a material, it triggers complex multiscale features and a cascade of interrelated processes. This renders the understanding of laser-material ablation complex.

The time it takes for excited electronic states to transfer their energy to phonons and thermalize depends on the specific material and specific mechanism within the material. When the laser-introduced excitation rate is low, in comparison with the thermalization rate, the details of the transient electronic states are not significant. Furthermore, one can consider the absorbed laser energy as being directly transformed into heat. Such processes are called photothermal and the material response can be treated in a purely thermal way. The resulting melting and resolidifaction processes can greatly alter the material's microstructure and properties [9-11].

When the laser introduced rate is high, in comparison with the thermalization rate, large excitations can build up at the intermediary states. Such excitation energies can be significant enough to directly break bonds. This is called photo-decomposition. It can be used for material texturing via what is often referred to as the photochemical processing of materials.

Biological implants are often used to reinforce or replace diseased or damaged tissues in human bodies. However, there is still a major challenge with these implants as their life-time is limited requiring continuous and costly retrieval and revision surgery to

reattach the implant. Recent advances in biomaterial engineering have limited the number of failures due to wear or fracture of the implant itself but loosening of the load bearing surfaces of the implants from the supporting hard tissue can still lead to malfunction. Abrasion between the loose implant and the bone surface can cause pain and further wear. Accumulation of debris particles can trigger a macrophage-induced inflammation response that can lead to bone loss (osteolysis) and further implant loosening.

Much of current implant research has focused on engineering biomaterials that allow for rapid integration with the supporting hard tissue, resist loosening, and shorten the recovery period. Biological cells and tissues mainly interact with the outermost atomic layers of an implant. Therefore, modifying only the surface morphology and chemistry is sufficient to elicit novel biological responses from existing materials. Laser processing is ideally suited for such an endeavor. The nano-scale and micro-scale surface features necessary for optimal adhesion to laser microgrooved surfaces need to be established.

Lasers provide excellent controllability, agility, and efficiency at removing small amount of metal from a substance. However, local heating during laser machining results in more subtle physical and chemical changes that may influence cell behavior. For example, contact guidance may be induced by microgrooves with spacings and depths that are comparable to the cell [7, 8, 12]. The spreading and proliferation of cells within microgrooves may also be influenced by the distribution of nano-scale features within the grooves [7, 8]. These are features that can be controlled by the use femtosecond lasers. However, there is still no fully accepted view on how femtosecond lasers influence micro-groove and nano-scale structure formation.

1.3 Objectives of this Work

This work will explore femtosecond laser-material interactions. With so many divergent views on the physics responsible for the material breakdown, the objective of this work will be to identify and provide alternative insights into the physical processes that occur during the interactions of femtosecond laser beams with materials. A physics-based model will be developed for the prediction of material removal during laser-material interactions.

In this work, an attempt will be made to prove that when femtosecond lasers are used for surface modifications, the physical and chemical properties of the material are retained. It will be shown that ionization and free electron heating completes in such a short time that the lattice temperature remains unchanged during the absorption of femtosecond pulses. Consequently, the underlying microstructure and properties of the surrounding materials should be unchanged.

References

[1]. J. Chen, S. Mwenifumbo, C. Langhammer, J.-P. McGovern, M. Li, A. Beye, W. Soboyejo, Wiley InterScience (2007).

[2]. L.V. Zhigilei, D.S. Ivanov, Appl. Surf. Sci.248, 433–439 (2005)

[3]. L.V. Zhigilei, Z. Lin, D.S. Ivanov, inProceedings of the 2006 ASME

[4]. Z. Lin, L.V. Zhigilei, Phys. Rev. B73, 184113 (2006)

[5]. L. J. Lewis, D. Perez, Applied Surface Science 255 (2009) 5101–5106(2007)

[6]. J. Chen, S. Mwenifumbo, C. Langhammer, J.-P. McGovern, M. Li, A. Beye, W. Soboyejo, Wiley InterScience (2007).

[7]. W. O. Soboyejo, B. Nemetski, S. Allameh, N. Marcantonio, C. Mercer, J. Ricci, Wiley Periodicals, Inc (2002)

[8].Anil Kurella, Narendra B. Dahotre, J Biomater Appl 2005 20: 5 DOI:10.1177/0885328205052974

[9]. A. Y. Vorobyev and Chunlei Guo, App Phy let 92, 041914(2008)

[10]. A. Y. Vorobyev, Chunlei Guo, Hindawi Publishing Corporation ,Advances in Mechanical Engineering Volume 2010, Article ID 452749(2009)

[11]. P. Campbell, J. Opt. Soc. Am. B10(12) (1993)

[12].Z. Feng ,Y. Lin, H. He & C. Hong, Chinese Science Bulletin(2009)

[13].J.H. Zhao, A.H. Wang, P. Campbell, M.A. Green, IEEE Trans. Electron Devices46(7), 1495(1999)

[14].H. Jansen, M. Deboer, R. Legtenberg, M. Elwenspoek, J. Micromech. Microeng.5(2), 115(1995)

[15].H. Nakaya, M. Nishida, Y. Takeda, S. Moriuchi, T. Tonegawa, T. Machida, T. Nunoi, Sol.Energy Mater. Sol. Cells34(1–4), 219 (1994)

[16].W. Zhou, M. Tao, L. Chen, H. Yang, J. Appl. Phys.102(10) (2007)

Chapter 2:

Laser physics

2.1 Introduction

The term “laser” is an acronym for (L)ight (A)mplification by (S)timulated (E)mission of (R)adiation. To understand the laser, one needs to understand the meaning of these terms. There exit different kinds of lasers but they all have a common feature. They all possess a material capable of amplifying radiations and this material is called the gain medium. By gain we mean the radiations acquire more energy passing through this medium. Simulated emission of radiation is the basic physical principle responsible for lasing action and was discovered by the great Einstein in 1916. A brief review of laser action is presented in this section.

A laser is an electromagnetic wave and has four key elements:

1) A medium exit, atoms or other material, which amplifies a light signal passing through it. Fig. 2.1a. This medium is known as the gain.
2) To boost up the signal even more, the amplifying material is usually enclosed by a highly reflecting cavity that will hold the amplified light. This reflecting cavity redirects the signal through the medium for repeated amplifications. Fig. 2.1b.
3) The amplifying medium amplifies the signal by converting its energy to light energy. If no provision is made to replenish the energy of the amplifier, the amplifying medium will lose its effectiveness and the light signal will not last long. An external heat source can serve as the backup for the amplifying medium. Fig. 2.1c.

4) We are interested in harnessing in the form of a beam at least part of the light stored in the cavity. To do this, an opening is created at one end of the amplifying medium. Fig. 2.1d.

Fig 2.1 summarizes the four basic elements described above and Fig. 2.2 is a schematic diagram of an operating laser embodying all the elements.

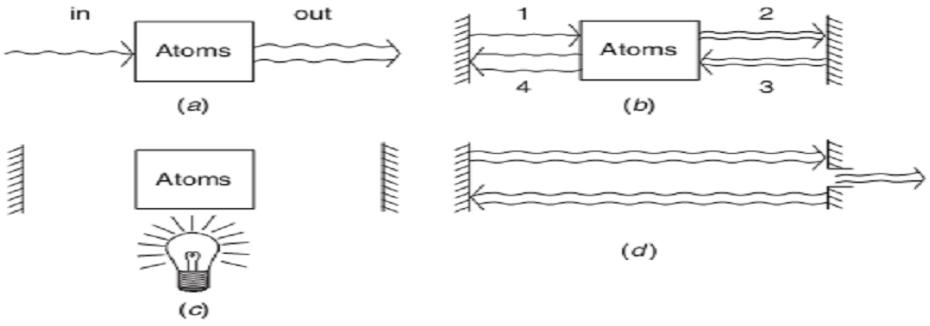


Figure 2.1 Basic elements of a laser

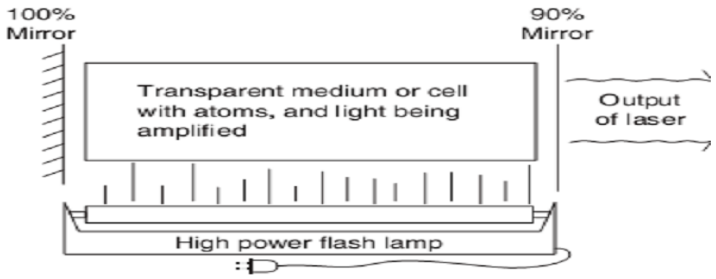


Fig 2.2 Complete laser system showing elements responsible for energy input, amplification, and output.

2.2 Fundamentals of Laser Physics

Lasers as mentioned above exhibit unique characteristics that make it ideal for so many applications most especially in the micromachining industry. It has three special properties that lead to its usefulness in many applications: coherence, monochromaticity, and collimation (directionality) as shown in Figure 2.3.

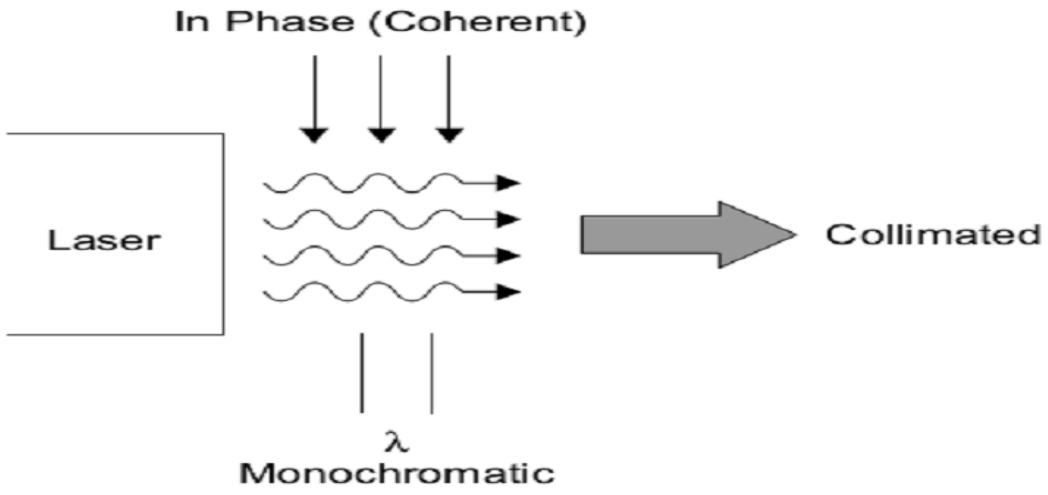


Figure 2.3 Properties of laser light.

Coherence is the most interesting property of laser light. This property states that all photons emitted from a laser are at exactly the same phase. Coherence is brought about by the mechanism of the laser itself in which photons are essentially copied. To stay in phase it is required that all emitted photons are at exactly the same wavelength (or very, very close). If some photons are at a different wavelength, the phase of those photons relative to others will be different and the light will not be coherent. They must also be highly directional, all moving in the same direction. The property of coherence, then, gives rise to the other two properties of laser light. In a laser beam, all photons

travel in lockstep with each other, cresting at the same time. The photons complement each other, rendering it high amplitude.

Monochromaticity is the ability of the laser to produce light that is at one well-defined wavelength. It is a requirement for coherence since photons of varying wavelengths cannot be coherent.

Collimation is the property of laser light that allows it to stay as a tight, confined beam for large distances. It can be thought of as the spread in a beam of light (called divergence). The simplest explanation for the highly directional output of the laser is in the mechanism of the laser itself.

Certain things need to be put in place for laser action to take place. Consider a situation where energy is injected into a system at thermal equilibrium to cause the population of atoms at the higher energy level to be greater than that of the lower level. Such a nonequilibrium condition is required for lasing action in almost all lasers. This phenomenon is known as population inversion and it is achieved through pumping.

Pumping can be accomplished by any number of means including electrical, thermal, optical, nuclear, or chemical. For laser action to take place, the excited atoms in the highly populated state undergo a transition, stimulated or spontaneous, to the lower energy states liberating energy equivalent to the energy difference between the states. Various terms are used to characterize the laser [1,2].

2.3 Modeling of laser-material interactions

In a drive to elucidate the complex mechanisms responsible for material breakdown when irradiated by a laser pulse, molecular and atomic level computer modeling has emerged as the most promising approach in the investigation of the complex and highly nonequilibrium processes involved. So many computational methods for simulation of laser interactions have been developed. When the laser pulse falls on a material, it triggers complex multi-scale features and a cascade of interrelated processes which makes computational description of short-pulse laser interactions difficult. Computer modeling of this diverse range of processes is challenging and requires a combination of different models and techniques. The size of the systems used in electronic structure calculations, however, is typically limited to several hundreds of atoms and does not allow for a realistic representation of the transition from the electronic excitation to the collective atomic dynamics responsible for the structural transformations in the irradiated material.

A good number of approaches, Continuum-level simulations, Direct Simulation Monte Carlo (DSMC) techniques, Hydrodynamic computational model, have been used so far to study laser ablation of materials. In a situation where the continuum modeling of laser materials interactions is hindered by the complexity and the highly nonequilibrium nature of the phenomenon, the classical molecular dynamics (MD) computer simulation technique has emerged as a promising alternative approach. MD simulation is capable of providing atomic level insights into the laser induced processes. This work uses an MD approach to model femtosecond laser-material interactions. It is therefore logical to have an overview of what it entails.

MD

Molecular dynamics is a computer simulation technique that allows one to predict the time evolution of a system of interacting particles. A detailed discussion of this method and the areas of its applicability can be found in several books devoted to atomistic simulation techniques, e.g., [7,8]. Briefly, MD allows one to follow the evolution of a system of N particles in time by solving a set of classical equations of motion for all particles in the system,

$$\frac{m_i\, d^2 r_i}{dt^2} = F_i, i = 1, 2, \ldots, N \qquad 2.1$$

Where m_i and r_i are the mass and position of particle *i* and F_i is the force acting on this particle due to the interaction with other particles in the system. The force acting on the *i*th particle at a given time can be obtained from the interparticle interaction potential $U(r_1,r_2,r_3,...,r_N)$ that, in general, is a function of the positions of all the particles.

$$F_i = -\nabla_i U\,(r_1, r_2, \ldots, r_N) \qquad 2.2$$

Once the initial conditions (initial positions and velocities of all particles in the system) and the interaction potential are defined, the equations of motion, (2.1), can be solved numerically. The result of the solution is the trajectories (positions and velocities) of all the particles as a function of time, $r_i(t),v_i(t)$, which is the only direct output of an MD simulation. From the trajectories of all particles in the system, one can easily calculate the spatial and time evolution of structural and thermodynamic parameters of the system. The main strength of the MD method is that the only input in the model is the function describing the interparticle interaction, $U(r_1,r_2,r_3,...,r_N)$, and no assumptions are

made about the character of the processes under study. This is an important advantage that makes the MD method to be capable of discovering new physical phenomena or processes in the course of a “computer experiment.” Moreover, unlike real experiments, the analysis of fast nonequilibrium processes in MD simulations can be performed with unlimited atomic level resolution, providing complete information on the phenomena of interest. The predictive power of the MD method, however, comes at a price of a high computational cost, which imposes severe limitations on the time and length scales accessible for the simulation. The record length-scale MD simulations of systems containing more than 10^{11} atoms have been performed with the use of thousands of processors on one of the world’s largest supercomputers [9], whereas long time-scale simulations of protein folding have been performed through distributed computing [10].

The limitations on the time and length scales that are accessible for MD simulations present a serious challenge for the modeling of laser induced processes that typically involve a collective motion of a large number of atoms or molecules in the surface region of the irradiated target. Moreover, since the electrons and quantum effects are not explicitly included in the classical MD, the optical properties of the irradiated material cannot be obtained in the course of the simulation, but have to be assumed in advance and provided as input to the model. Thus, the design of novel approaches aimed at extending the time and/or length scales of MD simulations and incorporating a description of the laser excitation into the MD model is required for an adequate modeling of laser materials interactions.

References

[1]. Csele .M , fundamentals of light sources and lasers, John Wiley & Sons, Inc., Hoboken, New Jersey, 2004

[2].P. W. Milonni, J. H. Eberly, Laser physics, John Wiley & Sons, Inc., Hoboken, New Jersey, 2010

[3]. Series in Plasma Physics, Applications of Laser–Plasma Interactions, CRC Press

[4]. N. B. Dahotre, S. P. Harimkar, Laser Fabrication and Machining of Materials, 2008 Springer Science + Business Media, LLC

[5]. William s. c. Chang, Principles of lasers and optics, Cambridge university press 2005

[6] optical society of America, Hand book of optics volume I, McGRAW-HILL , INC .1995

[7].M.P. Allen, D.J. Tildesley,Computer Simulation of Liquids (Clarendon,Oxford, 1990, 1987)

[8]. D. Frenkel, B. Smit,Understanding Molecular Simulation: From Algorithms to Applications(Academic, San Diego, 1996)

[9].K. Kadau, T.C. Germann, P.S. Lomdahl, Int. J. Mod. Phys. C17,(2006)

[10].http://folding.stanford.edu/

Chapter 3

3.1 Laser-material interactions

3.1.1 Introduction

As pointed out in chapter 1, many people have worked on laser-material interactions predicting various mechanisms responsible for the breakdown of the material. Zhigilei *et. al*, Perez *et. al*, and a host of others have all identified melting and resolidification as the chief cause of material breakdown when irradiated by laser energy. Soboyejo *et. al*, Jianbo *et. al*, and Mwenifumbo *et. al* all pointed out that micro/nano-scale features are created on material surfaces when irradiated by ultra-short laser pulses and these features enhances cell proliferation. With all these advances, laser-material interactions still remains a complex topic as it embodies various branches of physics. To be able to understand the processes which take place when laser energy falls on a material, we will need to identify what transpires within the material when the electromagnetic (laser) radiation falls on it. When light falls on a material, it may undergo reflection, absorption, refraction, scattering, and transmission. Understanding each of these phenomena goes a long way in identifying the cause of laser ablation. It is but logical to conclude that the most desirable feature in the laser processing industry is the absorption of the laser light by the material. Fig 3.1 depicts the various effects of laser material interaction.

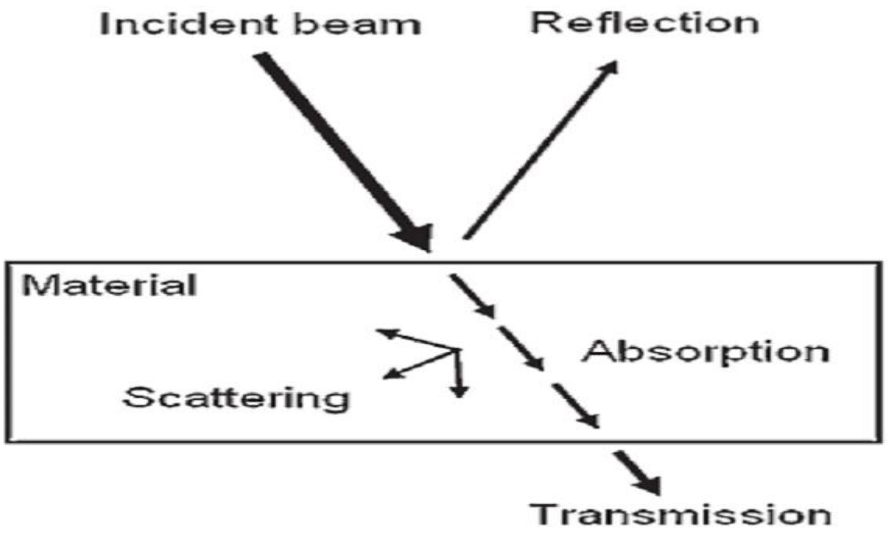


Fig 3.1. effects of laser interaction with a material

When the radiation is absorbed by the material, it can result to various effects including heating, melting, and vaporization depending on the laser parameters: intensity, wavelength, angle of incidence, pulse on time, etc, and the properties of the material such as its absorptivity and thermal conductivity. The basic understanding of the respond of a material when irradiated by the laser forms the basis for laser ablation of materials.

Laser radiation is an electromagnetic wave and thus carries an electric and a magnetic component. When the laser radiation falls on a material, its electric and magnetic component interacts with the electrons found in the material and thus transferring some of their energy to them. The increased energy of the electrons due to the absorbed radiations sets them into motion and according to the Lorentz force $\boldsymbol{F}$ law, the electromagnetic radiation exerts a force on the electrons given by:

$$\boldsymbol{F = eE + e\left(\frac{v}{c}\, X\, B\right)} \qquad \mathbf{3.1}$$

Where $\boldsymbol{E}$ is the electric field, $\boldsymbol{B}$ is the magnetic field, v is the velocity of electron and c is the speed of light. We can conclude that the electric field component of eqn. 3.1 is far greater than the magnetic component if we assume that they both carry the same amount of energy which is often the case in laser ablation of materials. With the increased energy of the system due to the absorption of the radiation, the free electrons witness an increase in their kinetic energy as well as the excitation energy of the bound electrons. The increased motion/vibrations results in the generation of heat. With continuous illumination of the target, particle might eventually be removed from the target.

When laser radiation is incident on a material, the intensity of the laser radiation gets attenuated inside the material following and exponential decay law generally expressed in terms of the Beer-Lambert law:

$$\boldsymbol{I(z) = I_o e^{-\mu z}} \qquad \mathbf{3.2}$$

I_0 is the incident intensity, $I(z)$ is the intensity at depth z, and μ is the absorption coefficient of the material. Significant reduction in strength of the laser radiation within the material occurs when the length of penetration, l, equals the reciprocal of the absorption coefficient of the material. This is given as:

$$\boldsymbol{l = \frac{1}{\mu}} \qquad \mathbf{3.3}$$

Eqn. 3.3 clearly shows that one can determine beforehand the maximum length within the material where appreciable lose in the laser intensity will occur.

As mentioned in the previous section, the most desirable feature in laser machining of materials is the absorptivity of the material for laser radiation. One can therefore say that the more the absorptivity of a material for laser light, the more easily damaged that material can be when irradiated by laser energy. By absorptivity (A) of a material we mean that fraction of the incident radiation that is absorbed at normal incidence and it is generally expressed, for opaque materials, as:

$$\boldsymbol{A = 1 - R} \qquad \boldsymbol{3.4}$$

R is the reflectivity of the material. As one would expect, the reflectivity of a material generally increases with increasing wavelength. Thus, materials are strong absorbers at shorter wavelengths. In any case, wavelength is not the only factor that determines the absorptivity of a material. A clear example to this effect is that of temperature as depicted in fig 3.2. As can be seen from the figure, the reflectivity of a material generally decreases with increasing temperature. This is to say materials are strongly reflective at low temperatures as oppose to the intuition idea that the reverse might be true. The idea of temperature to explain absorptivity of a material is of paramount importance in the laser processing of materials because laser-material interactions results in significant increase in the surface temperatures.

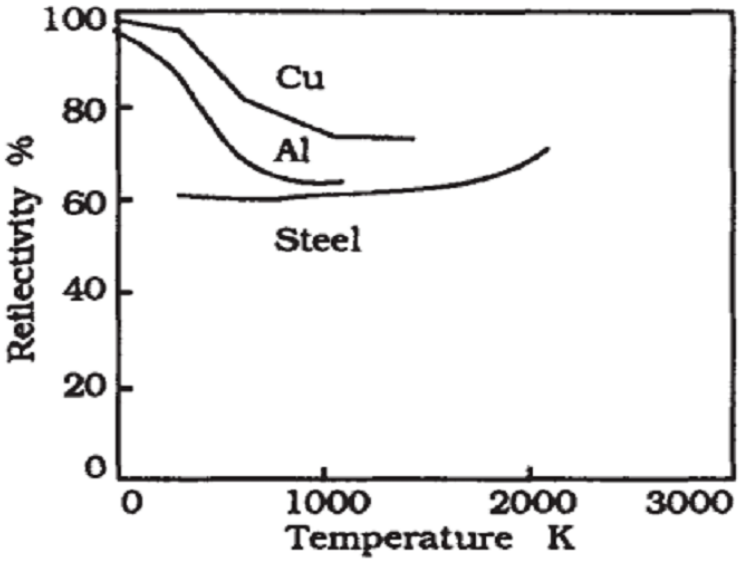


Fig3.2. Variation of reflectivity with temperature for 1.06 mm radiation (Steen 1991)

The absorbed laser energy by the material results in the generation of heat which is subsequent conducted into the material establishing as temperature distributions in the material. Various Physical effects such as heating, melting, vaporization, and plasma generation can take place in the material depending on the magnitude of the temperature rise which depend on the laser and material parameters respectively. All of these effects play important role during laser-material processing. Fig 3.3 summarizes these effects. Since heating, melting, and evaporation of materials are prime to laser ablation of materials, the next section, focuses on simplified analysis of laser heating, melting, and evaporation of materials

.

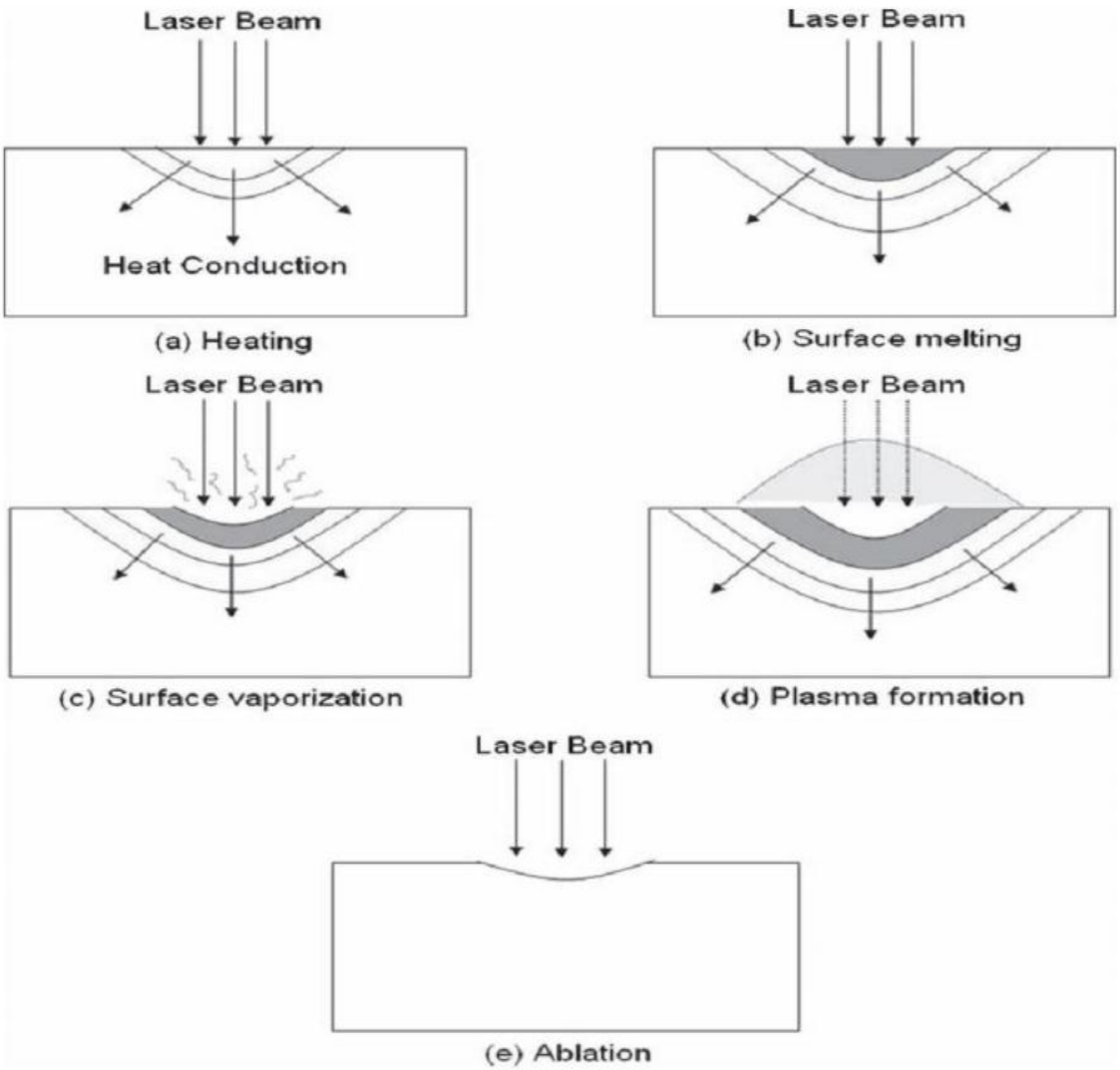


Fig 3.3. Various effects of laser material interaction: (a)heating, (b)surface melting, (c)surface vaporization, (d)plasma formation, and (e)ablation

3.1.2 Heating

Understanding the effects of laser irradiation on a material requires knowledge of the temporal and spatial variation of the temperature distribution within the material. In most

cases, the one dimensional heat equation is often used. When the one dimensional heat equation is used, the following assumptions are always made:

- Material is homogeneous
- The initial temperature of the material is constant.
- Heat input is uniform during the irradiation time.
- The convection and radiation losses from the surface are negligible.

The governing equation for the one dimensional heat transfer can be written as:

$$\frac{\partial T(z,t)}{\partial t} = \alpha \frac{\partial^2 T(z,t)}{\partial z^2} \qquad 3.5$$

T is the temperature at location z after time t and α is the thermal diffusivity of the material. Given appropriate initial conditions, this equation can be solved for analysis of the temperature evolution of the target.

As one would normally expect, the temperature of the material changes during irradiation with the laser. As depicted in fig 3.4, the temperature of the material increases with increasing irradiation time, reaches maximum temperature (Tmax) corresponding to pulse time (tp), and then decreases as the material solidifies.

3.1.3 Melting

As the laser power density increases or the pulse time, the temperature of the material increases as well and depending on the melting point of the material, it may be enough

to melt it. At this point, the temperature evolution of the material can be obtained using Fig. 3.4 below.

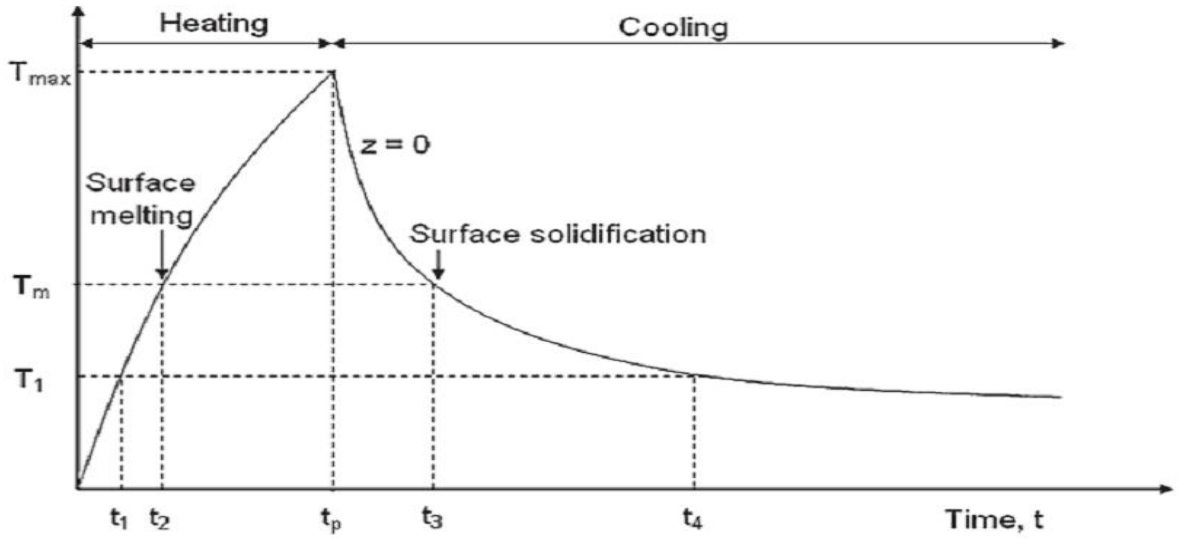


Fig. 3.4. temperature vs time

Figure 3.4 is a clear proof that the temperature evolution of the material is a function of the pulse duration and attains its maximum at pulse-on time tp. Beyond this time, when the laser is assumed to be turned off, the temperature of the material reduces as it undergoes resolidification up to the point t_3. Beyond t_3, the material simply cools down. The depth of melting of the material is also a function of the pulse-on time as well as the laser power density. At constant pulse time, it increases with increasing laser power density and at constant laser power density, it increases with increasing pulse time.

3.1.4 Vaporization

We have just shown in the previous section that the depth of melting is a function of the laser and surface parameters and as one would expect, it does not increase infinitely.

Each material has its melting and boiling point and once these points are reached, further addition of the laser energy serves as latent heat; a change of state occurs. When the surface temperature of the material reaches the boiling point, its depth of melting reaches a maximum value and any further increase in the laser power density or the pulse time causes the evaporative removal of material from the surface without further increase in the depth of melting. This is illustrated in Fig. 3.5 for the case of constant power.

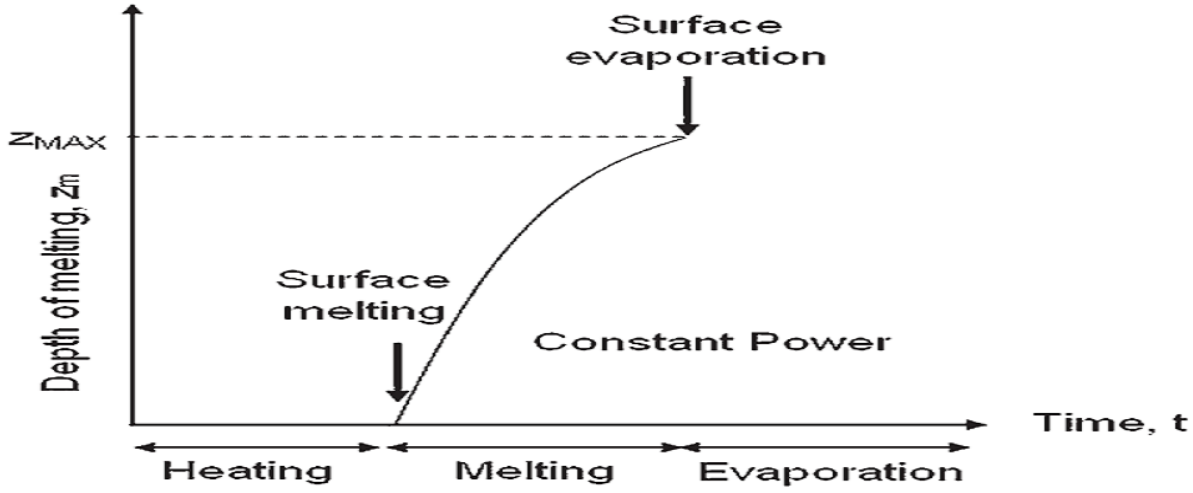


Fig3.5. Schematic of the variation of depth of melting with laser power

3.2 Theory of femtosecond Laser (Ablation) material interactions

3.2.0 Introduction:

Due to Challenges in identifying the physics principles responsible for material breakdown when irradiated by a laser pulse and the continuous divergent views as regards what transpires at each level of the material breakdown, the femtosecond laser

has emerged as the most promising tool to be used for this purpose. It provides excellent controllabilty, agility, and efficiency at removing small amount of metal from a substance. When femtosecond laser pulses are used for material modifications, the so called heat affected zone (HAZ) is minimized. This is often not the case with long laser pulses. Also with femtosecond laser pulses, one can argue that the energy transfer time from the electrons to ions by Coulomb collisions is significantly longer than the laser pulse duration as the target remains relatively cold during the pulse-on time t_p. Ionization and free electron heating completes in such a short time that the lattice temperature remains unchanged during the absorption of femtosecond pulses. Consequently, the underlying microstructure and properties of the surrounding materials is unchanged. HAZ is thus minimized.

To understand the complex mechanisms of femtosecond laser ablation of materials, it is important to develop analytical formulae which combine laser and target parameters which predict the ablation condition for an arbitrary material. An atom can only be removed from a solid using a laser pulse if and only if the laser energy is greater than the binding energy of the atoms. The initial state of the target has little or no effect on the absorbed laser energy. As mentioned in the previous sections, the laser energy is absorbed by the free electrons in the metal resulting in increased kinetic energy. When the energy absorbed by the electrons is greater than the Fermi energy, $\varepsilon_{F,}$ level of the system, charge separation occurs and the electrons can escape from the target.

The escaping electrons creates a charged imbalanced. This charge imbalance results in the creation of an electric field due to the charge separation. The electric field pulls the ions out of the target and at the same time, the force of the laser field, eqn. 3.1, in the

ablation layer pushes electrons deeper into the target. This creates a mechanism for ion acceleration into the target.

3.2.1 Penetration of laser field into a target and electron collision frequency

As mentioned in section 3.1.1, laser field is exactly an electromagnetic wave with the electric component dominating the magnetic component. The intensity of the laser radiation gets attenuated inside the material as expressed in terms of the Beer-Lambert law, eqn. 3.2,. If we assume that the intensity of an ultra-short laser pulse remain constant during it interaction with a target then the laser electric field in a similar fashion to the intensity expressed by the Beer-Lambert law decays exponentially with the depth into the target.

The electron collision frequency is very important in the study of laser ablation of materials. When the energy absorbed by the electrons is greater than the Fermi energy level, $\varepsilon_{F,}$ of the system, charge separation occurs and the electrons can escape from the target. This results in the formation of plasma in the ablation layer of the target. With continuous irradiation, the plasma disappears and a void is created as illustrated in fig 3.3. If the electron collision frequency ν_{ei} can be obtained, then electron-ion energy transfer time in the dense plasma can be approximated as

$$\boldsymbol{\tau_{ei}} \approx \frac{\boldsymbol{M}}{\boldsymbol{m_e}} \boldsymbol{v_{ei}^{-1}} \qquad \mathbf{3.6}$$

M is mass of atom and m_e is the electron mass. We can conclude from eqn. 3.6 that the electrons have no time to transfer their energy to the ions during the laser pulse as the electron-ion energy transfer time is greater than the pulse-on time. The target thus remains relatively cold during the laser pulse-on time and its density unchanged. The energy conduction time out of the target also exceeds the pulse duration. In fact, E. M. Lifshitz and L. P. Pitaevskii [3] have estimated the electron heat conduction time $\boldsymbol{t_{heat}}$ to be given by

$$\boldsymbol{t_{heat}} \approx \frac{\boldsymbol{l_s^2}}{\boldsymbol{k}}; \boldsymbol{k} = \frac{\boldsymbol{l_e v_e}}{\boldsymbol{3}} \qquad \boldsymbol{3.7}$$

Where l_{e} and v_{e} is the electron mean free path and velocity correspondingly and κ is coefficient for thermal diffusion.

The laser energy gets converted into heat as the free electrons in the target get more and more excited. This follows the energy conservation law given as:

$$\boldsymbol{c_e(T_e) n_e \frac{\partial T_e}{\partial t}} = -\frac{\boldsymbol{\partial Q}}{\boldsymbol{\partial z}} \qquad \boldsymbol{3.8}$$

$$\boldsymbol{Q = A I_0 e^{-2z/l}}$$

T_{e} is the electron energy, Q is the absorbed energy flux in the ablation layer, A is the absorption coefficient, I_0 is the incident laser intensity; n_{e} and c_{e} are the number density and the specific heat of the conductivity electrons.

For ablation to take place, the electron energy T_e must be greater or equal to the Fermi energy ε_F. With this in mind and assuming that $T_e \approx \varepsilon_F$, the time integration of eqn. 3.8 with $c_e \sim 3/2$, which is the saturation point for the electronic specific heat, yields an expression for the electron energy in the ablation layer given as:

$$\boldsymbol{T_e = \frac{4AI_0t}{3n_el}e^{-2z/l}} \qquad \mathbf{3.9}$$

3.2.2 Ablation mechanism: ions pulled out of the target by energetic electrons

As pointed out in section 3.2.0, the laser energy is absorbed by the free electrons in the metal resulting in increased kinetic energy. When the energy absorbed by the electrons is greater than the binding energy, ε_b, of ions in the lattice, charge separation occurs and the electrons can escape from the target. The escaping electrons creates a charged imbalanced. This charge imbalance results in the creation of an electric field due to the charge separation. The electric field pulls the ions out of the target and at the same time, the force of the laser field, eqn.3.1, in the ablation layer pushes electrons deeper into the target. This creates a mechanism for ion acceleration into the target. At high laser intensities, this electrostatic force is greater than the force which pushes the ions into the target. Bychenkov et al have shown that the magnitude of the electric field depends directly on the electron kinetic energy ε_e and on the gradient of the electron density n_e along the normal to the target surface.

3.2.3 Threshold of ablation for metals

We can conclude that electrons need a minimum energy in order to escape from the target. This energy must be greater or equal to the sum of the work function and the binding energy before ions can be pulled out of the target. This is to say the laser power density and the pulse-on time as pointed in section 3.1.4 play an important role in the eventual ejection of particles from the target. The sum of the work function and binding energy gives this minimum energy. With the help of the electron energy, eqn.3.9, the minimum energy is given as:

$$\boldsymbol{\varepsilon_e = \varepsilon_b + \varepsilon_{esc} = \frac{4}{3}\frac{AI_0 t_p}{ln_e}} \qquad \mathbf{3.10}$$

Where t_p is the pulse-on time and the rest of the terms are defined as in eqn. 3.9. The threshold laser fluence for ablation of metals is given as:

$$\boldsymbol{F_{th} \equiv I_0 t_p} \qquad \mathbf{3.11}$$

Where I_0 is the laser intensity. Making use of eqn. 3.10, 3.11 can be written as

$$\boldsymbol{F_{th} \equiv I_0 t_p = \frac{3}{4}\frac{(\varepsilon_b + \varepsilon_{esc}) ln_e}{A}} \qquad \mathbf{3.12}$$

Since we are considering the case of highly conductive perfect metals, their absorption coefficient A is related to the laser frequency ω, speed of light c, and the attenuation length l by

$$\boldsymbol{\frac{A}{l} \approx \frac{2\omega}{c}} \qquad \mathbf{3.13}$$

Making use of eqn. 3.13 in 3.12, an approximate formula for the ablation threshold can be obtained

$$F_{th} \equiv I_0 t_p \approx \frac{3}{8}\frac{(\varepsilon_b + \varepsilon_{esc})cn_e}{\omega} \equiv \frac{3}{8}\frac{(\varepsilon_b + \varepsilon_{esc})\lambda n_e}{2\pi} \quad 3.14$$

Eqn. 3.14 indicates a relationship between the threshold fluence and the laser wavelength. As expected, the threshold for laser fluence is directly proportional to the laser wavelength λ. Experimental work needs to be done to confirm this relation.

3.3 Molecular dynamics simulation of femtosecond laser-material interactions: (target Ti)

3.3.1 Introduction

Computer simulations have provided and are still providing important, if not essential, insights into the processes that transpire during laser ablation of materials. The physics of laser ablation has been studied in detail both experimentally and theoretically but the underlying mechanisms responsible for the eventual ejection of small amount of particles from the surface of the target when irradiated by the laser pulse still remains a puzzle. The complex nature of this problem is posed by the nature of the events that ultimately leads to ablation occurring on a wide range of length and time scales. The complex thermo-mechanical route taken by the material during ablation can be explained from computational simulation results. From Molecular Dynamics (MD) simulations performed on Titanium target, we identify in the following section various changes which take place when the target is irradiated with high laser fluences. From

the simulation results, the mechanisms of femtosecond laser melting, spallation and ablation of the target is inferred and the conditions that control the transitions between the three regimes established.

3.3.2 Computational model and simulation details:

The simulation of laser ablation of titanium (Ti) target was performed using cascade simulations, in lammps software, where the radiation event was modeled using MD simulations combined with two temperature model (TTM). The model account for the electron heat conduction in the metal target and provides an adequate representation of the fast heating and cooling of the surface regions of the target. It uses the well-known TTM to represent heat transfer through and between electronic and atomic subsystems. This model has as an added advantage the fact that it takes into consideration the effect of electron-ion interactions in the MD simulation which has always been neglected by most simulations on laser damage of materials. Electronic stopping and electron–ion interactions are included in the MD simulations by means of a friction term, with electronic stopping only applied at high velocities.

The material is modeled as a system of heavy atoms exchanging energy with a sea of light electrons, and the MD equation of motion has the form of a Langevin equation. Energy transport by the electronic subsystem in the model is described by the electronic temperature (T_e) evolution with the help of the heat diffusion equation

$$c_e \frac{\partial T_e}{\partial t} = \nabla(k_e \nabla T_e) - g_p(T_e - T_a) + g_s T'_a \qquad 3.15$$

Detail description of the various parameters in eqn. 3.15 can be found in reference [8]. C_e and K_e are the electronic specific heat and thermal conductivity respectively, g_p and g_s are coupling parameters. The second term on the right hand side represents energy exchange between the electronic and the atomic system due to the temperature difference, T_a and T_e, between them. The third term balances the energy lost by the atomic system due to electronic stopping. The simulation runs in such a way that at each timestep, energy is exchanged with the atomic system and the electronic energy is fed back into the atomic simulation via a Langevin thermostat.

The simulation cell is composed of 10 unit cells in the x and y directions, and 500 unit cells in the z direction making up approximately 200,000 atoms. In a bit to couple the MD simulation with the electronic energy and equally model the laser interaction with the target, the simulation cell is subdivided into 3 x 3 x 29 cells containing about 261 atoms each at constant temperature. These cells represent the grid for the integration of the heat diffusion equation. At each MD timestep the total energy lost by the atoms in each constant electronic temperature cell is added as a source term to the corresponding cell of the heat diffusion equation. The thermal and elastic properties of the lattice such as the lattice heat capacity, elastic moduli, coefficient of thermal expansion, melting temperature, entropy of melting and vaporization, etc., are all defined by the interatomic interaction potential, described by the embedded atom method (EAM) of Ref. [9, 10]. The particles thus interact with one another through the EAM potential. Periodic boundary conditions are used and the computational system is equilibrated to 300 K before introduction of the laser fluence. Laser energy into the target is modeled by giving the atoms at the surface of the simulation cell a high

temperature, equivalent to each laser fluence, at the start of simulation. Different laser fluences are used ranging from 100mJ/cm^2 to 500mJ/cm^2 and the ablation rate for each fluence studied. These laser fluences are sufficient and cover the range for which the target can undergo significant damaged. In the simulations, the electronic specific heat of Ti is assumed to saturate at $3K_B$ where K_B is the Boltzmann constant and the electronic thermal conductivity used is constant and is given by the room temperature value.

3.3.3 Results and Discussions

The simulation was done for laser fluences of 100mJ/cm^2, 200mJ/cm^2, 300mJ/cm^2, 400mJ/cm^2, and 500mJ/cm^2. These range of fluences used covered three different regimes of the material response to laser irradiation. At each laser fluence, a track of the ablation yield was made. A steady increase in the number of ejected particles was observed as the laser fluence and run time increases. This increase in the yield is marked by different changes in the phase of the target as explained in section 3.3.3.1. At 100mJ/cm^2, the laser energy is comparable to the melting point of target. The atoms get excited but only a few acquire sufficient energy to escape from the targets. At 500mJ/cm^2, the number of ejected particles skyrockets as the laser energy is sufficient to melt and vaporized the target within a few femtoseconds. There is no time for resolidification as experienced when nanosecond laser pulses are used. This is due to the fact that the sequence of events takes place within femtoseconds and thus the transition from melting to vaporization is almost instantaneous. Fig 3.6 show a plot of the ablation yield versus laser fluence for the first 70ps. A fraction of the number of ablated atoms from each laser fluence was also recorded and depicted in fig 3.7.

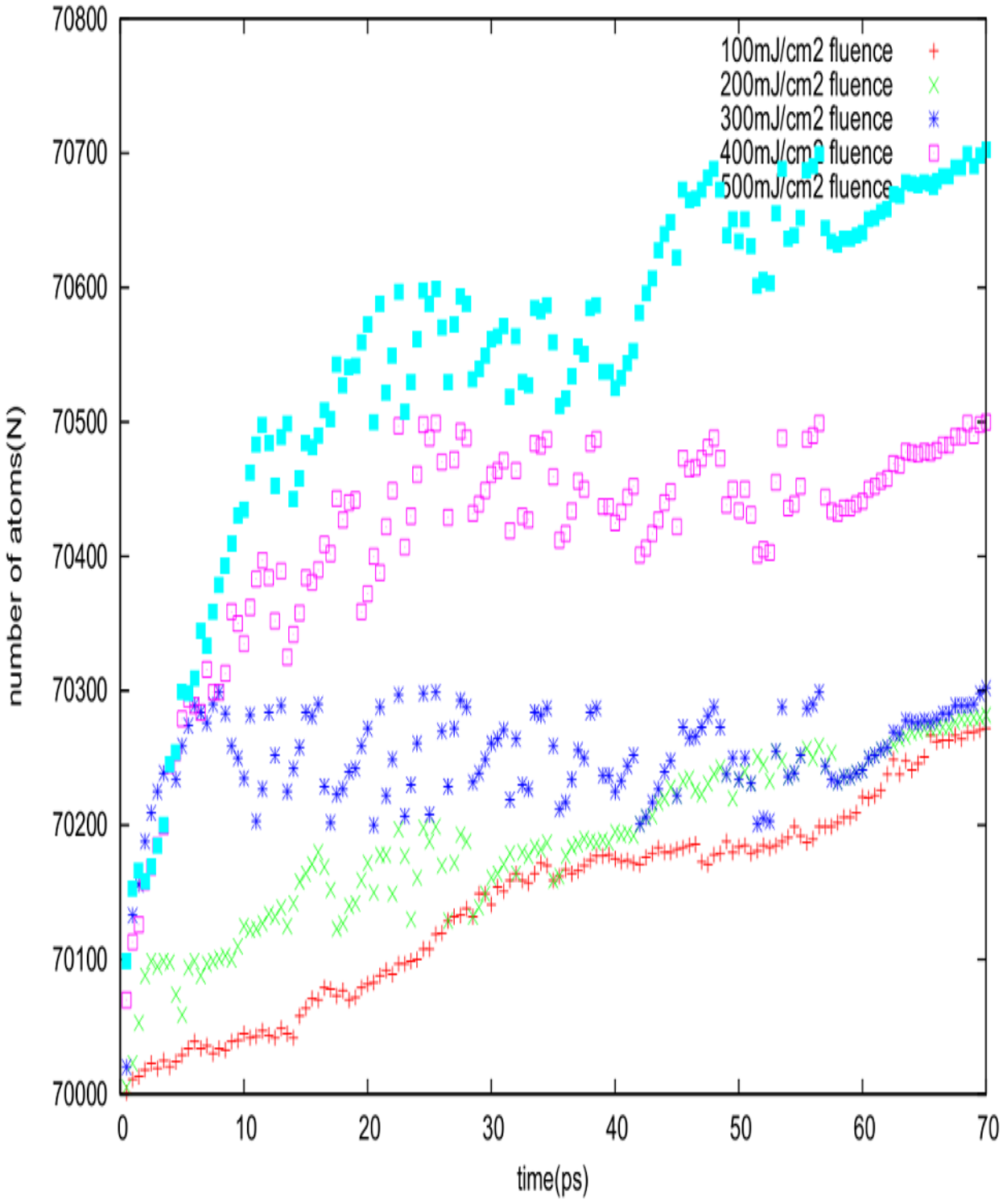


Fig 3.6. number of ejected atoms versus time.

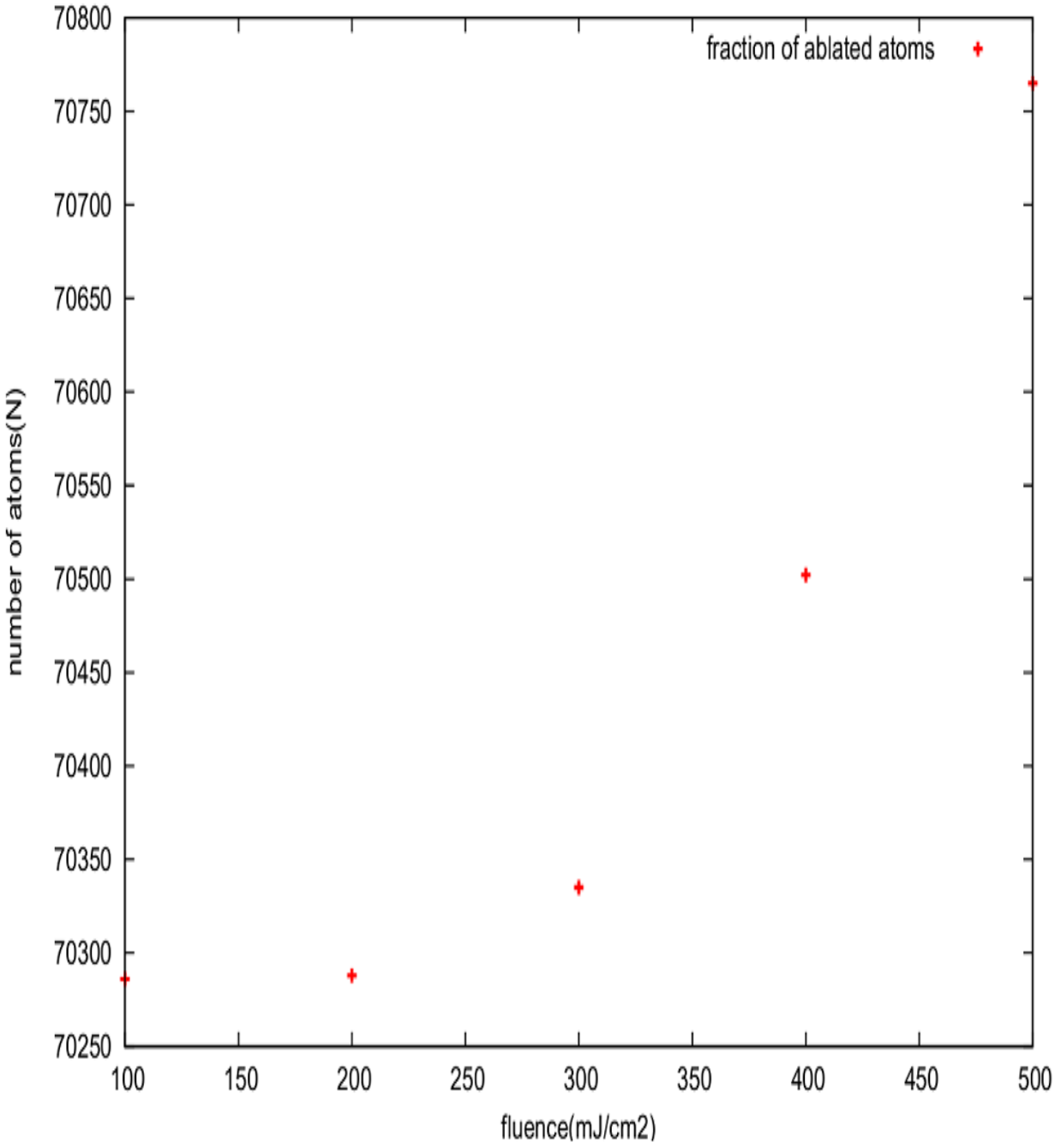


Fig 3.7 fraction of ablated atoms versus laser fluence

Knowledge of the temperature evolution of the atomic and electronic subsystem, pressure build up from the system as well as the energy evolution of the system was also obtained from the simulation results. The following analyses were made for the 100mJ/cm^2 laser fluence. A plot of the electronic temperatures for the system is presented in fig. 3.8. It is clear from the plots that the electronic temperature decays rapidly as run time increases because the electronic subsystem transfers it energy to the lattice subsystem. Fig 3.10 shows the temperature of the system with time respectively. From fig 3.10, the temperature of the system increases up to 2740k this value is greater than the melting point for Ti**.** The temperature dependence of the internal energy of the EAM Ti material is depicted in fig. 3.11. The linear relation between the temperature and the internal energy is an indication that more vibrations occur within the material as the laser energy increases. Fig 3.12a to 3.12f is a snapshot of the simulation process showing the ablation process of the target in the simulation cell after 10ps, 20ps, 30ps, 40ps, 50ps, and 60ps respectively.

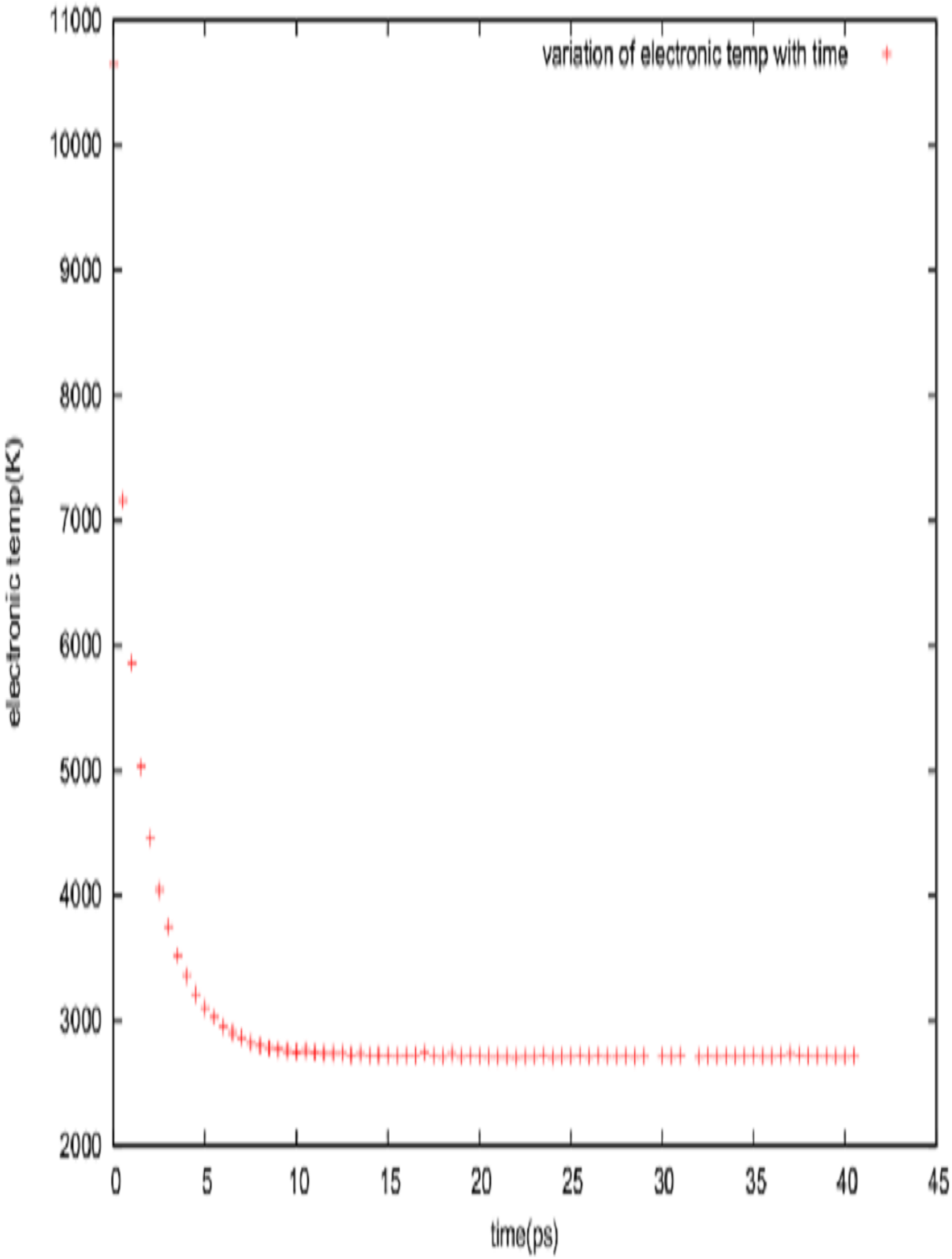


Fig 3.8 Variation of electronic temperature with time

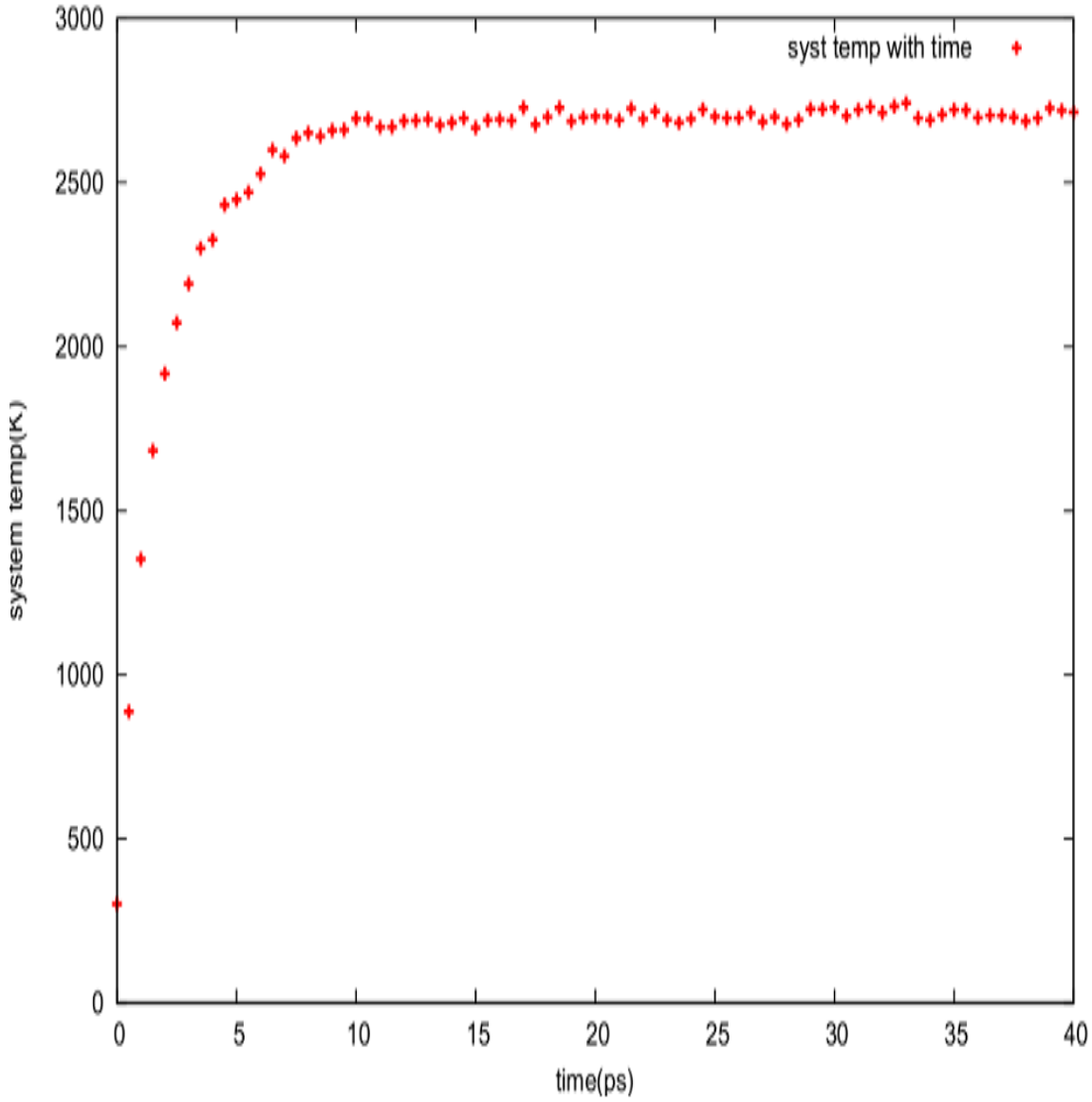


Fig3. 10. Variation of the tempereture of the system with time

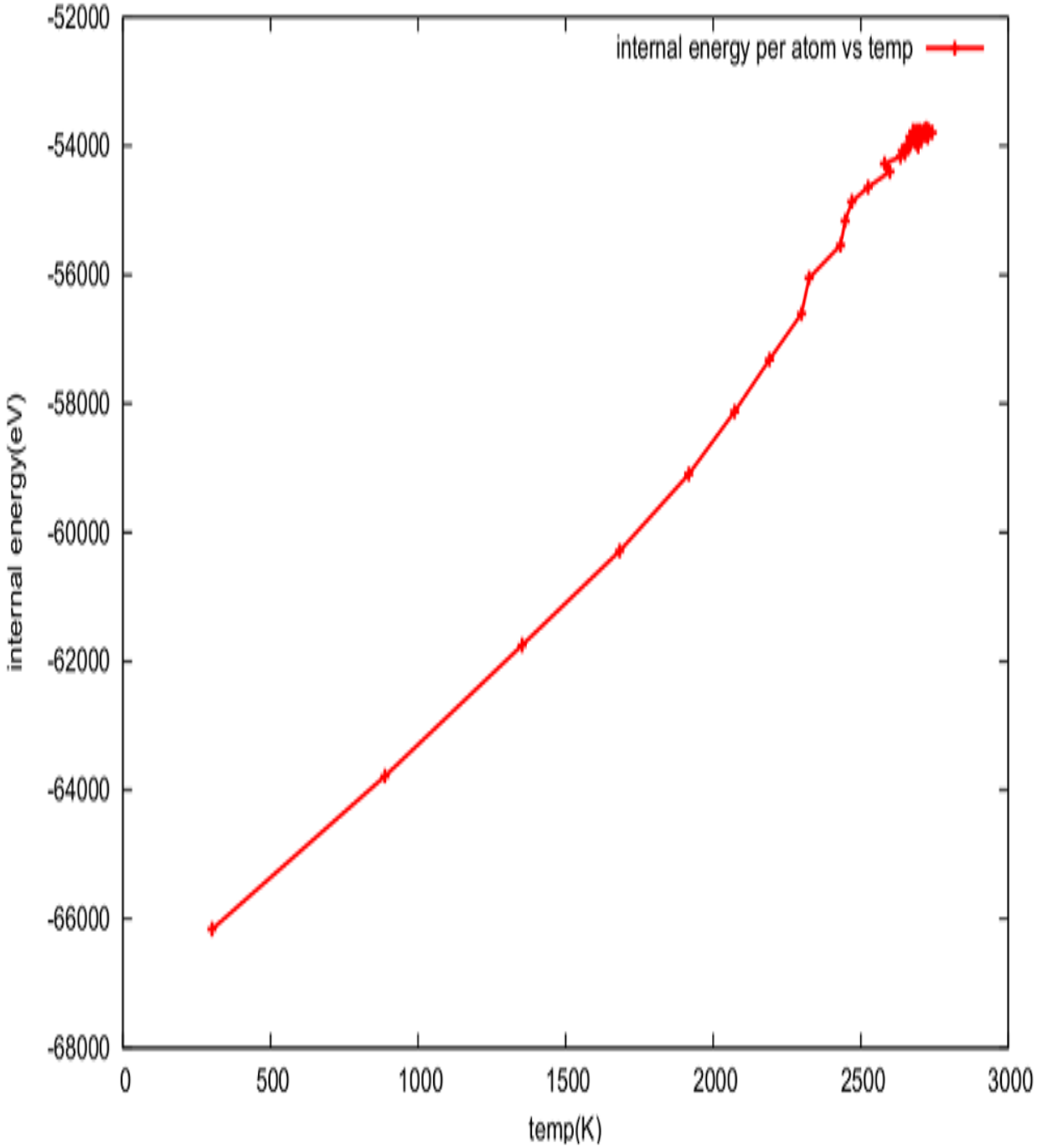
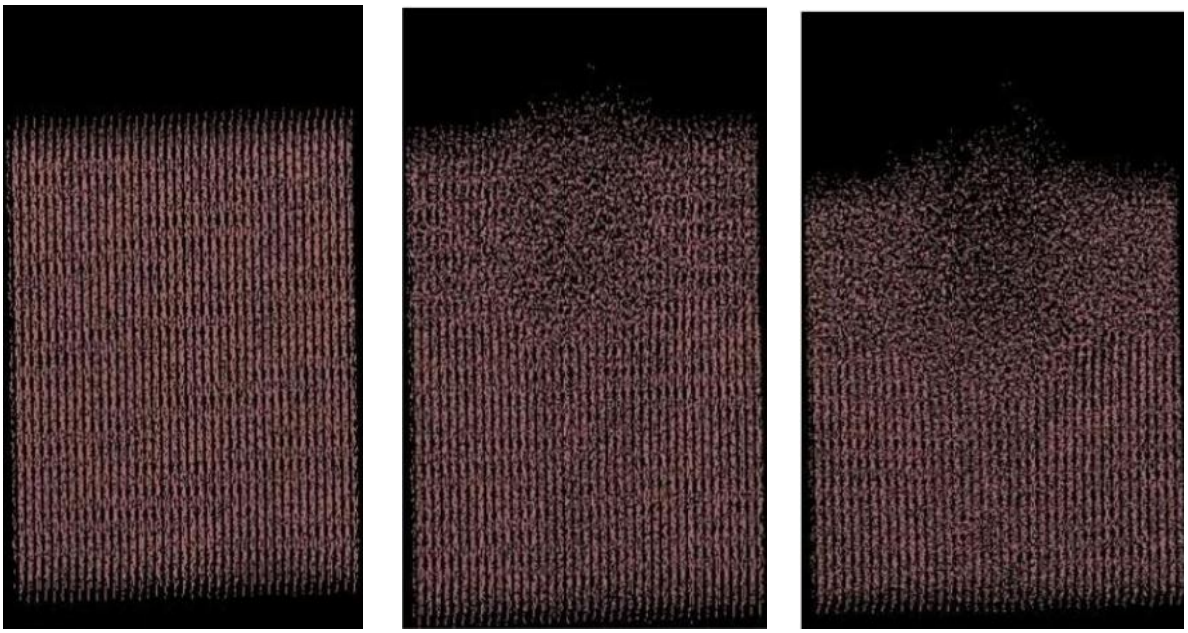
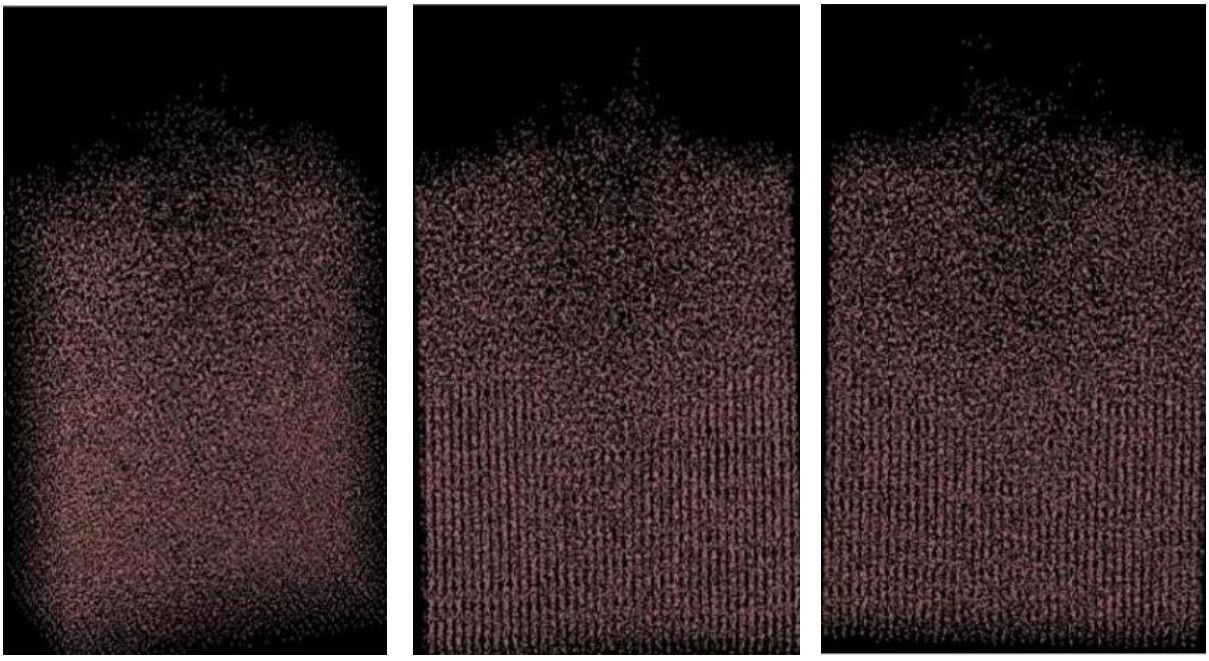


Fig 3.11. variation of the internal energy of atoms with temperature



a) 10ps b) 20ps c) 30ps



d) 40ps e) 50ps f) 60ps

fig 3.12. snapshops of simulation process

Interestingly, it can be inferred from the simulation results that different regimes of material response to laser irradiation for the given laser fluences used. These regimes are identified from the analyses of the fluence dependence of the total ablation yield. Three regimes are identified namely fast laser melting, photomechanical spallation of layers of material, and phase explosion of an overheated surface regime respectively. As pointed out in section 3.1, upon irradiation of the target by the laser, excitation of free and bound electrons occur and depending on the laser intensity and duration, different phenomena can take place in the material ranging from heating to eventual material removal from the target. In what follows, we draw conclusions from the simulations as regard the three regimes mentioned earlier.

3.3.3.1 Analysis of the three regimes: of melting, spallation, and phase explosion

Upon absorption of photons by the target, carriers are created and subsequently undergo a Drude-like dynamics, transferring their energy to the lattice in the form of phonons. The excited free and bound electrons upon absorption of the laser energy transfer their energy to the lattice due to the electron-phonon coupling. Heating of the crystal lattice takes place and the heating increases as the laser energy increases. This results in collapse of the crystal lattice in the form of melting. Resolidification of the melted material does not occur as the laser interaction time with the material is within femtoseconds. This was the case when the pulse was switched off as depicted in fig 3.4 of section 3.1.3.

Further increase in the laser fluence results in the separation of the melted material from the bulk of the target. This can be seen from the ablation yield graph plotted above when the yield smoothens. This actually follows a process as the rapid increase in the lattice temperature at initiation of the laser pulse takes place under conditions of the inertial stress confinement and results in the buildup of compressive stresses in the surface region of the irradiated target. These compressive stresses increase during the time of the lattice heating. Due to the free surface available for the target, relaxation occurs and the compressive stresses generate two fold waves; tensile and compressive waves which travel deeper into the target. As one would expect the strength of the compressive and tensile stresses increasing as the laser fluence increases and exceeds the dynamic strength of the melted material and cause separation of the melted layer from the target often called spallation.

Spallation has a threshold and once this threshold is exceeded by further increase of the laser fluence, separation and ejection of multiple layers from the target occurs. This is known as phase explosion. During phase explosion rapid decomposition of the overheated material into a mixture of vapor and liquid droplets occurs. The material gets ablated and craters are formed on its surface. Depending on the laser and material parameters, different dimensions of craters can be formed.

3.3.4 Conclusion

MD simulations combined with TTM are performed on Ti target and analyses of the ablation yield made. The evolution of the thermodynamic properties of the material are

also exploited and three ablation regimes, melting, spallation, and phase explosion identified. Form simulation results, it was found that the number of ejected particles from the target upon irradiation by the laser energy increases with increasing laser fluence. Experimental work need to be carried to confirm these results.

References

[1]. W. O. Soboyejo, B. Nemetski, S. Allameh, N. Marcantonio, C. Mercer, J. Ricci, Wiley Periodicals, Inc (2002)
[2]. W. L. Kruer, The Physics of Laser Plasma Interaction, Addison Wesley, NY, 1987.
[3]. E. M. Lifshitz and L. P. Pitaevskii, Physical Kinetics, Pergamon Press, Oxford, 1981
[4]. C. Kittel, Introduction to Solid State Physics (8^{th} edition)
[5]. W. L. Kruer, The Physics of Laser Plasma Interaction, Addison Wesley, NY, 1987
[6]. B. Luther-Davies, E. G. Gamaly, Y. Wang, A. V. Rode and V. T. Tikhonchuk, Sov. J.Quantum Electron. 22, 289 – 325 (1992)

[7].V. Yu. Bychenkov, V. T. Tikhonchuk, JETP 88, 1137 - 1142 (1999)

[8]. A.M Rutherford, D.M Duffy, J. Phys.: Condens. Matter19(2007) 496201 (9pp)

[9].The potential was taken from hcp (in C:\SIMULATION.MD\LAMMPS\Graeme\Ti)
[10]. G.J. Ackland, "Theoretical study of titanium surfaces and defects with a new many-body potential," Phil. Mag. A 66, 917-932 (1992).
[11]. C. Kittel, Introduction to Solid State Physics (8^{th} edition)
[12]. Csele .M , fundamentals of light sources and lasers, John Wiley & Sons, Inc., Hoboken, New Jersey, 2004
[13].P. W. Milonni, J. H. Eberly, Laser physics, John Wiley & Sons, Inc., Hoboken, New Jersey, 2010
[14]. E. G. Gamaly, A. V. Rode, V. T. Tikhonchuk, and B. Luther-Davies Phys. Rev. A 23 (2001)
[15]. M. D. Perry, B. C. Stuart, P. S. Banks, M. D. Feit, V. Yanovsky and A. M. Rubenchik, J. Appl. Phys. 85, 6803 - 6810 (1999).
[16]. S. Mwenifumbo, M. Li, J. Chen, A. Beye, W. Soboyejo, J Mater Sci: (2007)
[17]. J. Chen, S. Mwenifumbo, C. Langhammer, J.-P. McGovern, M. Li, A. Beye, W. Soboyejo, Wiley InterScience (2007).
[18]. L.V. Zhigilei, D.S. Ivanov, Appl. Surf. Sci.248, 433–439 (2005)
[19]. L.V. Zhigilei, Z. Lin, D.S. Ivanov, inProceedings of the 2006 ASME
[20]. Z. Lin, L.V. Zhigilei, Phys. Rev. B73, 184113 (2006)
[21] N. B. Dahotre, S. P. Harimkar, Laser Fabrication and Machining of Materials, 2008 Springer Science + Business Media, LLC
[22]. L. J. Lewis, D. Perez, Applied Surface Science 255 (2009) 5101–5106

Chapter 4

Case study

4.1 Introduction

Ultra-precision laser micromachining has excited vivid attention in various industrial fields and in medicine owing to the rapid progress in laser design capable of emitting powerful pulses with durations of less than a picosecond. The need of miniaturized structures is not only triggered by the silicon technology in microelectronics, but also by applications in telecommunication and medicine. Small lateral structural widths and high aspect ratios of cavities, grooves, etc. are required. Due to the high efficiency posed by femtosecond laser pulses for structuring of materials compared to other methods, in this chapter, we look at two applications of femtosecond laser textured surfaces. In the first case, focus is on the effect of texturing on the photo-optical properties of materials and in the second section, we look at it application in medicine with focus on enhanced biological interaction.

4.2 Surface texturing for enhanced photo-optical properties

4.2.1 Light trapping due to grooves in solar cells

With the continuous depletion of fossil fuel reserves around the world today, the biggest problem the world faces is finding a renewable energy source. Solar energy is the most abundant source of energy the earth can ever boost of but it is too expensive to harness compared to non-renewable energy sources. We know the efficiency of solar cells is relatively low. A way to increase the efficiency of solar cells will be to texture the cell

surface so that it traps light better and thus allowing more light to be absorbed and converted into electrical energy.

The backbone of PV cells is silicon and silicon is the second most abundant element on the planet. With this abundance of silicon and the availability of sun light, one would expect that solar cells should be the main source of electricity generation. This is not the case as solar cells cost too much to compete with fossil fuels and their conversion efficiency is relatively low. Mono-crystalline silicon wafer so far has the highest conversion efficiency compared to multi-crystalline silicon wafer.

One of the ways to increase the efficiency of the cell is by roughening or texturing the surface of the silicon wafer. This texturing reduces the reflection losses and improves on the light trapping capabilities of the silicon cell. This can be achieved through many means but the goal is to retain the chemical composition of the silicon cell after texturing and at the same time also reduce reflection and increase light trapping. For example, most commercial single crystalline solar cells are etched with potassium hydroxide to enhance light trapping [9], but the texture is limited to random pyramidal structures and the anisotropic etching does not apply to polycrystalline materials. Lithographic techniques combined with isotropic etching have been used to accurately define arbitrary nano-scale patterns to engineer opaque materials such as “black silicon" [10]. However, these processes would be too costly to apply to mass production [8]. Other techniques such as mechanical scribing [11] and solution based pattern deposition [7] have been investigated but may be difficult to integrate into certain manufacturing processes. In contrast, laser texturing is a non-contact technique which can be utilized on both crystalline and polycrystalline materials.

It is therefore our view that the most efficient way of doing the texturing and making sure that the chemical composition of the material is retained is through the use of lasers. An ultra-short pulse laser, femtosecond laser, is suited for this purpose as it impact time with the surface is very small, ~ fs, with adjustments made such that the penetration depth is just enough to tackle only the surface of the silicon cell. When ultra-short laser pulse is used, the so call HAZ is minimized and the properties of the material are retained. Figure 4.1 gives a general idea of how texturing would reduce the overall reflectivity of the cell. The triangles are the textured surface and they reduce the reflectivity by presenting a large fraction of inclined surfaces to the incident light. When the light strikes an inclined surface and reflects, it has a high probability to pass into the cell and be converted into electrical energy. This texturing is also used to lengthen the path that the light takes inside the cell. If the optical path is longer, the light ray has a better chance of getting absorbed in the silicon.

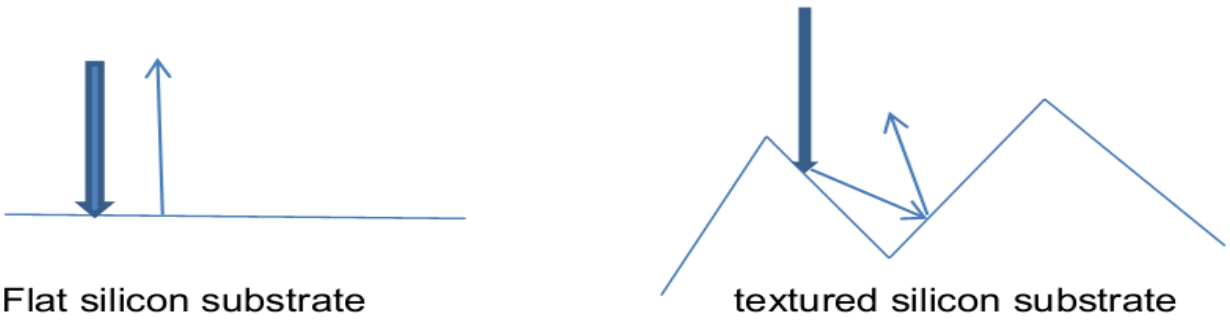


Fig 4.1. When light strikes the silicon substrate, some rays are reflected and never enter the silicon. A textured surface reducing this reflectivity by giving rays multiple opportunities to pass into the silicon

4.3 Surface texturing for enhanced biological interaction

For hard tissue replacement with metallic implants, it is necessary to have three crucial characteristics; cleanliness, stable oxide layer, and microscale morphology. When the first two conditions are satisfied, the third becomes a hard knock to crack as physical modification of the surface properties of a material requires diligent work. The purpose of this surface modification is to retain the key bulk properties of the material while modifying the surface to improve biocompatibility.

With the challenge posed by the tough nature of the materials used for bio-applications, it becomes obvious that special techniques have to be developed to modify these materials. Laser surface engineering stands out tall as the most efficient material processing method. This technique uses high power density available from focused and localized laser sources to melt, heat, or modify the material on and near surface. Femtosecond lasers promises to be the most efficient laser pulse to be used for this process as the so call HAZ is minimized and more micro/nano-scale features generated when femtosecond laser pulses are used compared to long laser pulses.

Biological cells and tissues mainly interact with the outermost atomic layers of implants. This therefore indicates that modifying only the surface morphology and chemistry is sufficient to elicit novel biological responses from existing materials. Several attempts to enhanced implant longevity have focused on the initial stages of cell adhesion and Osseo-integration (the process by which a direct structural and functional bone is formed between living bone and the surface of the artificial implant without intervening soft tissues). Initially, the surface of the newly fixed implant becomes conditioned by the

absorption of proteins which are active in cell adhesion, growth, and differentiation. Osseo-integration is then initiated by the osteoblast cells, which migrate to the conditioned implant surface and proliferate in the voids that exit between the implant and the exiting bone. The early activities of these osteoblast cells lay the groundwork for matured bone cells that will eventually be formed in that region.

It has been seen that surface texture and chemistry greatly influence the absorption of proteins and modify how the osteoblast and other cell attach and interact with the implant surface environment [3-6]. Thus optimizing these surface properties can increase the chances of successful Osseo-integration and also improve bonding of proteins and cells. Micro/nano-scale features created by ultra-short laser ablation can affect protein interactions associated with cell signaling, which regulates cell adhesion, proliferation, and differentiation. Also, these features influence the interaction of individual cell microfilaments and microtubules that form focal adhesion complexes. All this is achieved as a result of the increased surface area due to the micro/nano-scale features which provide more opportunities for focal attachment and causes cells to mechanically stretch or contract to align and organize with the features. This phenomenon is known as contact guidance. The alignment can be utilized to promote healthy regeneration of bones.

References

[1]. A. Y. Vorobyev and Chunlei Guo, App Phy let 92, 041914(2008)

[2]. A. Y. Vorobyev, Chunlei Guo, Hindawi Publishing Corporation ,Advances in Mechanical Engineering Volume 2010, Article ID 452749(2009)

[3]. S. Mwenifumbo, M. Li, J. Chen, A. Beye, W. Soboyejo, J Mater Sci: Mater Med (2007)

[4]. J. Chen, S. Mwenifumbo, C. Langhammer, J.-P. McGovern, M. Li, A. Beye, W. Soboyejo, Wiley InterScience (2007).

[5]. W. O. Soboyejo, B. Nemetski, S. Allameh, N. Marcantonio, C. Mercer, J. Ricci, Wiley Periodicals, Inc (2002)

[6].Anil Kurella, Narendra B. Dahotre, J Biomater Appl 2005 20: 5 DOI:10.1177/0885328205052974

[7].W. Zhou, M. Tao, L. Chen, H. Yang, J. Appl. Phys.102(10) (2007)

[8].S.A. Boden, D.M. Bagnall, Appl. Phys. Lett.93(13), 133108 (2008)

[9].J.H. Zhao, A.H. Wang, P. Campbell, M.A. Green, IEEE Trans. Electron Devices46(7), 1495(1999)

[10].H. Jansen, M. Deboer, R. Legtenberg, M. Elwenspoek, J. Micromech. Microeng.5(2), 115(1995)

[11].H. Nakaya, M. Nishida, Y. Takeda, S. Moriuchi, T. Tonegawa, T. Machida, T. Nunoi, Sol.Energy Mater. Sol. Cells34(1–4), 219 (1994)

Chapter 6

Summary and future work

Ultra-short laser micromachining has presented itself as a very useful tool in modifying the surface properties of materials in recent years. With its importance, so many theories have been developed all in an attempt to explain the physics responsible for the material damage. These theories are not without short comings as the ability to precisely deposit a large amount of energy into a material over a short time scale and in a spatially confined region near the surface pose a lot of challenges. When this is achieved, it allows control of local surface properties relative to bulk and relative to other regions on the surface. However, more importantly, the effect of this incident energy, the interaction time scales and other laser parameters can lead to material responses and changes that span multiple length scales. The Understanding of the capabilities and limitations of laser machining requires the knowledge of physical processes occurring during the laser beam interaction with materials. In this work, we identified the various mechanisms that are responsible for laser ablation of materials. The physics of this new regime of ablation consists in the ion acceleration in the electrostatic field created by hot electrons escaping from the target. Explicit analytical formulae for the ablation threshold, the electron temperature in the ablation layer, and the ablation rates for metals in terms of laser and target parameters are outlined. We also showed that the material evaporation rate is much higher than in the long pulse interaction regime. The ultra-short laser ablation can do a variety of fine jobs without any collateral damage to the rest of a target as oppose to long laser pulses. This is very much the case as we pointed out that HAZ was minimized when femtosecond laser pulses are used. The

theoretical background developed in this work for laser ablation allows the appropriate laser parameters to be chosen for any given material and the laser-target interaction process to be optimized.

In a bit to understand the mechanisms of femtosecond laser melting, spallation and ablation, MD simulations were performed using cascade simulations on titanium target. The model account for the electron heat conduction in the metal target and provides an adequate representation of the fast heating and cooling of the surface regions of the target. It uses the well-known two temperature model (TTM) to represent heat transfer through and between electronic and atomic subsystems. These simulations reveal that the ablation yield is directly proportional to the laser fluence. The conditions that control the transitions between the three regimes and the mechanisms of laser melting, spallation and phase explosion were identified from analyses of the ablation yield for the various laser fluences.

We then concluded with a looks at two applications of femtosecond laser textured surfaces in the photo-optics industry and in medicine. We showed that the optical properties of a material can be enhanced once its surface is textured as it increases the surface area and thus giving room for more light to be absorbed. Micro/nano-scale features on biological implant materials enhanced cell adhesion to surface and quicken recovery time and cell proliferation.

As a theoretical model, we need to carry out experiments to validate our model as well as run a check on the formulae used in this work. A lot of work still has to be done on the MD simulation of femtosecond laser ablation of Ti in order to identify the fluence

dependence with ablation depth as well as the compressive stresses which build up during the simulations. These stresses are great contributors to the eventual removal of material from the target. In line with texturing for enhanced biological interactions, experiments need to be carried out on different textured surfaces, grow cells on then and identify the micro/nano-scale features which lead to optimal adhesion and proliferation.

.

ALL GLORY TO GOD