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**ATOMISTIC STUDY OF MATERIAL DYNAMICS INDUCED BY LASER
AND ION IRRADIATION**

Year 2 from 3 years research duration

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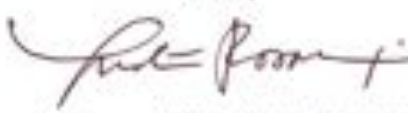
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SUMMARY

Laser assisted material processing has been used since decades ago. This method is one of the most popular techniques, and one of the promising tools to improve the technology of nano-scale device engineering. Laser ablation is a method to remove material by means of photon energy absorption. The application spreads in a very wide area in medical and engineering, such as tissue- or material-removal and material processing. However the study of the mechanism of laser-material interaction is still ongoing and the underlying theory has not completely been explored. Using the short pulse laser in femto-second pulse-width range, it is possible to probe experimentally the material responses in extremely short time duration (pico- to nano-seconds). This allows the detailed study of responses and gives one to one comparison between theoretical predictions and experiment results. However the initial processes take part at short time in tens to hundreds of femto-seconds after the laser irradiation is not completely known.

Another energy source that is also common for surface nano-machining is the ion-beam. In this case the ion is bombarding the surface, and the amount of deposited energy characterize the pattern on surface. The surface morphology is related to the type of bombarding ion, the fluence, and the geometrical configuration of ion beam, that is the angle of incidence. The potential application of ion beam for nano-lithography promising. Nowadays, the popular method is using the so-called *Focused-Ion-Beam* (FIB).

In this proposal we focus to study the processes of material at pico-second time scale using computer simulation methods and longer time scale using Smoothed-Particle-Hydrodynamics method. A so-called Two Temperature Model (TTM) has made an accurate computer simulation of the laser-material interaction possible, by coupling the electronic and lattice temperatures. The method has been used to simulate realistic material responses such as ablation mechanism, void formation and Coulomb explosion of material by high intensity laser pulses, as well as the *Swift Heavy Ion*.

The yearly plan of the proposed research is the following; In the first year we will start with theoretical study and modeling of electron dynamics. The electron will be approached from two approximations: the thermal diffusion model and the fluid flow model. In the second year, we will do the hydro-dynamics study of sputtering and pattern formation on surface. In this stage we plan to start comparing the theoretical observation with experiment data of surface nano-patterns. In the third year we will concentrate in further analysis of surface structures. In this stage we will have all the programming tools needed to simulate systems with various configurations.

Keywords: Laser Ablation, Ion Bombardment, Two-Temperature Model, Molecular-Dynamics, Smoothed Particle Hydrodynamics

1 Introduction

As electronic devices are getting smaller and smaller, the nano-fabrication technology has to be continually improved to operate in this scale with reliably high precision. In this order of size the fabrication is beyond the capability of conventional chemical etching techniques. This situation urge the exploration of new methods, among those are ion-assisted etching with *Focused Ion Beam*, femto-second laser ablation, and laser-assisted particle deposition [Gierak et al., 2001, Watt et al., 2005, Ahn et al., 2012]. However, the atomistic processes and mechanism occurs in nano-scale lithography are not completely explored. Those demanding applications trigger a more intensive study in the field of theory, computation, as well as experiment, with the expectation that more effective and economical method can be discovered.

From the theoretical point of view, the process occurs at surfaces is one of important discussions. Mechanisms at surfaces due to energy deposition by ion beam and photon (LASER) are still becoming question marks that have to be answered. Phenomenon, such as *Laser Induced Surface Structure* (LIPSS), has not been fully understood. Studies on this issue is still ongoing. Although the phenomenon is actually discovered more than a decade ago[Sipe et al., 1983, Zhakhovskii et al., 2008, Skolski et al., 2010].

With another method, ion-beam energy deposition induced also characteristic pattern on surfaces. Nevertheless, the mechanism is completely different compared with those induced by LASER. Some models have been proposed to explain the pattern formation, such as the Bradley-Harper theory [Bradley and Harper, 1988], and also a more recent *crater function* theory. These theories need to be examined in various conditions, in order to find out the limitations on different materials and different amount of energy deposition.

For a much smaller ion fluence, one finds a completely different mechanism. Here, the so called ion channeling plays role. The pattern induced by single ion has been able to visualized using recent microscopy technique, i.e. *Scanning Tunneling Microscopy*. The phenomena was discovered from both computational method and STM measurement [Redinger et al., 2010]. In this regime, it is discovered that the preexistent surface damage has important effects in ruling the damage at surface [Rosandi and Urbassek, 2006, Rosandi and Urbassek, 2007, Redinger et al., 2009].

1.1 Track Record on Ion and Laser Irradiation of Surfaces

We have already done the research in this field (ion/laser irradiation of surfaces) for many years. This is implemented in the MoU between two collaborating universities signed in 2010. We have built the theory of single ion impact at grazing incidence on metal surface corroborated with computation study and direct observation using *Scanning Tunneling Microscopy* experiment [Redinger et al., 2010]. Our work displayed in convincing manner the role of single impact of low energy ion as the initial process of surface nano-patterning. Beside metals, we also investigated the same phenomena occurred in semiconductor material[Rosandi and Urbassek, 2012]. Our theory is based on the atomistic view of the initial stage of nano-pattern formation, shown in figure 1. However, many questions still persist, one of those is the long time transient behavior of the