NUMERICAL SIMULATION OF SILICON NANOSECOND LASER ANNEALING BY COMSOL MULTIPHYSICS

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ABSTRACT
2D transient heat conduction model was created in COMSOL Multiphysics as a simulation of temperature change in material irradiated by a homogeneous KrF beam (248 nm, 27 ns) confined on the substrate (10 - 50 nm silicon surface). The aim of this work is to control the melting thickness (20-50 nm) for one laser pulse treatment, in order to recrystallized a surface layer which amorphized by ionic implantation and to reactivate the doping agents.
In this paper, the obtained results are shown and discussed in the case of bulk silicon. 'Gaussian' and 'gate' shapes are considered for the heat source time distribution. Values of thermal field in case of 'gate' shape were compared to the 'Gaussian' one. The returned result concerns mainly surface temperature versus time and laser fluence (i.e. energy density: 800-1300 mJ/cm²). Typically, over a laser fluence of 2000 mJ/cm², ablation process occurs on silicon surface.

1. INTRODUCTION

The importance of laser thermal processing (LTP) and thermal properties investigation of bulk and complex materials is still increasing.
Excimer laser crystallization is an efficient technology for obtaining high-performance poly-Si TFTs [**1**] for advanced flat panel display applications. In order to improve both the device performance and uniformity, high-quality poly-Si films with controlled grain size and location are required.

The aim of this work is to control the melting thickness (20-50 nm) by pulsed laser treatment, in order to recrystallized a surface layer which is firstly amorphized by ionic implantation, and to reactivate the doping agents of this one. For this, simulation by COMSOL Multiphysics is used to predict the melting kinetics by pulsed lasers. To accomplish this objective, several methods [**2-3**] have been developed utilizing spatially selective melting and lateral temperature modulation. A melt-mediated transformation scenario has been proposed [**4-5**] suggesting that the recrystallized Si morphology is determined by complex phase transformations. For laser energy densities (Fluences) causing partial melting, the maximum temperature [**6**] remains close to the melting point of amorphous silicon (a-Si). When complete melting occurs, substantial supercooling is observed, followed by spontaneous nucleation.

One of demo examples in COMSOL Multiphysics solves interaction of laser with Silicon sample but with considering negligible width of laser beam. In this example silicon is assumed to be semitransparent and Lambert-Beer law is used for the energy (photons) absorption in depth.

In the present paper one example of laser heating with dimensions 10x10x0.3 mm^3 is solved with affected area 2x2 mm^2 (Figure 1). The time resolution is in order of ns due to the pulse duration of the KrF laser which is closely 27 ns (FWHM) (Full Width at Half Maximum). The Numerical procedure is developed under COMSOL project and treated with 1.0 nm mesh size in the photon absorbing area (boundary 3) (Figure 2). In the *subdomain* zone the mesh size is close to 100 nm.

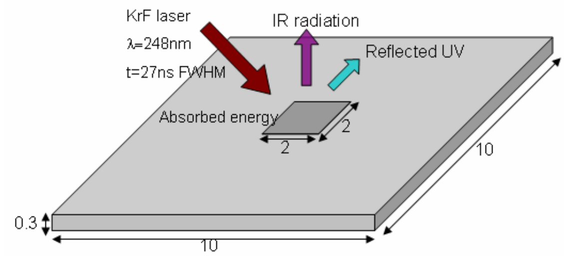


Figure 1. Schematic view of laser beam interaction with material surface (dimensions in mm)

The returned result concerns surface temperature versus time and laser fluence (energy density), and also temperature versus depth (y).

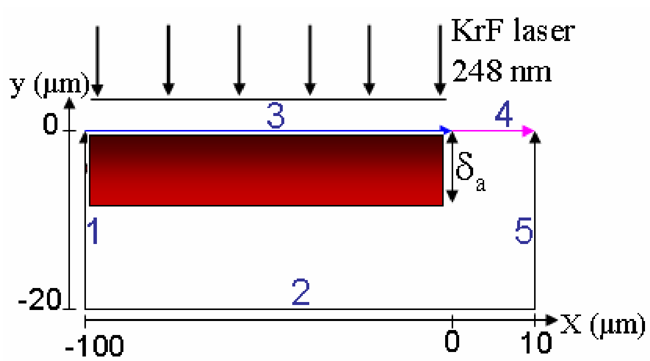


Figure 2. Sketch of selected part of bulk sample for modeling in COMSOL with numbers of boundary conditions.

2. GOVERNING EQUATIONS

The heat source is distributed in time with 'gate' and 'Gaussian' shapes (Figure 3). The returned results were almost simulated by conduction/diffusion models that are not well appropriate to the understanding of transport phenomena in the case of silicon.
Mathematical formulation of problem is described by volume equation of heat conduction

$$\rho C_p \frac{\partial T}{\partial t} - \nabla \left(k \nabla T \right) = Gt \tag{1}$$

Where ρ is material density, C_p specific heat capacity, T temperature, t time and k thermal conductivity. Gt is the heat source distribution in depth (Y) according to the Beer-lambert law (Figure 4), it's described by following equation :

$$Gt\left(y,t\right) = I\left(t\right).\left(1 - R\left(T\right)\right).\frac{e^{\frac{-y}{\delta a}}}{\delta a} \tag{2}$$

With:
$I(t)$ [W/cm²]: Time distribution of the laser beam intensity.
The sample can be simplified to 2D rectangle, x coordinate for width and y coordinate for depth (Figure 2). Only interface between heated and unheated part is solved i.e. a half of the sample is irradiated by laser and another half is not irradiated. As a source of heat it is used the energy absorbed in volume. The thermal conductivity and the heat capacity of solid and liquid silicon are respectively 148W/(m.K) and 710J/(kg.K), and 200W/(m.K) and 680J/(kg.K).
The specular reflectivity at $\lambda = 248\,nm$ and at 300 K on monocrystalline silicon is 61%. Melted silicon has the properties of a metal, i.e. high reflectivity, in general 73% [**7**]. The penetration depth δ_a under these last conditions is $\delta_a \approx 6\,nm$ [**8**], it depends on optical properties of semi-conductor (Si); refractive index n_1 and extinction coefficient n_2.

$$n = n_1 + in_2 \tag{3}$$

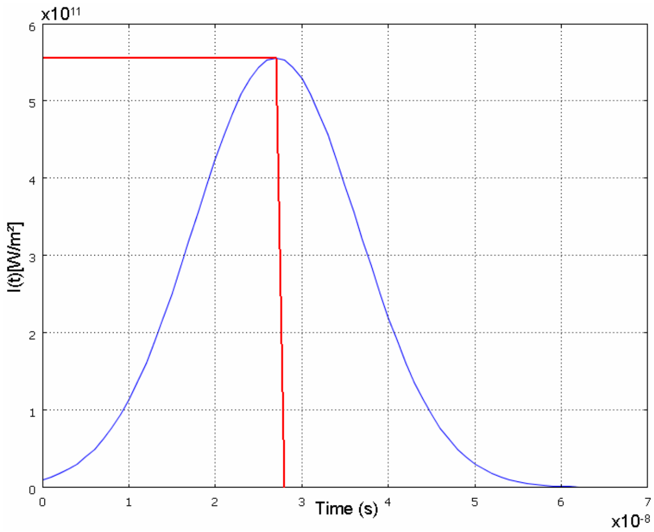


Figure 3: Time distribution of the incident heat flux density: Gate shape and Gaussian shape

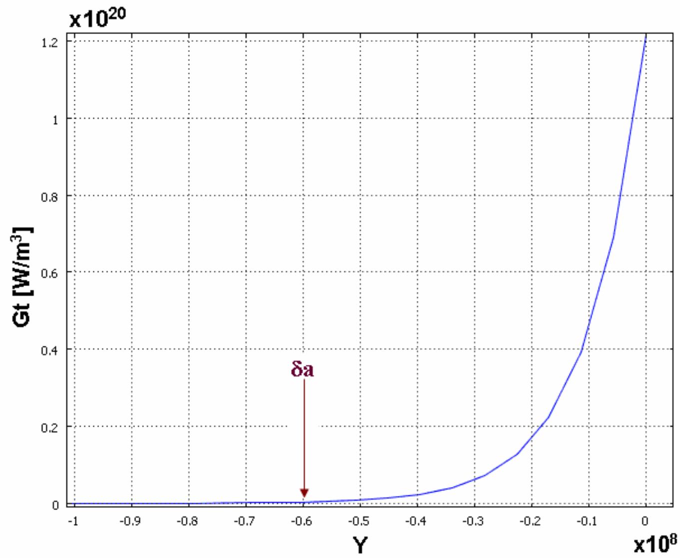


Figure 4: Heat source distribution in depth (Y): Beer-lambert law

Absorption coefficient α can be expressed by:

$$\alpha = \frac{2\omega n_2}{c} = \frac{4\pi n_2}{\lambda} = \frac{1}{\delta a} \tag{4}$$

Where ω is the circular frequency and c the speed of light. α is used in Beer-lambert law as following:

$$I(y) = I_0 . e^{-\alpha|y|} \tag{5}$$

Where $I(y)$ is the depth dependent laser intensity, I_0 is the intensity of the surface and $|y|$ is the depth as indicated in relationship (2).
Surface boundary condition for irradiated area (boundary 3 in figure 2) is described by equation (6)

$$\vec{n}.(k\nabla T) = q_0 + h(T_{\inf} - T) + \sigma.\varepsilon(T_{amb}^4 - T^4) \tag{6}$$

Where $\vec{n}$ is the normal vector, q_0 the surface heat flux, h the convective heat transfer coefficient, $T_{\inf}$ external temperature, σ Stefan-Boltzmann constant, ε emissivity and T_{amb} ambient temperature.
The unheated area (boundary 4) has a similar equation as the boundary 3 one excluding the heat source distribution term Gt. Left bottom and right side (boundaries 1, 2 and 5) are thermally insulated (adiabatic conditions), that means:

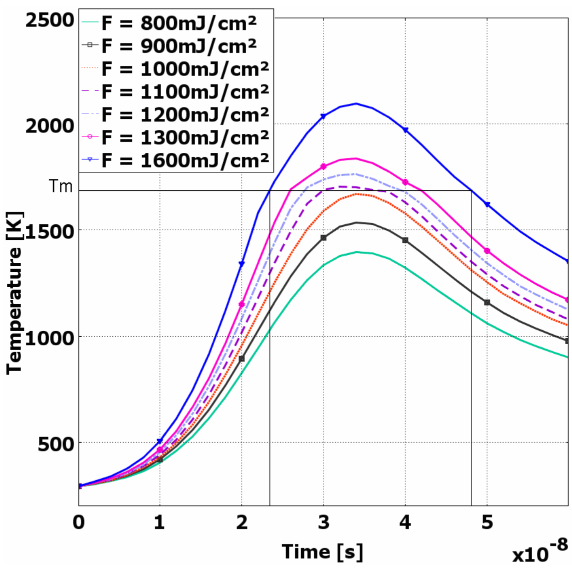
$$\vec{n}.(k\nabla T) = 0 \tag{7}$$

3. TECHNECAL COMSOL REALIZATION

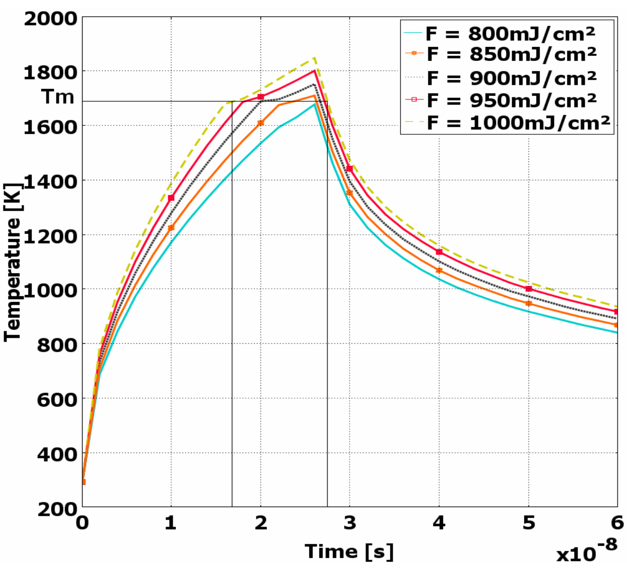
For the thermal model, *Heat transfer mode* and *Transient analysis* in *Conduction* type of heat transfer, have been chosen in order to solve the heat conduction problem. Sample geometry is made of a rectangle with dimensions in Figure 2.
In the section *global expressions* there are created variables and *constants* necessary for modeling laser pulse i.e. absorbed energy, affected area, shape of pulse (absorbed heat flux distribution in time) and material emissivity. The initial temperature of the *subdomain* is set to 293 K.
For the heat source, energy is absorbed in volume. Surface boundary condition includes thermal radiation and heat transfer to ambient room. Other boundary conditions were considered as thermal insulation (adiabatic conditions). Mesh elements in *subdomain* has maximal size of 100 nm. On the front surface (boundary 3) the finer element distribution with maximal size of 2 nm is used
In *solver parameters* time ranges from 0 to 60 ns with a step of 2 ns. For solving the default solver is used.
In *Postprocessing* mode there is selected *Cross-Section Plot parameters/Point* and inserted coordinates [-0.8e-4; 0] for surface temperature visualization.

4. SIMULATION RESULTS IN CASE OF CRYSTALLINE SILICON

The returned result concerns surface temperature versus time and laser fluence (Figure 5), temperature profile in depth (y) (Figure 6) for the gate shape and Gaussian shape time distribution.
Notice that for laser fluence lower than 1050 mJ/cm² (i.e. threshold of melting in case of gate shape), the execution time is close to few minutes. However, for higher laser fluence, when the melting process starts, the execution time increases dramatically to many hours (4 to 7 hours).



a)



b)

Figure 5. Point [-0.8e-4 ; 0] temperature versus time at different laser fluences (F). a) Gaussian shape, b) Gate shape

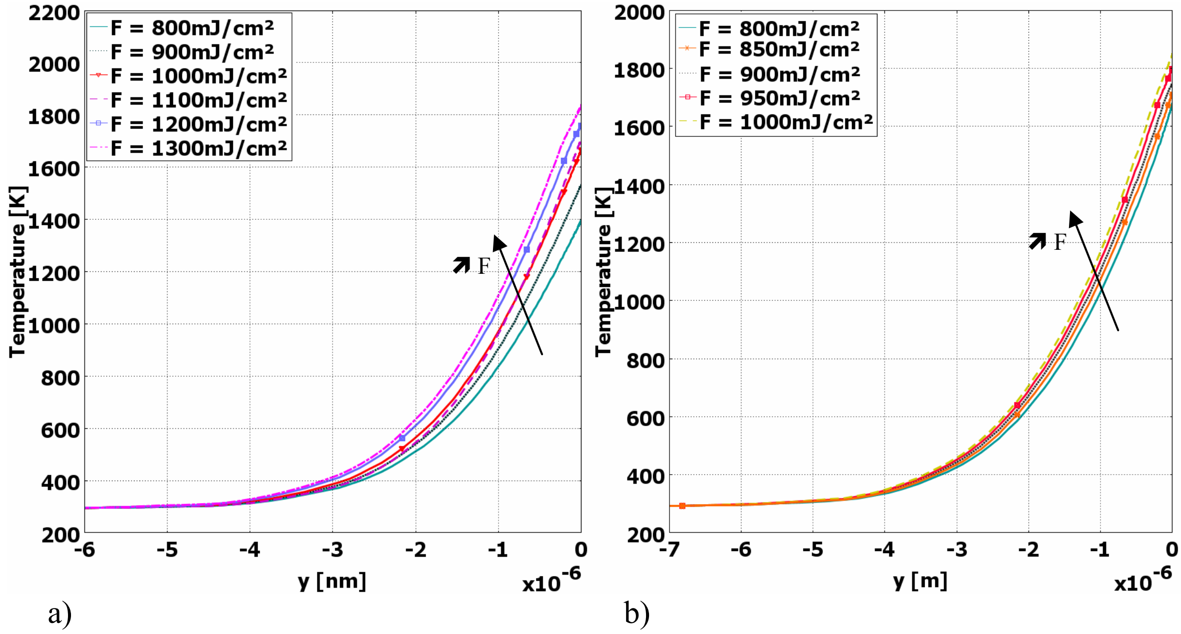


Figure 6. Temperature profile versus depth (Y) at time t = t_{max}. a) for Gaussian shape, b) for Gate shape

As increasing depth position (Y), the maximal temperature decreases dramatically to room temperature at 6 µm (Figure 6).
As reported in figures 5 and 7, in the case of gate shape time distribution, the melting phase starts for laser fluence F = 850 mJ/cm² However, the threshold of melting occurs in the case of Gaussian shape, for laser fluence higher than the last one (F = 1050 mJ/cm²). One should notice that for similar laser fluence higher than the lowest melting threshold (1050 mJ/cm² in case of Gaussian shape) the melted layer and phase duration are higher in the case of the gate shape (Figure 8 and Figure 5).

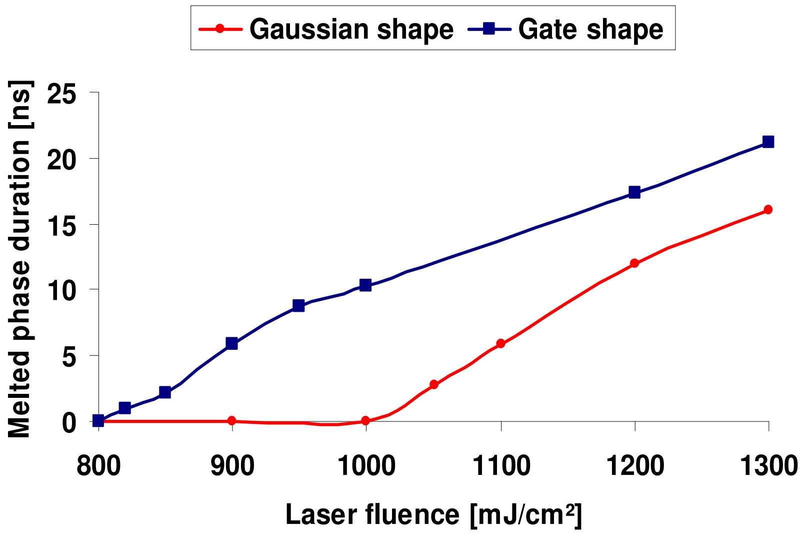


Figure 7. Melted phase duration versus laser fluence (F = 800 to 1300 mJ/cm²)

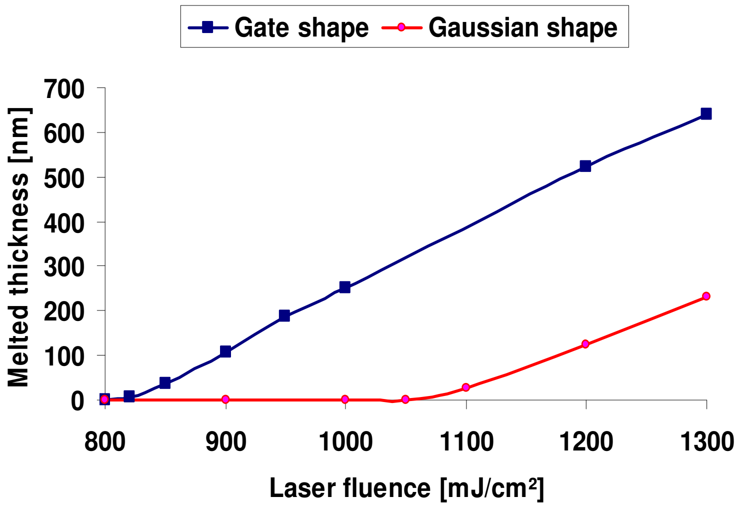


Figure 8. Melted thickness versus laser fluence (F = 800 to 1300 mJ/cm²)

5. CONCLUSION

Results on crystalline Si show different values of the melting pool and the melting duration under the pulsed laser treatment. Typical values of working laser fluences (i.e. 800 to 1300 mJ/cm²) give a melting pool close to 100 nm that is namely higher than the amorphous Si layer (20 nm). For a Gaussian shape time distribution (figure 8), the control of the melting kinetics is easier than in the gate shape one. However, in the first case, the melting threshold requires more energy.
The returned results show that investigation of melting kinetics should considered mainly in the range 800 to 1100 mJ/cm² (Figure 8), in order to refine the laser threshold and consequently to study the melting thickness sensitivity versus fluence in the vicinity of the melting threshold.
Effort of computing will be focalized on the congruence of the numerical resolution between the space and the time steps to better control very fine melted structures (2 nm) as announced from our first objective.
The melting kinetics (melted thickness and liquid/solid interface velocity) that is computed will be compared to the experimental results (TEM and MEB Techniques) in future work.

7. REFERENCE

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