COMSOL Multiphysics® Based Identification of Thermal Properties of Mesoporous Silicon by Pulsed Photothermal Method

I.El Abdouni [1], A. Melhem[1], N. Semmar*[1]

[1]GREMI-UMR 7344, CNRS Université d'Orléans, 14 rue d'Issoudun, BP 6744, 45067 Orléans Cedex 2, France

* Corresponding author: Nadjib.semmar@univ-orleans.fr

Abstract: The silicon is mainly known under its single-crystal shape and polycrystalline. Since a few decades, a new type of morphology is developed: the porous silicon (p-Si). Meso-porous silicon (Mp-Si) is one of promising materials for future microelectronic chips multi-functionalization systems, and for micro-sensing devices [1]. More particularly we are interested by the study of the thermal properties of those materials versus the specific morphology (porosity rate, and pore sizes). There are various analytical models that allow the thermal conductivity prediction, function of the porosity rate and the conductivities of the 2 phases (silicon and air). But those models are often based on a barycenter approach far from the real microstructure. That's why the modelling on Comsol is interesting to simulate the heat transfer in multi-layers geometries in 2 or 3 dimensions. For thermal properties investigation many experimental systems were developed based on the photothermal effect [2]. One of typical way is to induce a rapid surface temperature increase using pulsed laser beam acting like a heat source (volume or surface depending on the absorption coefficient) to finally create a model of this interaction. At least, it will be possible to determine the thermal parameters using the identification method (optimization by the least squares for example).

1. Samples, PPT Method and heat transfer

The samples used are single-crystal silicon <1 1 1> etched in various depths (0.2, 1, 10, 50 µm) .This porous silicon was obtained by electrochemical etching. Due to the complex surface of the meso-porous silicon which does not allow a homogeneous absorption of the incident photons, it is necessary to deposit a thin metallic layer (Titanium with 50% absorptivity). This 200 nm titanium layer (photothermal transducer) absorbs the incident photon, and creates a uniform heat source. With Comsol we model our samples in 2D axysymmetric case, 200 nm Titanium layer and the porous Si layer with thickness equal to the etching depth (from 0.2 to 50 µm), and then the bulk silicon with 50 µm depth.

Pulsed Photothermal Method (PPT) [4]:

The sample surface is beamed by a KrF laser pulse (λ = 248nm, τ_P = 27ns, f = 100mJ/cm²; S = 12 mm²) leading to a rapid increase of the temperature. Then the emitted IR flux is collected using a nitrogen cooled IR detector and converted to electrical signal. A calibration procedure allows finaly the plot of the surface thermal response. The surface temperature variation gives us informations about the thermophysical properties of the inspected material which are the density ρ, the heat capacity Cp and the thermal conductivity k (Figure 1). Moreover we have to consider the thermal resistance (Rth) between the Ti top-layer and the p-Si substrate as illustrated on fig.1.

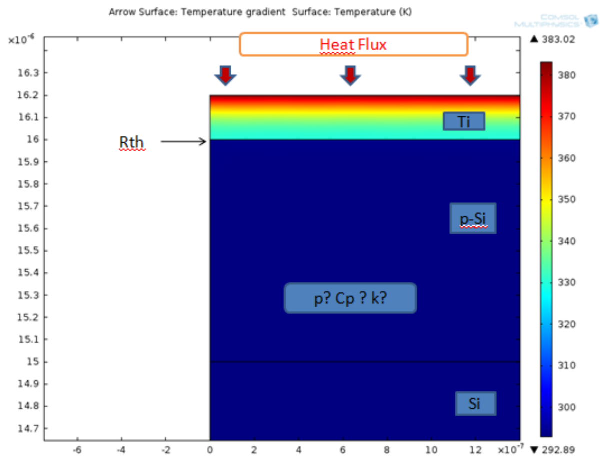

Figure 1 : View of the multi-layers sample for 1µm etched depth

The laser pulse is modeled by a Larson function [6]: (t) = (t/tm²) exp (-t/tm); (figure 2)

Tm = 8ns being the time when the maximum laser power amplitude is reached.

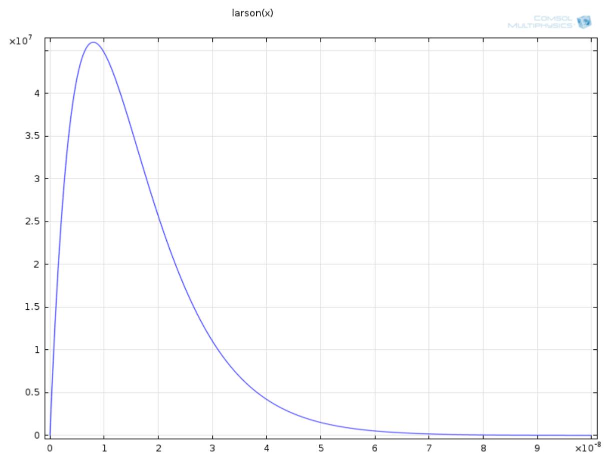

Figure 2: 'Larson' pulse time distribution

The Heat Transfer in Solids node in which Heat Flux is distributed on a surface of 12.56 mm² (figure 3) is employed in the multilayer domains. The equation which governs the conduction of heat is given by :

$$\rho \cdot C_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T)$$

To accelerate the computing time of our results we vary the different thermal parameters thanks to the Parametric Sweep.

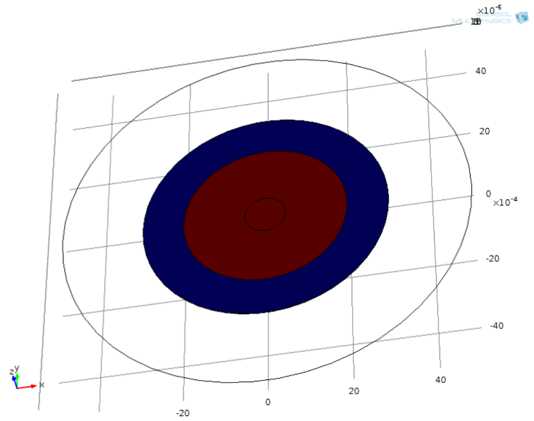

Figure 3: Top sight of our sample with laser spot (in red)

2. First results

The thermal properties of Titanium and bulk Silicium are known and listed in Comsol,
ρ(Ti)=4940kg/m³ ;Cp(Ti)=710J/kg/K;
k(Ti)=22W/m/K ;ρ(Sibulk)=2329kg/m³ ; Cp(Si bulk)=130J/kg/K ; k(Si bulk): 120 W/m/K
So the parameters which we make vary are the thermal properties of porous Si.

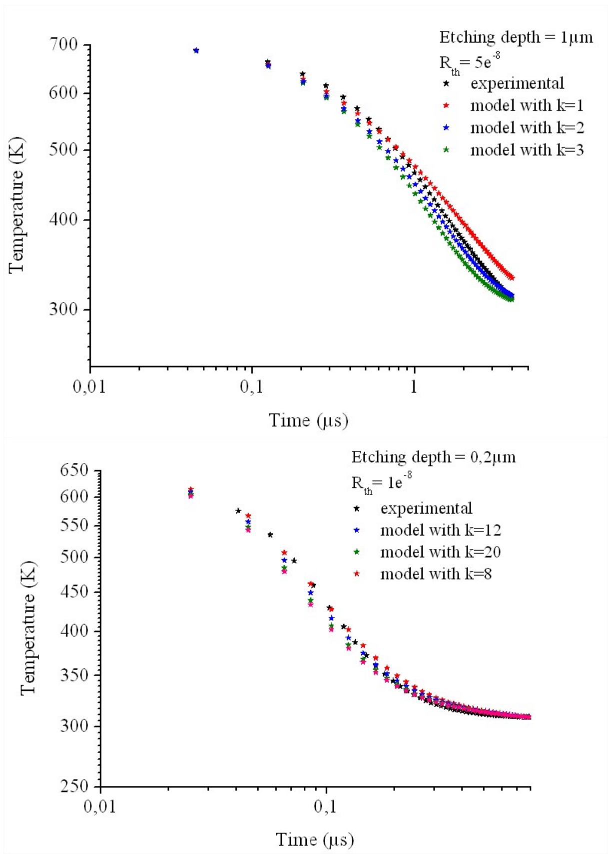

Figure 4: Surface temperature for 1µm (1) and 0.2µm depth etching (2) in log/log scale

With an optimized thermal resistance it seems that the best convergence with experimental relaxation curves occurs with the following parameters:

	ρCp(Sip)(J.kg/m³/K)	Rth	k(Sip)(W/m/K)	Tmax(K)	Relax time
0,2µm	1,6e^6	5,00E-08	(8;12)	645	0,3µs
1µm	1,2e^6	1,00E-07	(1;2)	685	3,5µs

For a depth etching of 0.2µm the approached thermal conductivity is between 8 and 12 J / K / m. For 1µm the value of the thermal conductivity with this Comsol model is between 1 and 2 W/K/m. Thermal resistances vary from 5e-8 m².K/W for 0.2µm to 1e-7 m².K/W for 1µm

We see that more we increase the etching depth, more the thermal conductivity of the porous silicon decreases. Indeed we increase the porous phase of our samples which possesses a lower thermal conductivity. The evacuation of heat is slower thus the maximum temperature and the time of relaxation to reach the adiabatic temperature increase.

3. Conclusion

This study focuses on the elaboration of a model to optimize the thermal properties of porous silicon which are very difficult to be estimated with analytical and experimental methods. We see that for the small etching depth the model is accurate with weak margins of errors.

4. Nomenclature

a: Absorption coefficient
ρ: Density (kg/m^3)
C_p: Specific heat (J/kg/K)
k: Thermal conductivity (W/K/m)
λ: Wavelength (nm)
f: Laser fluence(J/m²)

5. References

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