Investigation of Si(001) surface temperature throughout Laser-induced desorption process

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Abstract

Our study concentrates on the surface diffusion which is a thermally activated process that initiated by heating the substrate. More specifically, the study will investigate the Si(001) surface temperature throughout laser-induced desorption process. The nonlinear inhomogeneous heat conduction equation is solved numerically in one dimension by using the finite differences method as long as the temperature dependence of the physical(optical and thermal) functions prevents an analytical solution. All the effects are incorporated and highlighted especially the temperature- diffusion dependence on position and time.

Keyword:laser-induced surface heating , (LED), nonlinearinhomog-eneous(PDE).

Introduction

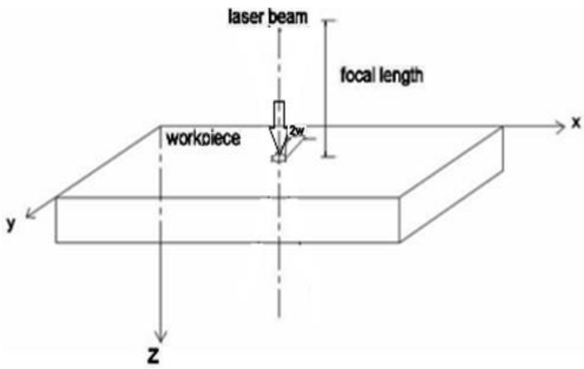
The idea of laser-induced thermal desorption (LITD) (M. Dürr, U. Höfer,2013, G. Mette *et al.*, 2013, F. H. Saeed, 2005, A. Vertes e*t al.*,1993), stems from early studies of the influence of laser radiation on small molecules adsorbed on solid surface. If the substrate absorbs the laser radiation, it heats up on a time scale comparable to the laser pulse length. The resulting temperature rise leads to the detachment of the adsorbed molecules. It was soon realized that Q-switched laser pulses (whose duration are on the nanosecond time scale) may lead to sub thermal velocity distribution of the desorbed particles (B. G. Koehler,S. M. George, 1991). Clearly, the evolution of substrate surface temperature plays a decisive role in the course of events in (LITD).

Recently, it was shown for recombination hydrogen desorption from Si(001) that the general difficulty can be circumvented by combining pulsed laser heating with scanning tunneling microscopy (M. Dürr, A. Biedermann *et al.*, 2002). The rearrangement of Silicon dangling bonds induced by pulsed laser heating of monohydride-covered Si(001) surfaces had been studied by means of scanning tunneling microscopy (C. H. Schwalb *et al.*, 2007).

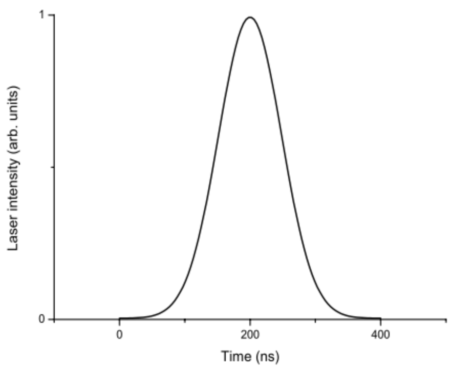
In our study, we investigate the time evolution of the Silicon surface temperature during one Gaussian laser pulse which is modeled by solving the one-dimensional heat conduction equation. This equation is solved numerically using finite differences methodbecause the temperature dependence of the optical and physical functions and coefficients of silicon prevents an analytical solution.

Formulation of the problem

Let us consider a thin film of thickness L as shown in Fig(1), a front surface z=0 is much larger than film thickness and the total laser radiation is completely absorbed at the surface and converted into heat, then it is possible to treat the interaction as a one-dimensional heat transfer process (J.K.Chen, J.E.Beraun, 2001).



(a)



(b)

Fig.(1). (a) Laserbeam impinging on a finite size sample, (b)

Gaussian profile of the laser intensity

The silicon heating calculations presented in this paper areper-formed using finite-difference method (D. M. Causon, C. G. Mingham, 2010). These calcula-tions incorporateboth a finite light penetration depth and temperature dependent of the optical and physical functions and coefficients.So the time evolution of the silicon surface temperature during one Gaussian laser pulse can be modeled by solving the one-dimensional heat conduction equation (C. H. Schwalb *et al.*, 2007),

$$\frac{\partial T(z,t)}{\partial t} = \frac{\partial}{\partial z}\left(D\,\frac{\partial T(z,t)}{\partial z}\right) + \frac{E(z,t)}{\rho C_p} \qquad (1)$$

with,

$$E(z,t) = [1 - R(T)]I_o\alpha(T)e^{-\alpha(T)z} \qquad (2)$$

is the laser power absorbed per unit volume $E(z,t)$ in unit of (J/cm^{3}sec), with R is the reflectivity,I_o(J/cm^2 sec) is the incident laser intensity, and α (cm^{-1}) is the absorption coefficient. Additionally, T(K) is the temperature, z(cm)is the depth of penetration, t (sec) is the time , C_p(J/g K)is the specific heat capacity, andD (cm^2 /sec) is the thermal diffusivity,

$$D = \frac{\kappa}{\rho C_p} \quad (3)$$

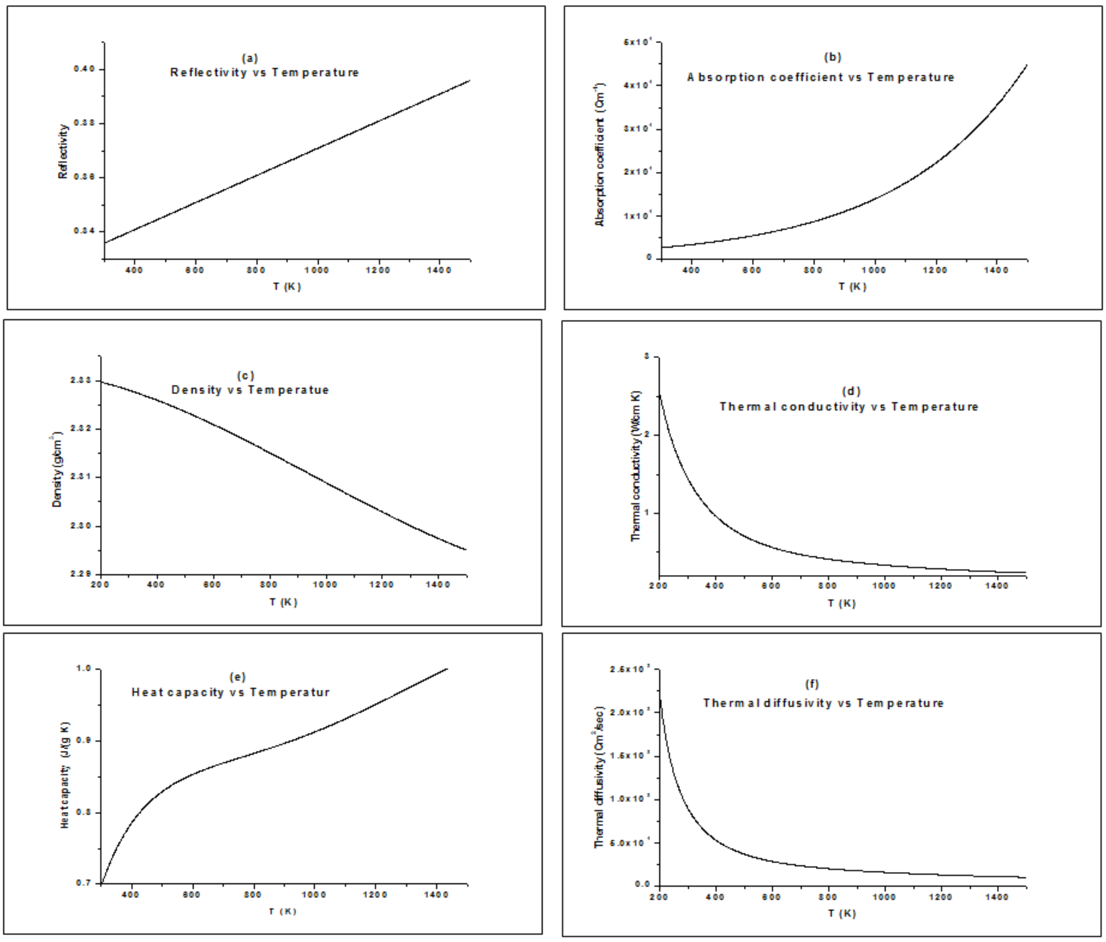
Where ρ(g/cm^3) is the density.

In our numerical calculations, the heat diffusion normal to the surface takesinto account the temperature dependent of the specific heat capacity C_p(T), thermal conductivity $\kappa(T)$, and the absorption coefficient $\alpha(T)$of silicon(O.Kimmelma *et al*., 2008, J. M. Dowden, 2009). Since the penetration depthof the laser pulse into the bulk is very small $(\approx 1\mu m)$, thermal diffusion into the bulk leads to a fast cooling of thesilicon surface within 10 ns, (see Fig.1,b) (C. H. Schwalb *et al.*, 2007). Becauseof the exponential dependence of both desorption and diffusion rates on surface temperature, one can conclude that mostof the processes will happen in a time window of only (3–4 ns) (J. H. G. Owen *et al.*, 1996, E. Hill, B. Freelon, and E. Ganz, 1999).

The optical and thermal parameters of silicon as a function of temperature: absorp-tion coefficient, reflectivity , heat capacity, density and thermal conductivity,and all calculated are shown in Fig(2). The curves represent empirical fits to several different sources of data (O.Kimmelma *et al*., 2008, J. M. Dowden, 2009,R.F. Wood and

G.E. GiIes, 1981, J.E. Moody and R.H. Hendel, 1982, S. De Unamuno and E. Fogarassy, 1989, P. Schvan and R.E. Thomas,1985, G.Rimvall, 1999).

The present study use finite difference methods (C. H. Schwalb *et al.*, 2007,D. M. Causon, C. G. Mingham, 2010, K. A. Nowakowski, 2005) to calculate laser induced silicon surface heating. The numerical calculation must be performed because the temperature dependence of the optical and physical parameters of silicon (Fig.2) in (eq.1) prevents an analytical solution (B. G. Koehler and S. M. George, 1991).



Fig(2) The optical and thermal parameters of silicon as function of temperature (B. G. Koehler and S. M. George,1991, D. M. Causon, C. G. Mingham, 2010, EMIS, Data review series No. 4, 1988).

Examination of the governing equation shows that the heat conduction equation requires evaluation of the first-order derivative with respect to time and the second order derivatives with respect to the coordinate directions z. The time derivative is commonly evaluated using a forward difference, and the spatial derivative is expressed using the central difference expr-ession because the error resulting from acentral difference is smaller than from a forward or backward difference. Consequ-ently, it is beneficial to use central difference method for the calculations whenever possible, so we must express the temperature at node j+1 at time t+dt explicitly in terms of the temperatures of the surrounding nodes at time t. This approach is called an explicit formulation , which allows for simplification through the finite difference mesh and solve for the temperature at succeeding time step, provided that the initial temperature of the entire grid is known.

Following the over mentioned procedure, we get:

$$T_{i,j+1} = T_{i,j} + r_1\left(T_{i-1,j} - T_{i,j} + T_{i+1,j}\right) + r_2\left(T_{i+1,j} - T_{i-1,j}\right)^2 + (1 - R\left(T_{i,j}\right)I_o\alpha\left(T_{i,j}\right)\exp(T_{i,j}z) \quad (4)$$

Where,

$$r_1 = D\left(T_{i,j}\right)\frac{dt}{(dz)^2} \quad (5)$$

$$r_2 = \acute{D}\left(T_{i,j}\right)\frac{dt}{(2dz)^2} \quad (6)$$

and,

$$\acute{D}\left(T_{i,j}\right) = \frac{\partial\acute{D}\left(T_{i,j}\right)}{\partial z} \quad (7)$$

Eq. 5 reveals that sufficient condition for convergence of eq.4 (D. M. Causon, C. G. Mingham, 2010 , K. A. Nowakowski, 2005) is,

$$0 \leq r_1 \leq 0.5 \tag{8}$$

so the stabilityof eq.4 depends on the relationship between material properties, the time incrementΔt and the spatial incrementΔz.

The model geometry of the problem is shown in Fig. 3

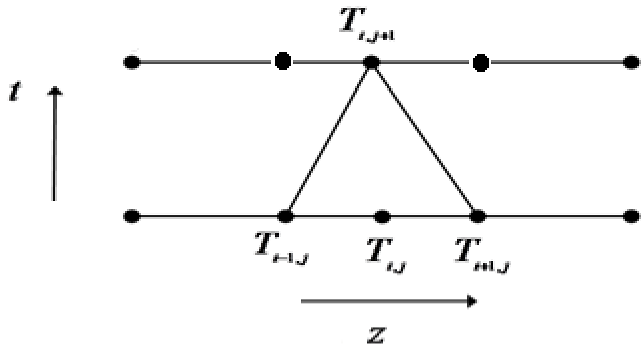


Fig.3Model geometry of the problem

Boundary conditions are the most important part of the model. They influence the programming and calculation results greatly. Specifying the suitable physical boundary conditions is the basis for successful computation.

The boundary conditions read as the following,

At $z = 0$,

$$T_{0,j+1} = \frac{T_{1,j+1}}{1+\Delta z} \tag{8}$$

and at$\boldsymbol{z = L}$,

$$\frac{\boldsymbol{\partial T}}{\boldsymbol{\partial z}} = -\boldsymbol{T} \tag{9}$$

i.e.,

$$\boldsymbol{T_{N_z,j+1}} = \frac{\boldsymbol{T_{N_z-1,j+1}}}{\boldsymbol{1-\Delta z}} \tag{10}$$

And the initial condition is,

$$T(z, 0) = 400\ K \quad (11)$$

The Results

The computer program that is design to study laser-induced silicon surface heating incorporates all the temperature-dependent optical and thermalparameters of silicon surface. Fig.(4) displays the temporal distribution induced by Gaussian laser pulse with a peak intensity of 30 $MW/cm^3$and time 10 n sec. The laser pulse, causes a rapid heating of the surface region (see also the contoure map in Fig.(5)). This figure makes sure that after the laser pulse has been absorbed, the surface temperature will be about 850 K within a few 10 n sec due to thermal diffusion.Notably, the maximum value of temperature induced by laser pulse depends on the initial surface temperature,the temperature dependence of the optical and thermalparameters of silicon and the time of pulse duration. One of the most interesting feature is the temperature diffusion dependence(see Fig.(6)). Finally Fig.(7) display the temperature profiles inside the material obtained at different heating times. It is obvious that the diffusion increases monoticaly with temperature. It is known that laser photons penetrate into the silicon bulk and are absorbed by band-gap transitions that create excited electron- hole pairs. These pairs diffuse to the surface and initiate photochemical desorption. Alternatively the pairs relax with life time on the order of 10^{-13} to 10^{-14} sec and transfer their energy to the silicon lattice. This energy transfer results in rapid lattice that may lead to thermal desorption.

Finally, as a future work, the time dependent laser intensity will be incorporated and the in additional to the diffusion the temperature-coverage dependence (F. H. Saeed, 2005) will be investigated. Since the coverage–surface temperature dependence has important role in determining the desorption kinetics

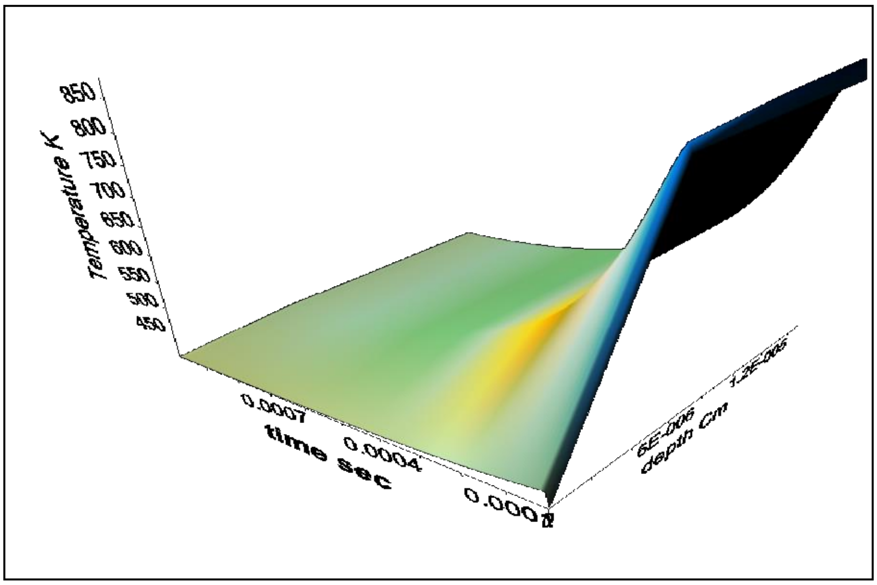


Fig.4. Temperature distribution inside Silicon with depth=10μm,induced by Gaussian laser pulse with a peak intensity of 30 MW/cm^2 and time=10 n sec.

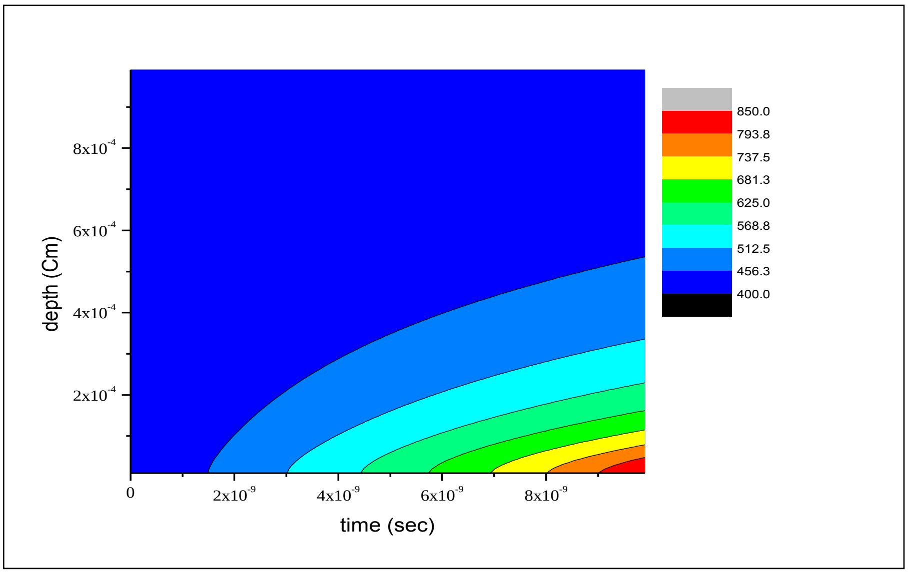


Fig.5.Temperature distribution inside Silicon (Contour map) (Fig.4)

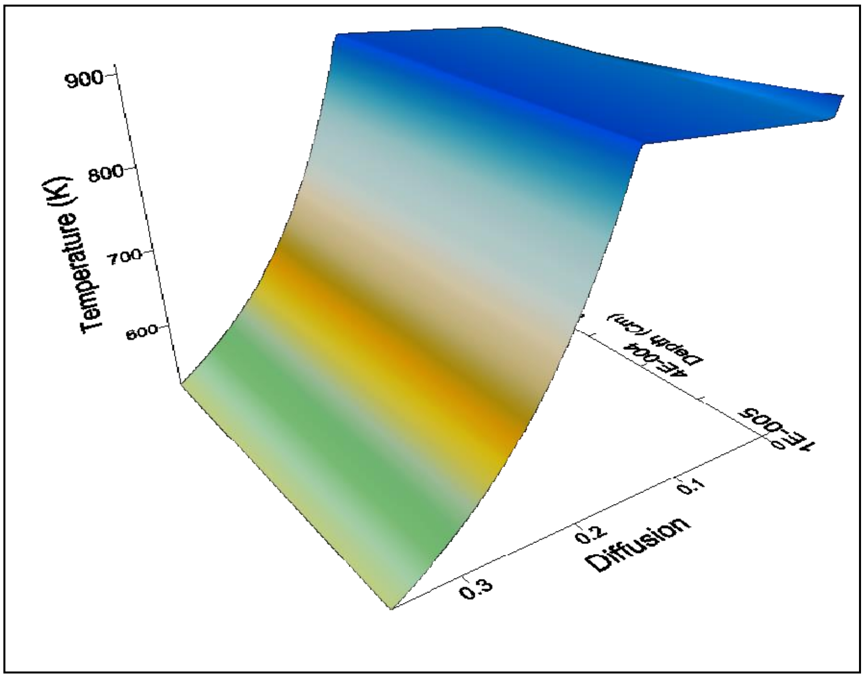


Fig.6. Temperature dependent diffusion (Fig.4)

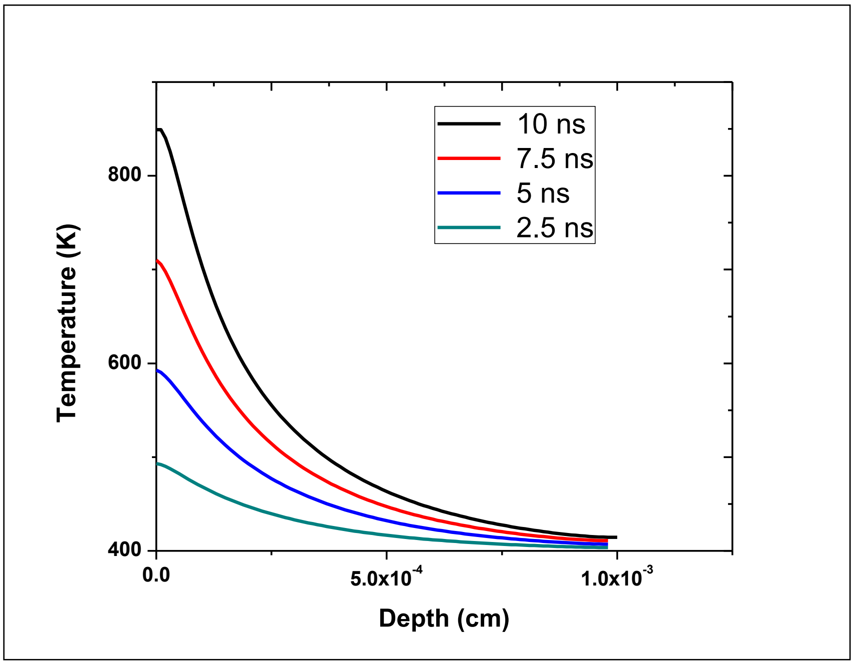


Fig.7. Temperature - depth dependence for different time

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فحص درجة حرارة سطح Si(001) خلال عملية القلع المحفزة بالليزر

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الخلاصة

تتركز دراستنا على عملية الانتشارعلى السطح التي تعد كعملية تنشيط حراري تبدأ من تسخين القاعدة. وبصورة خاصة ستفحص دراستنا درجة حرارة السطح Si(001) خلال عملية القلع يد المخ باستخدام طريقة الفروقات المحددة طالما ان اعتماد الدوال الفيزيائية (الحرارية والبصرية) تمنع اي حل تحليلي.تم تضمين وتسليط الضوء بصورة خاصة على اعتماد انتشار- درجة حرارة