Temporal profile of optical transmission probe for pulsed-laser heating of amorphous silicon films

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The transient temperature field development during heating of an amorphous silicon (*a*-Si) film, deposited on a fused quartz substrate by pulsed excimer laser irradiation is studied. Experimental optical transmission data are compared with heat transfer modeling results. The temperature-dependence of the material complex refractive index through the thin film thickness is taken into account.

Pulsed laser irradiation is employed over a wide spectrum of materials processing applications, including surface hardening, alloying, curing, synthesis of compound and semiconductor films. In semiconductor systems,[1] it is used to anneal ion-implantation surface damage, recrystallize amorphous and polycrystalline films, and enhance dopant diffusion. Recent studies[2] have shown that one of the most effective ways of removing submicron-sized particles from solid surfaces is achieved with the deposition of a liquid film on a substrate surface and the application of an ultraviolet (UV) excimer laser pulse on the surface. One of the main issues in improving this process is the control of the induced transient temperature field. Time-resolved optical transmission and reflection measurements have been reported for the investigation of the irradiation of crystalline silicon (*c*-Si) on sapphire structures at the picosecond[3] and the nanosecond,[4,5] time scales. This work presents an optical transmission probing technique for the transient, *in situ* monitoring of the temperature field in pulsed excimer laser irradiation of thin amorphous silicon (*a*-Si) films.

The sample is a 0.2 μm-thick amorphous silicon film deposited by electron beam evaporation of crystalline silicon in vacuum onto a 250 μm-thick fused quartz substrate. The substrate temperature is kept at 140 °C and the deposition rate at 10 Å/s. The uniformity of the thickness of the *a*-Si layer is monitored by surface profilometry. The sample is irradiated by a KrF ($\lambda=0.248$ μm) excimer laser beam. The laser beam fluence F is determined by measuring the pulse energy using an energy meter. An infrared probing diode laser beam ($\lambda=0.752$ μm) is incident normal onto the sample surface. The transmitted signal is captured by a fast photodiode and a digitizing oscilloscope.

The optical transmission measurement technique is based on the variation of the material optical properties with temperature. It has been reported[6] that the optical properties of submicron-thick, *a*-Si films do not vary significantly with temperature at the Nd:YAG, $\lambda=1.064$ μm laser wavelength. Recent studies[7] have revealed a significant variation of the optical properties of 0.2 μm-thick amorphous silicon films with temperature at the $\lambda=0.752$ μm diode laser light wavelength. Static reflectance $\mathscr{R}$ and transmittance $\mathscr{T}$ measurements yielded the following temperature dependence of the components of the complex refractive index, $\hat{n}=n-ik$, of the 0.2 μm-thick *a*-Si films used in this work, at the $\lambda=0.752$ μm wavelength, and in the temperature range of 293–650 K:

$$n=n(T)=4.0+1.3\times10^{-4}(T-293), \tag{1a}$$

$$k=k(T)=0.055+2.3\times10^{-4}(T-293). \tag{1b}$$

The temperature profile penetration is of the order of 1 μm, whereas the laser beam spot area on the sample surface is measured to be about 0.5 cm^2. Thus, it may be assumed that the heat transfer at the center of the laser beam is essentially one-dimensional. For temperatures below the melting temperature, the conductive heat transfer in the solid silicon layer is given by

$$\rho C_p \frac{\partial T}{\partial t}=\frac{\partial}{\partial x}\left(K\frac{\partial T}{\partial x}\right)+Q_{ab}(x,t). \tag{2}$$

In the above equation, x is the coordinate normal to the sample surface, ρ is the density, T is the temperature, C_p is the specific heat for constant pressure, K is the thermal conductivity. The variation of the material thermal properties[8] is considered. The energy absorption, $Q_{ab}(x,t)$, follows an exponential decay in the material:

$$Q_{ab}(x,t)=(1-\mathscr{R}_{\text{exc}})I(t)\alpha e^{-\alpha x}. \tag{3}$$

In the above equation, $\mathscr{R}_{\text{exc}}$ is the reflectivity of the *a*-Si layer for the excimer laser light, I is the incident laser beam intensity, and α is the absorption coefficient.

The amorphous silicon complex refractive index at the KrF excimer laser light wavelength ($\lambda=0.248$ μm) is taken as $\hat{n}=n-ik=1.69-i2.76$.[9] The absorption coefficient is given by $\alpha=1.398\times10^6$ cm^{-1}. The corresponding optical penetration depth in the thin film is of the order of a few nanometers. The temperature dependence of the ma-

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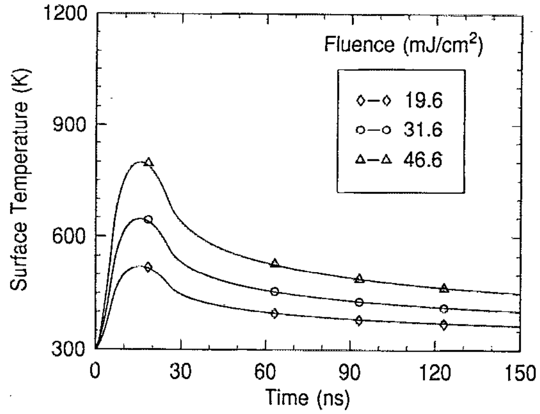

FIG. 1. Surface temperature histories for a 0.2 μm-thick amorphous silicon layer, irradiated with an excimer laser ($\lambda=0.248$ μm) for laser fluences $F=19.6$, 31.6, 46.6 mJ/cm^2. The laser pulse length $t_l=26$ ns. The solid lines show calculated data.

terial optical properties at this wavelength is expected to be small. It is reasonable to assume that no interference effects modify the local energy absorption in the thin film, as the case has shown to be[10] in pulsed ruby ($\lambda=0.694$ μm) and frequency doubled Nd:YAG ($\lambda=0.532$ μm) laser irradiation of silicon layers, and in absorption detection of defects in a-Si:H films.[11] The reflectivity $\mathscr{R}_{\rm exc}$ is thus considered constant and can be calculated using the expression for the normal incidence reflectivity of bulk material surfaces, $\mathscr{R}_{\rm exc}=[(n-1)^2+k^2]/[(n+1)^2+k^2]=0.545$. Measurements of the laser pulse temporal profile have shown that the pulse fluence F is distributed in a triangular shape, with the pulse length $t_l=26$ ns, and the peak intensity occurring at $t_p=6$ ns.

$$\begin{aligned} I(t)&=\frac{2Ft}{t_l t_p}, && 0<t<t_p.\\ I(t)&=\frac{2F(t_l-t)}{t_l(t_l-t_p)}, && t_p<t<t_l.\\ I(t)&=0, && t_l<t. \end{aligned} \tag{4}$$

Convection and thermal radiation losses are negligible for the high incident laser pulse intensities used (of the order of 10^{11} W/m^2), and time scales considered in this work. The temperature penetration in the structure is small, so that the bottom substrate surface remains at the ambient temperature T_∞.

$$\left.\frac{\partial T}{\partial x}\right|_{x=0}=0, \tag{5a}$$

$$T(x=d_{\rm Si}+d_s,t)=T_\infty. \tag{5b}$$

where $d_{\rm Si}$ and d_s are the thicknesses of the a-Si layer and the substrate correspondingly. Initially the structure is isothermal at the ambient temperature.

$$T(x,0)=T_\infty. \tag{6}$$

The heat conduction is solved numerically by an implicit finite difference algorithm. The a-Si layer was discretized into $N=20$ equal increments. A time step, $\Delta t=2\times10^{-12}$ s was used in the calculations. The a-Si layer is partially transparent for the probing laser light wavelength ($\lambda=0.752$ μm). The temperature field in the semiconductor film induces changes in the material refractive index [Eqs. (1a) and (1b). Such changes were accounted for in the picosecond irradiation of thin c-Si films[3] by assuming an average film temperature for the fitting of the measured optical properties. In this study, the semiconductor film is treated as a stratified multilayer structure,[12–14] composed of N layers of varying complex refractive index. The $m=1,\ldots,N$ layers within the a-Si film are absorbing and have a temperature dependent complex refractive index, given by Eqs. (1a) and (1b). The substrate is represented by the $m=N+1$ layer, and is transparent to the probing laser light, having a refractive index that is real, $\hat{n}_{N+1}=1.46$. Utilizing the formalism of the characteristic transmission matrix, the lumped structure reflectivity and transmissivity can be obtained. The mth layer of thickness d_m, having a complex refractive index $\hat{n}_m=n_m-ik_m$, is represented by the 2×2 matrix $\mathscr{M}_m$ whose elements are complex:

$$\mathscr{M}_m=\begin{pmatrix} \cos\left(\frac{2\pi}{\lambda}\hat{n}_m d_m\right) & \frac{i}{\hat{n}_m}\sin\left(\frac{2\pi}{\lambda}\hat{n}_m d_m\right) \\ i\hat{n}_m\sin\left(\frac{2\pi}{\lambda}\hat{n}_m d_m\right) & \cos\left(\frac{2\pi}{\lambda}\hat{n}_m d_m\right) \end{pmatrix}. \tag{7}$$

The multilayer transmission matrix $\mathscr{M}$ is:

$$\mathscr{M}=\prod_{m=1}^{N+1}\mathscr{M}_m. \tag{8}$$

The reflection and transmission Fresnel coefficients, r and t_r, are:

$$r=\frac{[\mathscr{M}(1,1)+\mathscr{M}(1,2)]-[\mathscr{M}(2,1)+\mathscr{M}(2,2)]}{[\mathscr{M}(1,1)+\mathscr{M}(1,2)]+[\mathscr{M}(2,1)+\mathscr{M}(2,2)]}, \tag{9a}$$

$$t_r=\frac{2}{[\mathscr{M}(1,1)+\mathscr{M}(1,2)]+[\mathscr{M}(2,1)+\mathscr{M}(2,2)]}. \tag{9b}$$

The structure reflectivity $\mathscr{R}_{\rm prb}$ and transmissivity $\mathscr{T}_{\rm prb}$ for the probing laser in terms of r and t_r, follow:

$$\mathscr{R}_{\rm prb}=|r|^2, \tag{10a}$$

$$\mathscr{T}_{\rm prb}=|t_r|^2. \tag{10b}$$

The amorphous silicon layer was irradiated by laser pulse fluences, $F=19.6$, 31.6, and 46.6 mJ/cm^2. Figure 1 shows predicted surface temperature histories for these fluences. The peak temperature occurs approximately at a time of 15 ns. The temperature profiles across the thickness of the silicon layer are shown in Fig. 2 for a laser fluence, $F=31.6$ mJ/cm^2. The experimental transmissivity signal was normalized by the steady state value before heating.[15] The predicted transmissivity was also normalized by the transmissivity at a temperature, $T_\infty=300$ K. This normalization is consistent with the measurement of the complex refractive index of the layer from reflectivity and transmis-

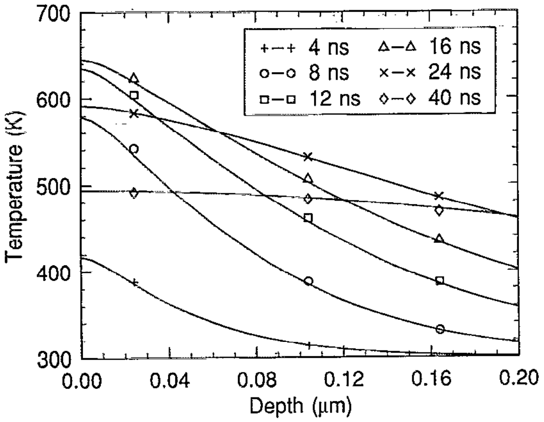

FIG. 2. Temperature profiles in a 0.2 μm-thick amorphous silicon layer, irradiated with an excimer laser. The laser fluence $F=31.6$ mJ/cm^2, and pulse length $t_l=26$ ns. The solid lines show calculated data.

sivity data. The comparison between experiment and model for the laser beam fluences, $F=19.6$ and 31.6 mJ/cm^2 is shown in Figs. 3(a) and 3(b). It can be stated that the model captures accurately the experimental trend. The calculated peak temperature for the fluence, $F=31.6$ mJ/cm^2, is approximately 650 K, (Fig. 1). At higher fluences, the agreement is not as good [Figs. 3(c)]. For the fluence $F=46.6$ mJ/cm^2, temperatures well above 650 K are predicted (Fig. 1). At such high temperatures $n(T)$ and $k(T)$ values could not be measured from steady-heating experiments.[7] Hence, there is much uncertainty to extend linearly the results in Eq. (1) into regions of high temperatures.

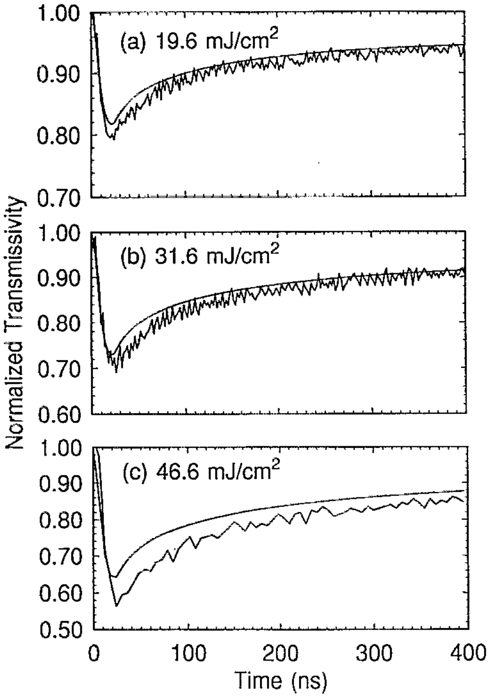

FIG. 3. Comparison between the numerical prediction and the experimental transmissivity signal at different laser beam fluences. The smooth line represents the calculated curve and the noisy line is the experimental signal.

Variations of the thin film thickness by ±0.01 μm, cause absolute transmissivity departures of about 40% from the values that correspond to the nominal 0.2 μm amorphous silicon layer thickness used in this work. The use of the normalized transmissivity measurements reduces the deviation to about 10%. Numerical computations have shown that variation of the thin film thermal diffusivity by 50% does not appreciably affect the magnitude of the transient transmissivity. The long-term temperature field depends mainly on the substrate thermal properties. The detailed shape of the pulse intensity temporal profile and the related experimental uncertainty do not seem to be important in the comparison of the theoretical model with the experiment. The optical transmission measurements presented in this work accurately capture the transient temperature field in excimer laser irradiated amorphous silicon films.

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