THERMALLY INDUCED STRESSES AND STRAINS IN LASER PROCESSING OF THIN FILMS

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ABSTRACT

The stresses and strains induced in thermal laser processing of substrates and thin films on substrates, are obtained in terms of single integrals by solving the thermoelastic equations using a Gaussian profile laser as the heating source. This analysis is applied to silicon thin films on fused silica and sapphire substrates. In part, this study shows that defects can form in the films because the stresses induced during high temperature laser processing of silicon and similar materials can exceed the yield stress under certain experimental conditions.

INTRODUCTION

During laser processing of surfaces, thermal heating will cause the formation of stresses and strains throughout the heated material, which must be analyzed because of their potential long term effects. In the extreme case, damage to the material system may result by the formation of defects. However, even the creation of built-in-stresses and strains without defects can alter properties. For example, laser-induced elastic strains will perturb phonon frequencies, thereby complicating in-situ temperature measurements by Raman microprobe analysis [1].

In this paper, solutions of the thermoelastic equations for local heating of isotropic substrates by a TEM_{00} Gaussian laser beam are presented. These solutions are extended to the case of thin films on substrates, as in Reference [1], to assess potential contributions to material damage by defect formation.

SOLUTION – THERMOELASTIC EQUATIONS

The temperature rise due to a focused laser beam with cylindrical symmetry, has been obtained by Lax [2] by solving the heat flow equation under steady state conditions. In the particular case of a TEM_{00} Gaussian beam with power P_0, beam waist ω, and intensity

$$I(r, z=0) = \frac{P_0}{\pi\omega^2} e^{-r^2/\omega^2} \tag{1}$$

Table I Total strains and residual stresses in a substrate heated by a gaussian laser beam.

$$\varepsilon^s_{rr} = -\varepsilon_0 \int_0^\infty \left(J_0(\lambda R) - \frac{J_1(\lambda R)}{\lambda R}\right) F(\lambda) \left[A(\lambda)\exp(-\lambda Z) - B(\lambda)\exp(-WZ) - C(\lambda) Z \exp(-\lambda Z)\right] d\lambda$$

$$\varepsilon^s_{\theta\theta} = -\varepsilon_0 \int_0^\infty \frac{J_1(\lambda R)}{\lambda R} F(\lambda) \left[A(\lambda)\exp(-\lambda Z) - B(\lambda)\exp(-WZ) - C(\lambda) Z \exp(-\lambda Z)\right] d\lambda$$

$$\varepsilon^s_{zz} = \varepsilon_0 \int_0^\infty J_0(\lambda R) F(\lambda) \left[\left(\frac{2W}{\lambda} B(\lambda) - A(\lambda)\right)\exp(-\lambda Z) - \frac{W^2}{\lambda^2} B(\lambda)\exp(-WZ) - C(\lambda) Z \exp(-\lambda Z)\right] d\lambda$$

$$\sigma^s_{rr} = -\sigma_0 \int_0^\infty J_0(\lambda R) F(\lambda) \left[\left(\frac{2W}{\lambda} - 1\right) B(\lambda)\exp(-\lambda Z) - \frac{W^2}{\lambda^2} B(\lambda)\exp(-WZ) - C(\lambda) Z \exp(-\lambda Z)\right] d\lambda$$
$$+ \sigma_0 \int_0^\infty \frac{J_1(\lambda R)}{\lambda R} F(\lambda) \left[A(\lambda)\exp(-\lambda Z) - B(\lambda)\exp(-WZ) - C(\lambda) Z \exp(-\lambda Z)\right] d\lambda$$

$$\sigma^s_{\theta\theta} = \sigma_0 \int_0^\infty J_0(\lambda R) F(\lambda) \left[\left(A(\lambda) + B(\lambda)\left(1 - \frac{2W}{\lambda}\right)\right)\exp(-\lambda Z) + \frac{W^2 - \lambda^2}{\lambda^2} B(\lambda)\exp(-WZ)\right] d\lambda$$
$$- \sigma_0 \int_0^\infty \frac{J_1(\lambda R)}{\lambda R} F(\lambda) \left[A(\lambda)\exp(-\lambda Z) - B(\lambda)\exp(-WZ) - C(\lambda) Z \exp(-\lambda Z)\right] d\lambda$$

$$\sigma^s_{zz} = \sigma_0 \int_0^\infty J_0(\lambda R) F(\lambda) \left[B(\lambda)(\exp(-\lambda Z) - \exp(-WZ)) - C(\lambda) Z \exp(-\lambda Z)\right] d\lambda$$

where $\varepsilon_0 = \frac{1+\nu}{1-\nu} \frac{2\alpha' W}{\sqrt{\pi}} T_{max}$, $\sigma_0 = \frac{E}{1+\nu} \varepsilon_0$

and $A(\lambda) = \frac{\lambda^3 - (W+2\lambda)(1-\nu)(W-\lambda)^2}{(W^2-\lambda^2)^2}$, $B(\lambda) = \frac{\lambda^3}{(W^2-\lambda^2)^2}$ and $C(\lambda) = \frac{\lambda^3}{(W+\lambda)(W^2-\lambda^2)}$

Table II Total strains and residual stresses in a laser heated thin film on a substrate.

$$\varepsilon^f_{rr}(r) = \varepsilon^s_{rr}(r, z=0)$$

$$\varepsilon^f_{\theta\theta}(r) = \varepsilon^s_{\theta\theta}(r, z=0)$$

$$\varepsilon^f_{zz}(r) = \frac{\nu^{(f)}}{\nu^{(f)}-1} [\varepsilon^s_{rr}(r, z=0) + \varepsilon^s_{\theta\theta}(r, z=0)] + \frac{1+\nu^{(f)}}{1-\nu^{(f)}} \alpha'^{(f)} T(r, z=0)$$

$$\sigma^f_{rr}(r) = \frac{E}{(1-\nu^{(f)2})} (\varepsilon^s_{rr}(r, z=0) + \nu^{(f)} \varepsilon^s_{\theta\theta}(r, z=0) - (1+\nu^{(f)}) \alpha'^{(f)} T(r, z=0))$$

$$\sigma^f_{\theta\theta}(r) = \frac{E}{(1-\nu^{(f)2})} (\nu^{(f)} \varepsilon^s_{rr}(r, z=0) + \varepsilon^s_{\theta\theta}(r, z=0) - (1+\nu^{(f)}) \alpha'^{(f)} T(r, z=0))$$

$$\sigma^f_{zz}(r) = 0$$

incident on a semi-infinite elastic substrate, the resultant temperature rise takes the form

$$T(R, Z, W) = \frac{\alpha P_0(1-R_0)}{\pi K} \int_0^{\infty} J_0(\lambda R)\, F(\lambda)\, \frac{W e^{-\lambda Z} - \lambda e^{-WZ}}{W^2-\lambda^2}\, d\lambda \tag{2}$$

with α the absorption coefficient, K the thermal conductivity, and R_0 the surface reflectivity, each assumed to be independent of temperature for a given substrate [2]. Here, $F(\lambda)$ is the Bessel transform of the laser lineshape f(R), so that

$$F(\lambda) = \int_0^{\infty} J_0(\lambda R)\, R\, e^{-R^2}\, dR = \frac{1}{2} e^{-(1/4)\lambda^2} \tag{3}$$

Use has also been made of the normalized coordinates $R = r/\omega$, $Z = z/\omega$, and $W = \alpha\omega$. This temperature rise may now be included as the driving term in the thermoelastic equations, to yield the thermally induced stresses and strains.

The thermoelastic equations themselves are obtained from the stress-strain relations and from the equations of equilibrium for an isotropic system. Using stress functions Ω and Ψ defined in terms of the stresses σ and total strains ε by Youngdahl [3], they take the form

$$\nabla^2\Omega = \frac{1}{2(1-\nu)} \left(-\frac{\partial^2\Psi}{\partial Z^2} + 2(1+\nu)\alpha'\omega^2 T \right) \tag{4}$$

$$\nabla^2\Psi = 0 \tag{5}$$

where α' is the thermal expansion coefficient, and ν is Poisson's ratio. Equations 4 and 5 are easily solved for the substrate [1] and expressed directly in terms of the residual stresses and total strains, where the total strain is the sum of the elastic strain and the thermal strain, yielding the relations in Table I. Note that the off-diagonal elements of the stress and strain tensors are identically zero for all but the rz components, which will also be ignored since they are very small [1].

These solutions may now be extended to the case of a thin film on a substrate. It is assumed that the thin film is sufficiently thin so that it does not perturb the stresses and strains in the substrate and that radial thermal conduction in the film is negligible relative to that in the substrate. Then, the resultant stresses and strains in the substrate are determined by linear superposition of two separate thermal driving terms, corresponding to laser absorption at the surface due to the thin film (of thickness d) and absorption within the substrate. For heating at the surface, the temperature rise of Equation (2) is used in the $W \to \infty$ limit with diminished effective incident power, $P_0^{eff} = P_0(1-e^{-\alpha_f d})$. This expression ignores multiple reflections in the film, which could be included when necessary. For heating due to absorption in the substrate, the temperature rise of Equation (2) is used with $P_0^{eff} = P_0 (1 - R_1) e^{-\alpha_f d}$, where R_1 is the reflectivity at the film/substrate interface, again ignoring multiple reflections. From the solutions for the stresses and strains in the substrate obtained using both thermal heating terms, the stresses and strains in the thin film are now determined by matching boundary conditions to the substrate.

The planar strains in the film may be obtained from the continuity of planar total strains at the film/substrate interface. Film strain in the z direction is derived from the stress-free condition ($\sigma_{zz}^f(r) = 0$) for the film/air interface using the corresponding stress-strain relation. The remaining two diagonal film stresses are found by direct substitution of the other known quantities in the stress-strain relations.

The six solutions for stress and total strain within the film are given in Table II in terms of the quantities of Table I and Equation 2, where E is Young's modulus and where the s and f superscripts refer to the substrate and the film, respectively. The elastic strains $\bar{\varepsilon}$ may be obtained directly from the total strains by subtracting the thermal strain α' T(r, z=0) from each component. Note that since the film is assumed to be very thin, all physical quantities within it are independent of z.

The expressions in Table II for stress and strain within the film may be numerically integrated, with the results displayed in Figures 1-3 for a silicon film on sapphire, a silicon film on fused silica, and for a silicon substrate (or, equivalently, a silicon film on a silicon substrate). Only the $W \rightarrow \infty$ (W = 15) case has been shown, corresponding to total laser absorption within the thin film.

The three cases are plotted for different effective laser powers, chosen so that the ratio $[P_0^{eff}(1-R_0)]/\omega K_{substrate}$ was held constant. In particular, the ratio was chosen so that the maximum temperature rise, $T_{max} = T(R=0, Z=0, W=\infty) = [P_0^{eff}(1-R_0)]/(2\sqrt{\pi}\ \omega K_{substrate})$ determined from Equation (2), would correspond to heating the silicon thin film to the melting point temperature of 1420°C ($T_{total} = T + T_{ambient} = 1420°C$). The other physical quantities which have been used are: $\nu = 0.42$, $E = 1.13 \times 10^{12}$ dyn/cm^2, $\alpha' = 4.0 \times 10^{-6}$/°C for silicon; $\nu = 0.17$, $E = 7.58 \times 10^{11}$ dyn/cm^2, $\alpha' = 5.5 \times 10^{-7}$/°C for fused silica; and $\nu = -0.02$, $E = 3.65 \times 10^{12}$ dyn/cm^2, $\alpha' = 8.6 \times 10^{-6}$/°C for sapphire, with all of these constants assumed to be independent of temperature.

As seen from the figures, the qualitative trends are similar for silicon thin films on either a silicon or fused silica substrate. However, results for silicon thin films on sapphire are quite different, due to the relatively large difference in the physical quantities for sapphire compared to the other two materials (particularly for Poisson's ratio).

Of course, since the laser increases the temperature everywhere within the film, the film expands in all directions. This is demonstrated by the positive values for the total strains everywhere. However, since the thin films are primarily influenced by the substrate, the relative magnitudes of the individual stress and strain components depend entirely on the particular

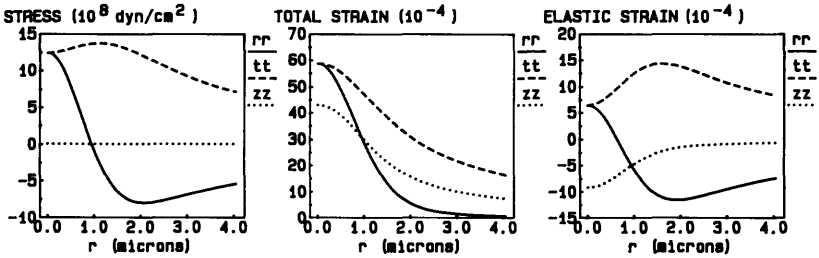

Figure 1. The residual stresses, total strains, and elastic strains are shown as a function of r for a silicon thin film on sapphire, using $\omega = 1$ μm, $T_{max} = 1400$ K, and $W = 15$. Note that rr, tt, and zz in the figure correspond to the rr, θθ, and zz components, respectively.

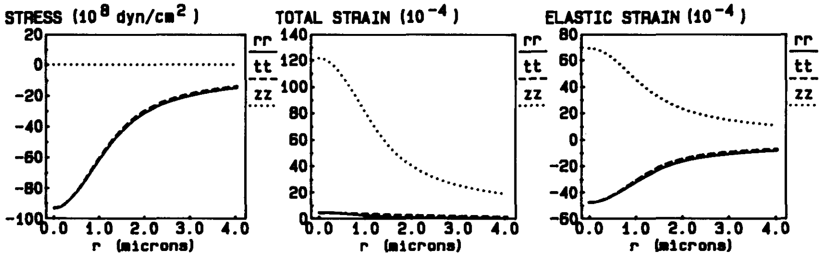

Figure 2. Same as Fig. 1 but for a silicon thin film on fused silica.

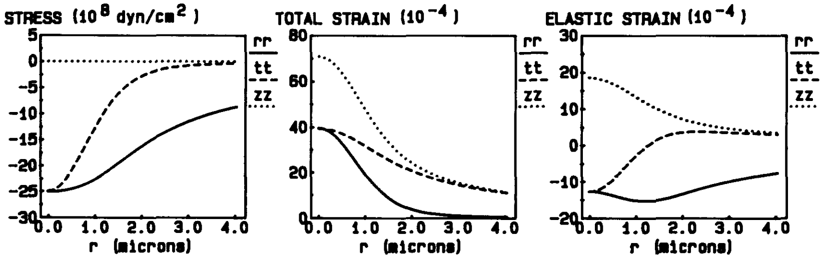

Figure 3. Same as Fig. 1 but for a silicon thin film on silicon. These results are identical to those obtained in Ref. [1] for a silicon substrate.

film/substrate system. As a result, a silicon film on sapphire is under tensile stress near beam center (positive residual stress) and has relatively less bowing (or displacement) in the vertical direction ($\varepsilon_{zz} < \varepsilon_{rr}, \varepsilon_{\theta\theta}$), since the thermal expansion coefficient of the substrate is greater than that of the film. For silicon on fused silica, on the other hand, the planar stress is compressive, and the strain is greater vertically than in the planar direction ($\varepsilon_{zz} > \varepsilon_{rr}, \varepsilon_{\theta\theta}$), since the thermal expansion coefficient of the substrate is here less than that of the film. For silicon on silicon, again the stress is compressive, and $\varepsilon_{zz} > \varepsilon_{rr}, \varepsilon_{\theta\theta}$ since expansion in the planar direction is inhibited by decreasing temperature in the substrate away from the beam center.

This analysis has assumed that the silicon films have no built-in stresses when under ambient conditions, with no laser incident. However, because silicon films are often deposited at elevated temperatures ($T_{dep} \sim 640$ °C), adhering silicon films on sapphire will actually be under compressive stress at ambient temperature, while silicon films on fused silica will be under tensile stress. Qualitatively, this means that laser heating will counterbalance the built-in-stress of the system (which is compressive for silicon on sapphire) at low laser powers, and will generate stress in the opposite sense (tensile for silicon on sapphire as in Figure 1) only at higher laser powers. However, since the laser does not heat the surface uniformly, the cross-over from compressive to tensile stress (for silicon on sapphire) or tensile to compressive stress (for silicon on fused silica), will actually take place when the laser heats the substrate at r=0 to a temperature slightly higher than T_{dep}. A more refined treatment would require inclusion of the built-in stresses in solving the thermoelastic equations.

DEFECT FORMATION

Defects will occur when laser heating leads to either tensile or compressive conditions if the magnitude of the stress exceeds certain yield conditions. Two types of damage are possible: that within the bulk of the film or substrate and that at the film/substrate interface. Only damage within the silicon thin film will be considered here.

Material damage will occur when the stress in the material exceeds a certain yield stress. For many materials, the yield stress is a function of the rate of strain [4], with

$$\sigma_E = C_0\left(\frac{\partial|\bar{\varepsilon}|}{\partial t}\right)^{1/n} \exp\left(\frac{U}{nk_B T_{total}}\right) \qquad (6)$$

where U is the activation energy for glide movement, and C_0 and n are constants. For the silicon thin films under consideration, U = 2.3 eV, n = 2.1 and $C_0 = 1.7 \times 10^5$ (dyn/cm^2)s$^{1/n}$, and for laser heating by a scanning Gaussian beam, with scan velocity $|v|$, then the dwell time of the laser over a distance of the spot size ω is $\frac{\omega}{v}$, so that $\left|\frac{\partial|\bar{\varepsilon}|}{\partial t}\right| \approx \frac{v}{\omega}|\bar{\varepsilon}|$.

In silicon, stress in excess of the yield stress will result in dislocations on the {111} slip planes in the <110> slip directions. The stresses within the silicon thin films may therefore be projected along the twelve combinations of slip directions on slip planes, for comparison with the yield stress. This analysis was performed in Reference [1] for the case of a silicon substrate (or equivalently a silicon film on a silicon substrate). It was demonstrated that for laser powers such as those considered here (where $T_{max} \sim 1400°C$) defects will form when the laser scan speed is less than ~ 10 mm/sec, corresponding to the fastest demonstrated speeds for direct laser writing.

Similar limiting conditions may be obtained for silicon thin films on sapphire and fused silica. In particular, it may be shown that for silicon on sapphire, the minimum possible scan speed with no defect formation is decreased by approximately a factor of two vis-a-vis that for Si on Si, whereas for silicon on fused silica this minimum is increased by more than a factor of four. Therefore damage is more likely during laser heating of Si films on fused silica and less likely for Si films on sapphire than for laser heating of Si substrates.

Of course, the scan velocities may be decreased without producing damage if the effective laser power is decreased, thereby decreasing T_{max}. Moreover, inclusion of built-in stresses will allow for even greater temperatures and even slower scan speeds with no defect formation, since built-in stresses and stresses due to laser heating have opposite signs, as stated above.

CONCLUSIONS

The stresses and strains induced during laser processing of thin films on substrates have been evaluated in this study. Results indicate that in certain experimental regimes thermoelastic stresses may be large enough to induce material damage. More refined treatment of this problem could include built-in stresses, deviations from isotropic structure and perfect elasticity, temperature-dependent optical and thermal parameters, the relaxation of the ideal thin film assumptions, and a more detailed model of defect formation.

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