

MORPHOLOGICAL AND STRUCTURAL CHANGES IN LASER CVD OF SILICON: COMPARISON OF THEORETICAL TEMPERATURE CALCULATIONS WITH EXPERIMENTAL RESULTS

D. MILNE, J.I.B. WILSON

Department of Physics, Heriot-Watt University, Riccarton, Edinburgh EH14 4AS, Scotland, UK

T.T. RANTALA and J. LENKKERI

Microelectronics and Material Physics Laboratories, University of Oulu, SF-90570 Oulu, Finland

Received 30 May 1989; accepted for publication 29 June 1989

The paper considers to what extent theoretical calculation of the laser induced temperature profile in a substrate can be used to predict the morphology and structure of silicon tracks deposited by pyrolytic LCVD. The micron scale tracks are deposited from silane using a focussed argon ion laser onto a substrate consisting of 1000 Å SiO₂ upon a 300 μm thick, 100 mm diameter, [100] silicon wafer. The influence of various experimental parameters such as scan speed, laser power, gas pressure and gas composition on the temperature profile and on the deposited silicon track is investigated.

Temperature profiles and their time evolution are simulated by numerically solving the heat diffusion equation using a finite difference approach. The track deposition is simulated using experimental temperature and pressure dependent growth rates. Gaussian shaped low laser power track profiles are well reproduced but the volcano like structures of high power deposition are not explained by the present model alone. The calculations are found to explain, at least qualitatively, the observed relationships between various experimental parameters.

1. Introduction

Pyrolytic laser chemical vapour deposition (LCVD) has in recent years attracted much interest for use in the production of microelectronics [1–3] due to its ability to directly deposit high quality material on a variety of substrates with high spatial resolution and high deposition rate. The maskless nature of the process, with its corresponding cost savings, has resulted in the application of pyrolytic LCVD to integrated circuit prototype construction being one of the most important possible future applications. If however this is to occur then the process must be well characterised both experimentally and theoretically for a variety of conditions. Further, for ease of integration into conventional processing, both the precursor materials and the substrates must be commonly used in device construction. An investigation of the pyrolytic LCVD of silicon from silane onto conventional substrates is then of fundamental importance.

2. Experimental

The experimental setup has been described in detail elsewhere [4], but briefly involves moving an absorbing substrate under a focussed argon ion laser beam in a silane atmosphere. The substrate used consists of a 300 μm thick, 100 mm diameter, [100], p-type silicon wafers with a uniform 100 nm coating of thermally grown oxide SiO₂. Substrates of this type are commonly used in conventional microfabrication. The influence on the deposit morphology and structure, of the gas pressure, laser power and scan speed were investigated using scanning electron microscopy (SEM) and scanning profilometry (Sloan Dektak). These results were then compared with those from theoretical calculation.

3. Calculations

The theoretical results are simulations of the time evolution of the stationary temperature dis-

tributions using a straightforward model [5–7]. The simulation is based on the numerical solution of the heat diffusion equation

$$c\rho \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + p, \quad (1)$$

in rectangular coordinates. The procedure is described in ref. [5] in detail, but briefly the model consists of a Gaussian laser beam perpendicular to a substrate with a $1/e$ beam width of 8 or 12 μm . The physical parameters used for glass (SiO_2) and silicon were given in refs. [5,6]. Thus, the absorption coefficient of glass is zero. Interference of laser light in the 0.1 μm glass and its possible enhancement of absorption were not included, giving a constant absorption of $\sim 60\%$, which was slightly dependent on the temperature of the topmost silicon layer. The step length of the numerical grid in the horizontal direction varied from 1 to 4 μm ranging to 28 μm , and in the vertical direction the steps were 0.5, 0.1, 0.4, 0.5, 1, ..., 4 μm ranging to 14 μm , where the boundary conditions were applied. The temperature gradient was assumed to have a $1/r^2$ -behaviour at the boundary.

Compared to the previous calculations [5–7], we have extended the simulations to include the growth of the silicon using the experimental data of Doppelbauer and Bauerle [8] for the temperature and pressure dependent growth rates. However, due to the very different time scales of the evolution of the temperature distribution and track growth, the simultaneous simulation of both was too time consuming, with the stationary temperature distribution being found in a few microseconds, whereas meaningful growth took place in about a millisecond. Therefore, the procedure consisted of sequential short simulation steps of temperature evolution and growth.

Simulations showed that the stationary temperature distribution in the bare SiO_2/Si substrate does not differ much from that of the Si substrate without the glass layer, requiring about 1.5 W to melt the surface for the 8 μm beam width. Simulating the vertical growth rate of silicon through short temperature and growth steps in sequence as described above, revealed that the deposition of silicon on the transparent glass surface greatly enhances the absorption of low incident powers,

which increases the growth rate versus time. At high incident powers, 1.7 W, the calculated thickness is a linear function of the dwell time, because the melting point of silicon will be reached almost instantaneously.

Calculations for stationary temperature profiles have also been made for a $0.5 \times 5 \mu\text{m}^2$ track on the SiO_2/Si substrate. From these it can be concluded that heat conduction along the track has only a small effect in lowering the temperature in the growth region, but instead the increase in power absorption has a stronger effect in raising the surface temperature at the growth region.

4. Results

Typical SEM and corresponding Dektak results are shown in fig. 1. It can be seen that as the power is increased the track profile changes from a flat topped structure to a “volcano” like one. Such a change has been reported by Bäuerle et al. [9] who ascribed the formation of the central depression to surface melting and the resulting difference in surface tension between the hot center and cooler sides causes a parting of the deposit into two peaks. Other authors however have ascribed the formation of such “volcano” structures to: (1) surface melting and subsequent enhanced vaporization at the hotter center [10], (2) gas-phase, diffusion-limited, induced starvation of reactants in the central region vis-a-vis the higher rate of reactant replenishment at the sides of the deposited line [11,12], (3) nonlinearities in the absorption–desorption processes [12], and (4) nucleation effects [13]. The simulations of the silicon growth (see fig. 2) reveal nearly Gaussian thickness profiles for low incident powers and flat topped profiles when the melting point of silicon is reached. To explain the volcano like profiles a more sophisticated model should be used.

Plotted in figs. 3 and 4 is the variation in thickness and width respectively against incident power, where the thickness is taken as the average of the measured minimum and maximum thickness. The results show that both are linear, but limit at high power, probably due to conversion from the kinetic to the diffusion limited region.

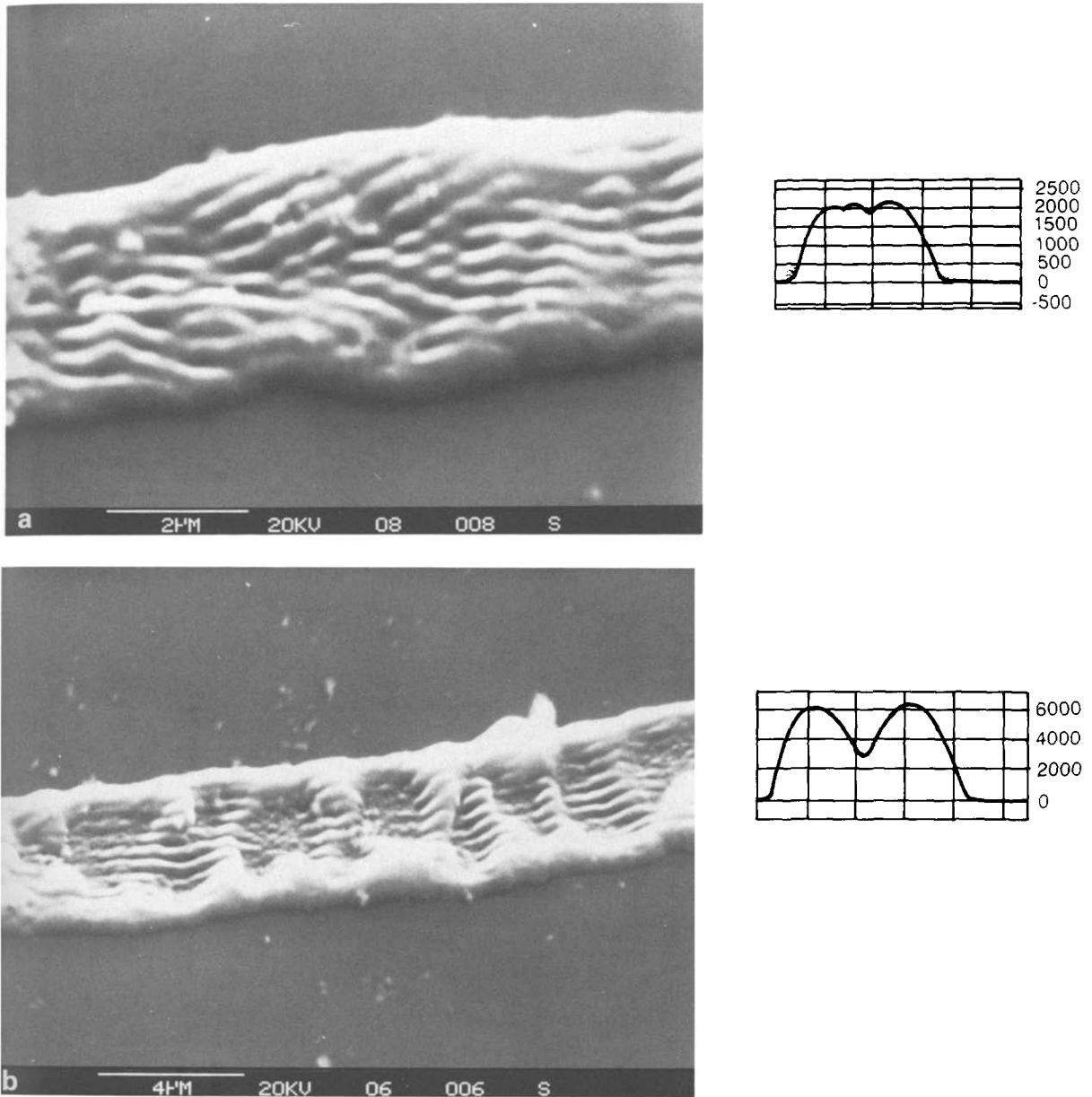


Fig. 1. Change in morphology of deposited tracks with incident power: (a) 1.33 W, (b) 2.13 W. Gas pressure = 200 Torr, scan speed = $200 \mu\text{m s}^{-1}$.

The width is found to be independent of scan speed whilst the thickness varies linearly with the inverse of the scan speed but do not extrapolate to the origin. This may arise from a delay caused by the nucleation, but the calculations of the growth on the glass layer exhibit a very similar effect

although nucleation has not been taken into account. This delay in the theoretical results arises from the fact that a critical thickness of the silicon is required before sufficient absorption occurs to result in an increasing temperature and hence growth rate. However, in reality there is a further

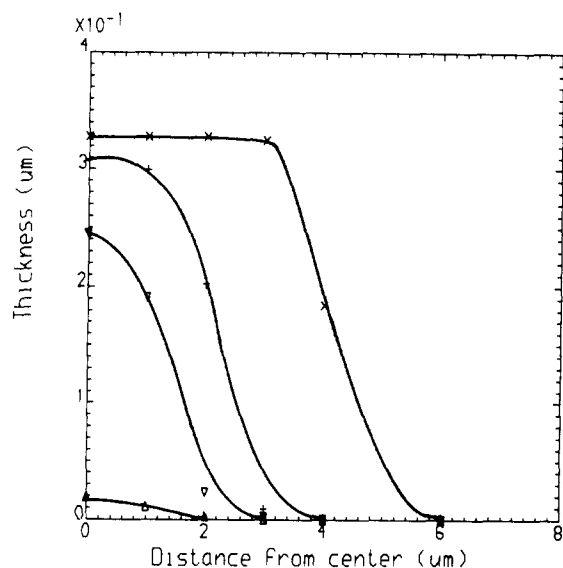


Fig. 2. Theoretical calculations of deposit profiles for various incident powers; (Δ) 1.8 W, (∇) 1.9 W, (+) 2.0 W, ($\times$) 2.5 W. The dwell time is 7.5 ms and the beam width is 12 μm .

delay resulting from nucleation, which causes the experimental tracks to be thinner than predicted. In order to consider this in the model one must combine it with some kind of Monte Carlo simulation of the nucleation phase (e.g. use the simula-

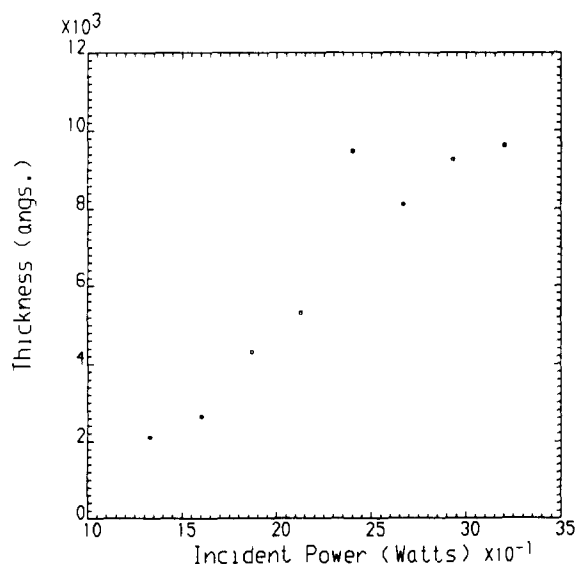


Fig. 3. Variation in thickness versus incident power. Scan speed = 200 $\mu\text{m s}^{-1}$, pressure = 200 Torr.

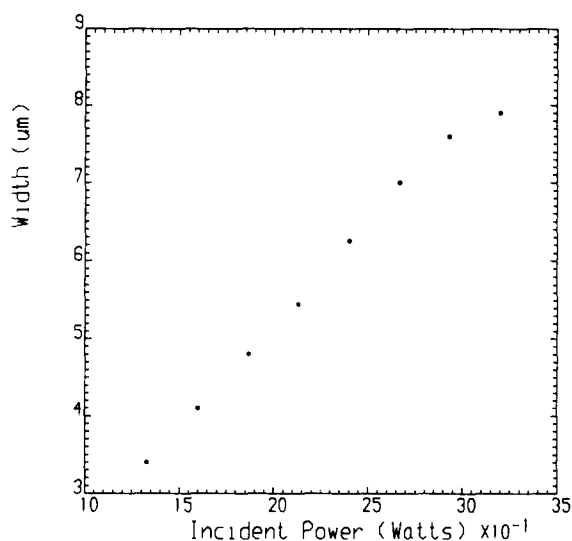


Fig. 4. Variation in width versus laser power. Scan speed = 200 $\mu\text{m s}^{-1}$, pressure 200 Torr.

tion of Kotechi and Herman [13]). This however is complex and beyond the scope of this discussion. The experimental data and theoretical calculations are compared in fig. 5, where an effective step length of 1.4 μm for the laser beam transfer was

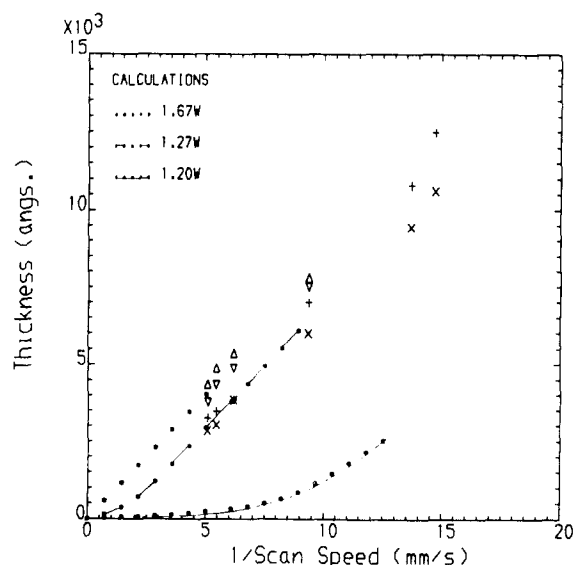


Fig. 5. Variation in thickness versus 1/scan speed, for various incident powers: (Δ) 2.4 W, (∇) 2.0 W, (+) 1.73 W, ($\times$) 1.33 W. Gas pressure = 200 Torr.

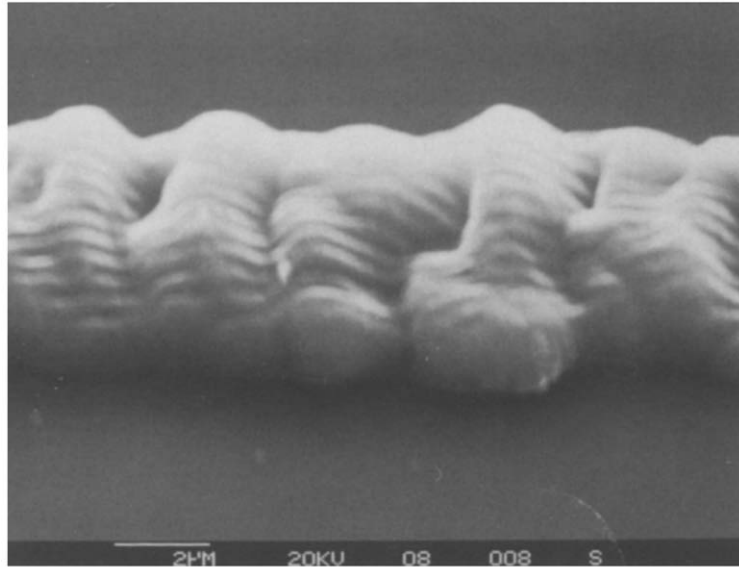


Fig. 6. Silicon track showing periodic superstructure. Incident power = 1.73 W, scan speed = $68 \mu\text{m s}^{-1}$.

assumed in order to match the experimental scan speed and the dwell time used in the calculations.

Interestingly as the scan speed is lowered a periodic superstructure in the deposited material becomes apparent as shown in fig. 6. Structures of this kind are also found if the substrate cleaning procedure is altered from the normal acetone/methanol/Decon/deionised water sequence followed by baking at 100°C for 2 h to one in which the substrate is cleaned using the same sequence but baked for 24 h under flowing dry N_2 . Such structures have been observed by other groups who have explained them by: (1) a periodic exothermic reaction, analogous to that for self-sustained “explosive” recrystallization of amorphous films, whose periodic spacing was independent of scan speed and laser power [14], (2) a periodic variation in the thermal conductance along the deposited track, where the periodic spacing was dependent on the laser power, scan speed and gas pressure [15], or (3) a periodic variation in the surface reflectivity [15,16], where the periodic spacing was power and scan speed dependent. Preliminary results show that in our case the period of the superstructure is power and gas pressure independent, but is dependent on the scan speed. Results also show that tracks showing such struc-

tures have similar relationships for their thickness and width against power and gas pressure. However, in general the tracks are thinner than tracks without such periodic structures, as shown in fig. 7.

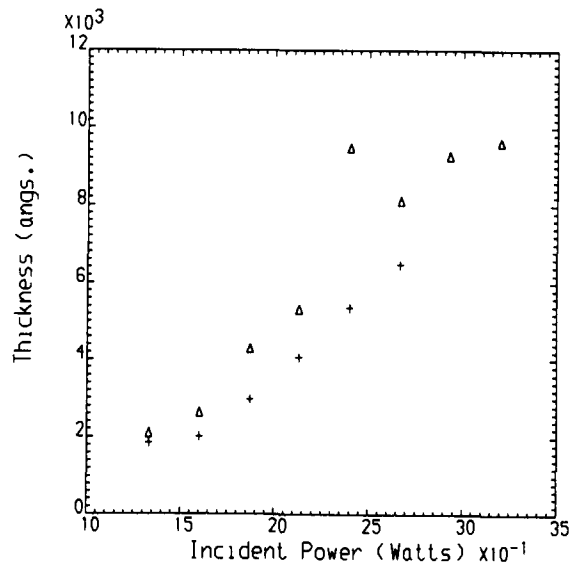


Fig. 7. Variation in thickness versus incident power for tracks with (+) and without (Δ) superstructure.

In light of the calculations the heat conduction along the deposited track does not seem to have influence large enough to cause such variation in the growth temperature that it could lead to the observed periodic superstructure. The temperature distribution in front of the growing track could possibly cause a periodic structure through the temperature dependence of the nucleation rate. If there exists a critical temperature above which the nucleation is slower than at lower temperatures the growth does not easily proceed just in front of the deposited track but rather at some distance where the temperature is initially lower.

5. Conclusions

- Both track thickness and width are linear with power and saturate at high powers.
- Width is independent of scan speed, whilst the thickness is linear with $1/\text{scan speed}$.
- Nucleation is important in determining the morphology of the deposited material, with those tracks deposited on a clean substrate exhibiting a periodic superstructure.
- The spacing of this superstructure is independent of gas pressure and incident power, but does depend on scan speed.
- Simulations at the present sophistication level cannot be used for quantitative analysis or to predict complex track structure, like volcano shape, but they are very helpful in the analysis of experimental results.

Acknowledgements

We would like to thank Dr. Phil John for many useful discussions and Mr. Iain Drummond for building the deposition system. We also acknowl-

edge SERC for its financial support. T.T. Rantala and J. Lenkkeri would like to thank Professor S. Leppävuori for his interest in their work.

References

- [1] D. Bäuerle, *Appl. Phys. B* 46 (1988) 261.
- [2] R.M. Osgood and T.F. Deutsch, *Science* 227 (1985) 709.
- [3] I.P. Herman, in: *Laser Processing and Diagnostics*, Ed. D. Bäuerle (Springer, Berlin, 1984) p. 396.
- [4] D. Milne, A. Black, J.I.B. Wilson and P. John, *Electron. Letters* 24 (1988) 19.
- [5] T.T. Rantala and J. Levoska, *J. Appl. Phys.*, in press.
- [6] J. Levoska, T.T. Rantala and J. Lenkkeri, *Appl. Surface Sci.* 36 (1989) 12.
- [7] J. Lenkkeri, J. Levoska, T.T. Rantala and S. Leppävuori, in: *Laser Assisted Processing*, Eds. L.D. Laude and G. Rauscher (Materials Research Society, Pittsburgh, PA, 1989) p. 65.
- [8] J. Doppelbauer and D. Bäuerle, in: *Interfaces Under Laser Irradiation*, Eds. L.D. Laude, D. Bäuerle and M. Wautelet (Nijhoff, Dordrecht, 1986) p. 277.
- [9] D. Bäuerle, P. Irsigler, G. Leyendecker, H. Noll and D. Wagner, *Appl. Phys. Letters* 40 (1982) 819.
- [10] I.P. Herman, R.A. Hyde, B.M. McWilliams, A.H. Weisberg and L.L. Wood, in: *Laser Diagnostics and Photochemical Processing for Semiconductor Devices*, Eds. R.M. Osgood, S.R.J. Brueck and H.R. Schlossberg (North-Holland, Amsterdam, 1983) p. 9.
- [11] S.D. Allen, *J. Appl. Phys.* 52 (1981) 6501.
- [12] D.C. Skouby and K.F. Jensen, *J. Appl. Phys.* 63 (1988) 198.
- [13] D.E. Kotechi and I.P. Herman, in: *Photon, Beam, and Plasma Stimulated Chemical Processes at Surfaces*, Eds. V.M. Donnelly, I.P. Herman and M. Hirose (Materials Research Society, Pittsburgh, PA, 1987) p. 65.
- [14] R.B. Jackman, J.S. Foord, A.E. Adams and M.L. Lloyd, *J. Appl. Phys.* 59 (1986) 2031.
- [15] Y.C. Du, U. Kempfer, K. Piglmayer and D. Bäuerle, *Appl. Phys. A* 36 (1986) 167.
- [16] Y. Kalafati, I. Reshetnikov and I. Serbinov, in: *Proc. 5th Soviet Union Meeting on Application of Metalorganic Compounds for Producing Non-Organic Films and Materials*, 1987, p. 22 (in Russian).