Thermal Diffusivity of Heavily Doped Low Pressure Chemical Vapor Deposited Polycrystalline Silicon Films

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The thermal diffusivity of heavily doped low-pressure chemical vapor-deposited (LPCVD) polycrystalline silicon films is measured using polycrystalline silicon microbridges. The thermal diffusivity is extracted from the time dependence of the resistance of electrically heated microbridges in a high-vacuum chamber. The resistance decay is measured by heating the microbridge on a half cycle of a square wave and monitoring its resistance change in the other. The diffusivity obtained using this technique is $0.17 \pm 0.01 \text{cm}^2\text{s}^{-1}$, a value consistent with previous measurements of the thermal conductivity.$^{(1,2)}$

1. Introduction

The thermal diffusivity of heavily doped LPCVD polycrystalline silicon films is an important parameter in the design of polycrystalline-silicon-bridge flow sensors,$^{6-6}$ since diffusivity is needed to compute their transient response. We describe an experiment carried out to determine this parameter through the use of electrically heated microbridge resistors. Figure 1 shows the cross section and top view of a polycrystalline-silicon microbridge of the type used in our experiments. Bridges of three different lengths (180, 230, and 280 $\mu$m) made of polycrystalline silicon measuring 1.3 $\mu$m in thickness and 3 $\mu$m in width were elevated 3 $\mu$m above the silicon substrate.
2. Fabrication

The fabrication process for the microbridges starts with 100 mm silicon wafers coated with a 3-layer sandwich made by subsequent depositions of 1 \( \mu \)m-thick LPCVD phosphosilicate glass (PSG), 0.2 \( \mu \)m of undoped glass, and 2.8 \( \mu \)m of PSG. The top PSG layer is patterned and time-etched with 5:1 buffered hydrofluoric acid (BHF) to form a mesa, the middle undoped glass layer acting as an etch barrier. A 1.3 \( \mu \)m-thick layer of in-situ P-doped LPCVD polycrystalline silicon is subsequently deposited at a pressure of 300 mTorr and a temperature of 650\(^\circ\)C with flow rates of SiH\(_4\) and PH\(_3\) of 120 and 1 sccm, respectively. The microbridges are then defined using CCl\(_4\) plasma etch. This is followed by a high-temperature annealing step at 950\(^\circ\)C for 30 minutes which activates the dopants in the polycrystalline silicon. The final resistivity of the annealed samples is 10\(^{-3}\) \( \Omega \)-cm. Conventional aluminum metallization follows, and a time-controlled PSG etch in 5:1 BHF frees the bridge in a technique first described by Howe and Muller.\(^7\) The PSG etch is stopped when the polycrystalline silicon bridge is freed completely. Oxygen-plasma etch then cleans away the aluminum-protecting photoresist and completes the process, which is described more fully in reference 5. Figure 2 shows a SEM photograph of a polycrystalline silicon bridge.
3. Theory

Ohmic dissipation is used to heat the microbridge resistor. If the bridge is heated in high vacuum, we can assume that heat is transported only by conduction through the heavily-doped polycrystalline silicon bridge arms because the thermal radiation and free-molecule air conduction are negligible\(^{(1)}\) even when accounting for the enhanced transfer of energy\(^{(8,9)}\) caused by radiation tunneling through the gap beneath the microbridge. Under this condition, the transient heat-conduction equation in the microbridge using the coordinate system in Fig. 1 is

\[
\frac{\partial^2 u}{\partial x^2} + \delta \xi u = \frac{1}{\alpha_p} \frac{\partial u}{\partial t} - \delta, \tag{1}
\]

where \( u = T(x) - T_o; \) \( T_o \) is the substrate temperature; \( \xi \) is the linear temperature coefficient of resistance; and \( \alpha_p \) is the thermal diffusivity of polycrystalline silicon. The parameter \( \delta \) is the power-generation term

\[
\delta \triangleq \frac{J \rho_o}{\kappa_p}, \tag{2}
\]

where \( J \) is the current density through the microbridge, \( \rho_o \) is the resistivity at temperature \( T_o \), and \( \kappa_p \) is the thermal conductivity of polycrystalline silicon. For long microbridges, the temperature at the supports is essentially \( T_o \); therefore, eq. (1) is solved subject to the boundary and initial conditions:
\[ u(x = 0, t) = u(x = L, t) = 0 \]  
\[ u(x, t = 0) = f(x). \]

For a step in the current density at \( t = 0 \), all coefficients in eq. (1) are constants, and the general solution is

\[ u(x, t) = \frac{1}{\xi} \left( \frac{\cos \sqrt{\delta \xi} (x - L/2)}{\cos \sqrt{\delta \xi} L/2} - 1 \right) + e^{\alpha_p \delta \xi t} \sum_{n=1}^{\infty} B_n \sin \left( \frac{n \pi x}{L} \right) e^{-\alpha_p (n \pi / L)^2 t} \]

\[ = u_{ss}(x) + u_n(x, t), \]

where

\[ B_n = \frac{2}{L} \int_{0}^{L} [f(x) - u_{ss}(x)] \sin \left( \frac{n \pi x}{L} \right) dx. \]

The microbridge resistance is

\[ R_b(t) = R_0 (1 + \xi \bar{u}(t)), \]

where

\[ \bar{u}(t) = \frac{1}{L} \int_{0}^{L} u(x, t) \, dx. \]

Performing the integration in Eq. (7) and substitution in Eq. (6) yields

\[ R_b(t) = R_0 \left[ \frac{\tan (\sqrt{\delta \xi} L/2)}{\sqrt{\delta \xi} L/2} + \sum_{n=1}^{\infty} \frac{(1 - (-1)^n)B_n}{n \pi} e^{-\alpha_p (n \pi / L)^2 - \delta \xi t} \right] \]

\[ = R_0 \left[ A + \sum_{n=1}^{\infty} C_n e^{-\tau_n t} \right], \]

where

\[ \tau_n = \frac{L^2}{\alpha_p n^2 \pi^2 - \delta \xi L^2}. \]

Note that only odd terms are present in the summation. At sufficiently long times, the contribution of the high-order eigenfunctions to the sum become negligible, and \( R_b(t) \) decays with a time constant corresponding to \( \tau_1 \):

\[ R_b(t) \approx A + Be^{-t/\tau_1}, \quad t > \tau_3. \]

If the power generation term \( \delta \) is small compared to \( \pi^2 / L^2 \), then

\[ \tau_1 \approx \frac{L^2}{\alpha_p \pi^2}. \]
Hence, we can extract $\alpha_p$ from measurements of the transient resistance decay.

The circuit of Fig. 3 is used to measure the decay of the microbridge resistance. This circuit is driven by a square wave voltage waveform $V_g$ of period $2\Delta$. In the negative cycle of the input signal, the diodes D1 and D2 are forward biased; hence the full voltage signal is applied to the microbridge, heating it up for a time $\Delta$. In this half cycle, the amplifier stage has a gain of unity. For small changes in $R_b$, the current of the bridge is

$$I_{b_1}(t) = \frac{V_g}{R_b(t)} \approx \frac{V_g}{R_o}. \quad (12)$$

In the positive cycle, diodes D1 and D2 are in reverse bias, hence the bridge current is

$$I_{b_2} = \frac{V_g}{(R_1 + R_b(t))} \approx \frac{V_g}{R_1}, \quad R_1 \gg R_b(t). \quad (13)$$

The resistor $R_1$ is chosen such that the power generation $\dot{\delta}$ is negligible, and eq. (11) applies. Since $I_{b_2} \ll I_{b_1}$, the resistance $R_b(t)$ in this cycle decays to a lower value, and the small voltage across $R_b$ is amplified by the noninverting amplifier stage with gain $G$ set by the feedback resistors $R_2$ and $R_3$. The output voltage of the circuit is

$$V_o(t) = GV_b(t) = I_{b_1(t)}R_b(t)\left(1 + \frac{R_3}{R_2}\right) \approx R_b(t) \frac{V_g}{R_1} \left(1 + \frac{R_3}{R_2}\right) \propto R_b(t). \quad (14)$$

Therefore, $V_o(t)$ has the same time dependence as $R_b(t)$. 

Fig. 3. Circuit used for the thermal diffusivity experiment.
Since the generator signal is periodic, \( R_b(t) \) is a periodic function of time; hence \( u(x, t) \) is also periodic. In order to find the unknown initial temperature \( f(x) \) of eq. (3) and the coefficients \( C_n \) we use the periodicity condition

\[
u(x, t) = u(x, t + 2\Delta).
\] (15)

Because two different currents, \( I_{b1} \) and \( I_{b2} \), both approximately constant over each half cycle, are applied to the microbridge, we solve the differential equation of eq. (1) for the negative and positive cycles of \( V_x \) with \( \delta_1 \) and \( \delta_2 \), respectively. Since the temperature \( u(x, t) \) must be continuous at all times, and using the periodicity condition of eq. (15), it is straightforward to show that if

\[
\frac{\pi^2}{L^2} > \delta_1 \gg \delta_2,
\] (16)

the coefficients \( C_n \) Eq. (8) are

\[
C_n \approx -\frac{4\delta_1 \xi(1 - (-1)^n)}{n^2 \pi^2 \left[n^2 \pi^2 - \delta_1 \xi L^2\right] \left[1 - e^{-\alpha L^2/n^2 - \delta_1 \xi L^2}\right]} \propto \frac{1}{n^4}.
\] (17)

Therefore, the ratio of the first and third components in the summation is

\[
\frac{C_1}{C_3} \approx \frac{1}{81}.
\] (18)

For sufficiently long \( \Delta \), the exponential term in the denominator of Eq. (17) can be neglected, and the ratio of \( C_1 \) to the sum of \( C_n \) is

\[
\sum_{n=1}^{\infty} C_n \approx \frac{8\delta_1 \xi L^2}{\pi^2 (n^2 - \delta_1 \xi L^2)} \left[\frac{\sqrt{\delta_1 \xi L/2}}{\tan\sqrt{\delta_1 \xi L/2} - \sqrt{\delta_1 \xi L/2}}\right],
\] (19)

which for the limit \( \delta_1 \to 0 \) becomes

\[
\lim_{\delta_1 \to 0} \frac{C_1}{\sum_{n=1}^{\infty} C_n} = \frac{96}{\pi^4} = 0.986.
\] (20)

Thus the higher-order terms \( \sum_{n=3}^{\infty} C_n \) only contribute 1.5\% of the total change in \( R_b(t) \).

4. Experiments

All the polycrystalline silicon bridges are first bonded in 64-pin dual-in-line packages (DIPs). The temperature coefficient of resistivity for the polycrystalline silicon, \( \xi \), is found from measurements of the resistance of polycrystalline-silicon resistors constructed on the same substrate as the microbridges as a function of
temperature. The samples were heated up to temperatures of 300°C. Figure 4 shows a linear plot of $\Delta R/R_o$ as a function of temperature. The regressional line has a slope $\xi \approx 1.2 \times 10^{-3} K^{-1}$.

The determination of the diffusivity $\alpha_\phi$ is based upon measurements of the output voltage $V_o$ of the circuit of Fig. 3 during the positive cycle of the input waveform. The measurement is performed with the polycrystalline silicon microbridges in a high-vacuum chamber at a pressure of 2 $\mu$Torr. Initially, the generator voltage $V_g$ is set to zero and gradually increased until a decay in $V_o(t)$ in the positive cycle is observed. The output-voltage waveform is then captured and stored with a Tektronix 7854 digital scope. Measurements of this type were performed for three microbridges 180, 230 and 280 $\mu$m long. The voltage waveform $V_o(t)$ showing the exponential decay in resistance for the 230 $\mu$m microbridge is plotted in Fig. 5.

If the time $\Delta$ is much larger than $\tau_1$, from eqs. (10) and (11) we see that the thermal diffusivity of polycrystalline silicon can be extracted from the slope of a curve of the function

$$F = \frac{L^2}{\pi^2} \ln \left( \frac{V_o(t) - V_o(t_1)}{V_o(t_o) - V_o(t_1)} \right) = -\alpha_\phi (t - t_o), \quad t_o < t < t_1, \quad (t_1 - t_o) < \Delta,$$

(21)
Fig. 5. Output voltage $V_o(t)$ of the circuit of Fig. 3 using a 230 $\mu$m-long microbridge resistor. The exponential decay of the signal is generated by the cooling of the microbridge resistor.

Fig. 6. Plots of Eq. (21) as a function of time for microbridges 180, 230, and 280 $\mu$m long. The slope of the regresional line indicates $\alpha_p = 0.17 \pm 0.01$ cm$^2$s$^{-1}$. 
where \( t_o \) is an arbitrary initial time sufficiently far from the leading edge of the positive waveform to allow for the decay of the high-order terms in the summation of eq. (8). The time \( t_1 \) is chosen such that the resistance \( R_h(t_1) \) is within 0.1% of its steady value. Figure 6 shows plots of \( F \) from eq. (21) as a function of time for three microbridges of different lengths. Note that all data fall on a straight line of slope \(-\alpha_p\), where \( \alpha_p = 0.17 \pm 0.01 \text{ cm}^2\text{s}^{-1} \).

The thermal diffusivity \( \alpha_p \) can be defined in terms of the thermal conductivity \( \kappa_p \), density \( \rho_m \), and heat capacity \( C_p \) by

\[
\alpha_p \triangleq \frac{\kappa_p}{\rho_mC_p}.
\]  

(22)

The density of the film is found by measuring on an analytical balance the weight difference of a wafer with a polycrystalline silicon film of known thickness before and after etching. This measurement gives \( \rho_m = 2.3 \text{ g cm}^{-3} \), the same density as found for single-crystal silicon.

The thermal conductivity of polycrystalline silicon films was measured earlier and found to be approximately 0.3 W cm\(^{-1}\) K\(^{-1}\). Using these two values, we obtain a value of \( C_p \) of 0.77 J g\(^{-1}\) K\(^{-1}\), very close to the bulk silicon value of 0.7 J g\(^{-1}\) K\(^{-1}\). This result supports our experimental finding that, at the temperature of the experiments, \( C_p \) is essentially a function of the atomic density of the film which is unchanged by the presence of the grain boundaries.

5. Conclusions

The thermal diffusivity of heavily doped LPCVD polycrystalline silicon films has been found from measurements of the transient decay in the resistance of electrically heated microbridge resistors under high vacuum. The measured value of \( \alpha_p \) is \( 0.17 \pm 0.01 \text{ cm}^2\text{s}^{-1} \), which agrees well with measurements of film density and earlier measurements of the thermal conductivity of heavily doped polycrystalline silicon films.

References