THERMAL STABILITY OF UNDOPED POLYSILICON LAYERS

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Abstract
The grain size of as-deposited and annealed polysilicon layers has been investigated by scanning electron microscopy. Intentionally undoped layers were prepared by low pressure chemical vapor deposition (LPCVD) at temperature of 640 °C. Primary recrystallization of the layers has been observed during annealing at temperatures in range from 900 °C to 1150 °C. The activation energy of the silicon self interstitials diffusion along the grain boundaries was calculated as 2.2 eV. The difference in the grain-growth process was observed for the undoped layers grown either on (i) lightly boron doped substrate or (ii) on the substrate heavily doped with antimony.

Introduction and experimental

Grain boundaries in the polysilicon layer are energetically favorable sites for the metal impurities and act as metal traps. Hence, the gettering ability of the polysilicon strongly depends on the size of the grains. The thermal cycles during subsequent steps of a device fabrication induce the recrystallization of the layer.

The silicon wafers were sliced from two Czochralski-grown ingots, one lightly doped with boron ($7 \cdot 10^{13}$ atoms/cm^3) and another heavily doped with antimony ($5 \cdot 10^{19}$ atoms/cm^3). The 150 mm wafers have the crystallographic orientation (100) and thickness 525 µm. The polysilicon layers were grown using the LPCVD technique. The layers thickness was 1.1 µm. The wafers were annealed under the ambient atmosphere for 0.5 hr at temperatures from 650 °C to 1150 °C. The non-annealed wafers were used as the reference samples. Layers cross-sections were studied using a Scanning Electron Microscope (SEM) with an electron beam acceleration voltage of 10 kV.

Results and discussion

It was shown that while the boron (p-type) doping has a negligible effect on the recrystallization process, the presence of the n-type dopant in the layer enhances the recrystallization process [1]. Wada and Nishimatsu [2] reported the primary recrystallization of the polysilicon layers proceeds via the grain boundary-induced growth. The elementary process behind the primary recrystallization is the diffusion of silicon self-interstitials along the grain boundary region. In this case, the grain size d increases as the square-root of the annealing time t [1] following the equation:

$$d^2 = d_0^2 + \frac{2ab^2\lambda D_1\gamma}{k_B T} \cdot \exp\left(\frac{-\Delta G}{k_B T}\right) \cdot t\,, \qquad (1)$$

where d_0 is the initial grain size, a is the geometric factor, b is the lattice constant, λ is the grain boundary energy, k_B is the Boltzmann constant, T is the annealing temperature, D_1 is the diffusivity of silicon self interstitials in bulk, ΔG is the difference in the diffusion activation energy between the grain boundary and bulk and γ is the constant equal to $1.0 \cdot 10^{-11}$ [1].

The grain size was estimated from SEM images. The dependences of the grain size on the annealing temperature are shown in Fig. 1. The grain size does not change significantly for annealing temperatures up to 900 °C for both layers deposited on (i) the lightly boron doped substrates and (ii) the heavily antimony doped substrates. The primary recrystallization was observed between annealing at 900 °C and 1150 °C. At 1050 °C and above the grain size is significantly higher for the layers deposited on the heavily antimony doped substrates. We attribute this to the enhancement of the grain growth by the antimony dopant diffused from the substrate into the layer. At temperatures above 1000 °C the time necessary for the dopant diffusion through the whole polycrystalline layer is much shorter than the annealing time and layer behaves as the doped layer during the recrystallization.

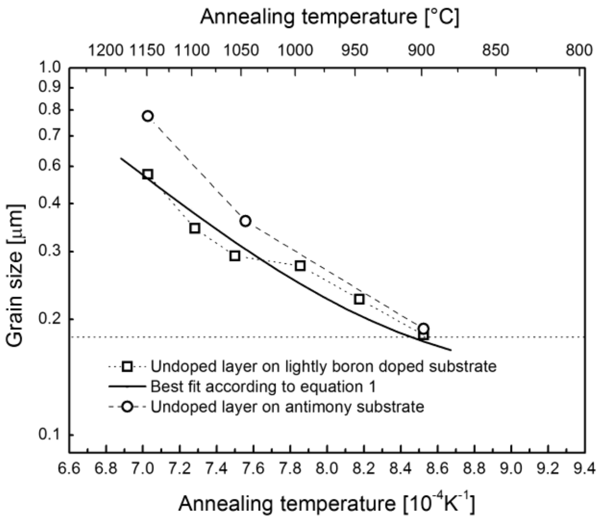

Fig. 1 The grain size of layers annealed for 0.5 hr at various temperatures. The dashed lines are to guide the eye only. The grain size measured on the reference sample and after annealing at 650 °C does not differ significantly from the size measured at 900 °C. This fact is represented by the horizontal dotted line.

The measured grain sizes for the undoped layer on the lightly boron doped substrate (open squares) and their best fit according to equation 1 (solid line) are plotted in Fig. 1. The ΔG value obtained from this simulation is 1.7 eV. The uncertainty in ΔG determination estimated from the variance of the measured grain size is approximately ± 0.2 eV. The activation energy of diffusion along the grain boundaries calculated from the ΔG value is approximately 2.2 eV. To get this, we used the value of the activation energy for the silicon atoms self-diffusion in silicon bulk as 3.9 eV [3].

Conclusions

Our results demonstrate that the undoped polysilicon films show negligible changes in the structure and the grain size after the annealing at temperatures below 900 °C. The primary recrystallization was observed between annealing at 900 °C and 1150 °C.

The activation energy of the silicon self interstitials diffusion along the grain boundaries was calculated to be approximately 2.2 eV. The different grain-growth mechanism was found to be a consequence of antimony diffusion into the polysilicon layer.

References

1. L. Mei, M. Rivier, Y. Kwark, and R. W. Dutton, J. Electrochem. Soc. 129 (1982) 1791.
2. Y. Wada, S. Nishimatsu, J. Electrochem. Soc. 125 (1978) 1499.
3. S. W. Jones, Diffusion in Silicon, ICKnowledge LCC, Georgetown, MA, 2006.