(4B-4)

Theoretical Model to Explain Dopant Segregation to the Grain Boundaries and Grain Growth

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1) Introduction

Because of the wide application of polycrystalline silicon in integral circuit technology, poly-silicon properties have been the focus of increasing attention by many researchers. Dopant segregation to the grain boundaries and grain growth phenomena are especially important properties of polycrystalline silicon. But up to this time, these two properties have been investigated separately [1), 2)]. In this paper, a theoretical model is proposed to systematically explain both of these two properties.

2) Experiment [2)]

Polycrystalline-silicon films were deposited to a thickness of approximately 0.2μm onto 0.2μm oxidation films. Arsenic and phosphorus atoms with 1×10^{16} cm^{-2} dose were ion implanted into the films at an energy of 180keV and 90keV, respectively. All films were then annealed at 1000℃ for 20min, and some were subsequently further annealed at 800, 850, or 900℃ for 20min, respectively. Hall measurements were used to estimate the number of active dopant atoms within the grains, and the number of atoms segregated at grain boundaries as a function of annealing temperature. After 1000℃ annealing for 20min, the grain sizes increased to approximately 0.26μm for phosphorus doped polycrystalline silicon and 0.59μm for arsenic doped polycrystalline silicon.

3) Theory

3-1) Theoretical model to explain dopant segregation

The phenomena of surface or interface segregation in a multicomponent has been described by equalizing the chemical potential of surface atoms and bulk atoms. Mandurah [2)] developed a theoretical model to explain the segregation phenomena of polycrystalline silicon by considering the number of lattice sites on both bulk and grain boundaries. The number of lattice sites is an obscure parameter especially on the grain boundaries. Assuming that the density of silicon atoms is equal on both bulk and grain boundaries, the chemical potential can be formulated differently with Mandurah's work, and we obtain

$$C_p^s=(C_pC_{Si}^sK)/(C_{Si}^b+C_{Si}^sK), \qquad (1)$$

where $K=\exp(Q/RT)$, C_p is dopant concentration per unit volume, C_p^s is dopant concentration on grain boundaries per unit volume, C_{Si}^s is silicon atom concentration on bulk per unit volume, C_{Si}^b is silicon atom concentration on grain boundaries per unit volume, Q is heat of segregation, R is Boltzman constant, and T is temperature. In Eq. (1), there are no obscure parameters. The heat of segregation of arsenic and phosphorus in polycrystalline silicon calculated using Eq. (1) is 14kcal/mol and 10kcal/mol, respectively. Fig. 1 is a plot of carrier concentration as a function of final annealing temperature.

3-2) Calculation of surface free energy

We assume a surface strain, which becomes larger with increasing atoms segregated at grain boundaries, causes the grain growth. By using Eq. (1), the surface free energy is defined as

$$G=-RTC_p^s\ln(C_p^b/C_p^s) . \qquad (2)$$

The grains grow to the size where the surface free energy becomes minimum. Result of computation by Eq. (2) is shown in Fig. 2 , which is a plot of the surface free energy as a function of the grain size. The result shown in Fig. 2 is in a good agreement with the tendency of the experimental results.The grains of boron doped polycrystalline silicon do not grow because there is no dopant segregation.

4) Conclusion

A theoretical model has been proposed to explain both dopant segregation to the grain boundaries and grain growth phenomena systematically. Comparing the theoretical calculation with the experimental results, we

confirmed that the surface strain, which becomes larger with increasing atoms segregated at grain boundaries, causes the grain growth.

Reference

1) Y. Wada et al. , J. Electrochem. Soc.,125, 1499 (1978). 2) M.M.Mandurah et al. , J. Appl. Phys. , 51, 5755 (1980).

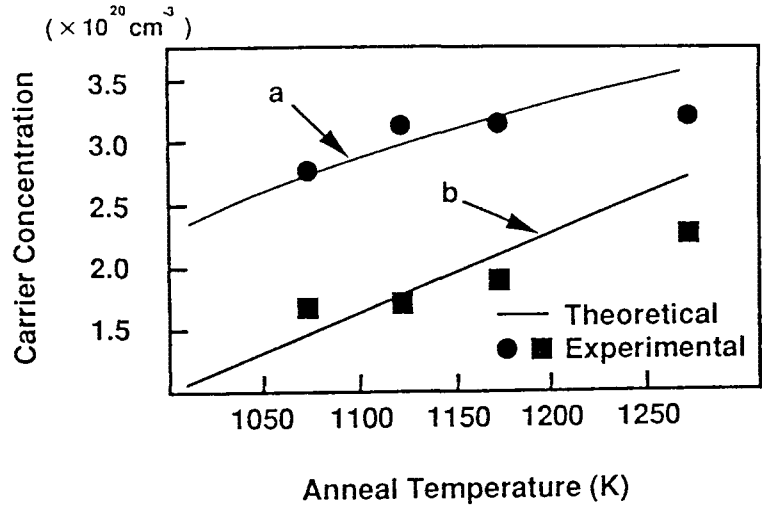

Fig. 1. Carrier concentration in the polycrystalline-silicon films as a function of post annealing temperature. The experimental data is plotted with theoretical curve.

a. Heat of segregation is 10kcal/mol for theoretical calculation of phosphorus doped poly-silicon.

b. Heat of segregation is 14kcal/mol for theoretical calculation of arsenic doped poly-silicon.

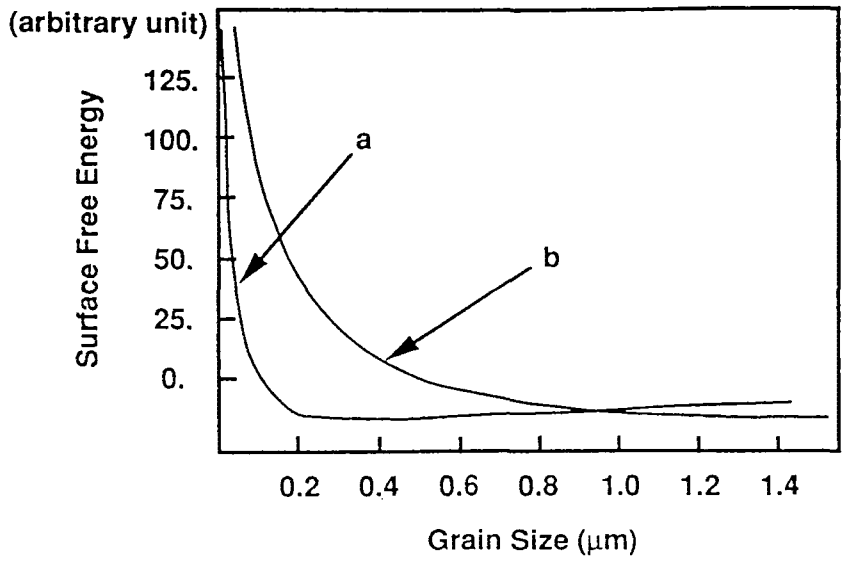

Fig. 2. Theoretical calculation of surface free energy.The grain growth stops at the grain size where surface free energy becomes minimum.

a. Heat of segregation is 10kcal/mol for theoretical calculation of phosphorus doped poly-silicon.

b. Heat of segregation is 14kcal/mol for theoretical calculation of arsenic doped poly-silicon.

Experimental grain-size is 0.26μm for phosphorus doped poly-silicon, and 0.59μm for arsenic doped poly-silicon after 1000℃ annealing for 20min.