THE EFFECT OF ANNEALING ON THE CHARACTERIZATIONS OF THE GRAIN-BOUNDARY OF SILICON FILMS

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Motivation

Silicon films are the subject of intense fundamental and applied research, due to their wide use in modern microelectronics and solar power. It is known that the structure of silicon films determines their electrophysical, optical, and other properties, which is important in terms of their practical application in microelectronics, solar energy, spintronics. The important element of the film structure is grain boundaries. The characteristics of grain boundaries are determined by film formation conditions and subsequent treatments, in particular, annealing.

In this paper, we analyzed the types of grain boundaries and grain boundaries joints, and estimated the relative energy of grain boundaries in phosphorus-doped silicon films depending on the temperature and annealing time.

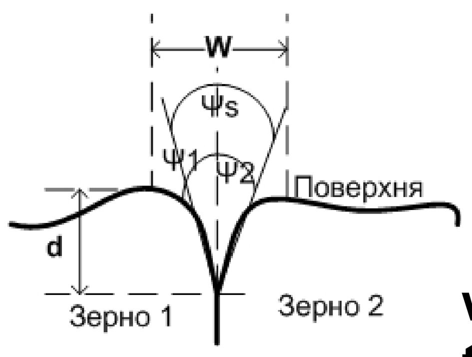
Experimental

Silicon films were prepared by low-pressure chemical vapour deposition on thermally oxidized (100 nm oxide thickness) (100) Si wafers. The deposition temperature was equal to 630^{0}C. The film thickness was 500 nm. Samples were doped with phosphorus (10^{21} cm^{-3}). Films were annealed for 30 min and 3 hours in a nitrogen atmosphere at a temperature ranging from 950^{0}C to 1200^{0}C.

The most common way to experimentally probe relative grain-boundary energies is to measure the geometry of the grooves that form where the boundaries intersect a free surface. Under the assumption of full surface isotropy, the condition for mechanical equilibrium of the triple line is:

$$\gamma_{rel} = \gamma_b/\gamma_s = 2\cos(\Psi_S/2),$$

$$\Psi_S = \Psi_1 + \Psi_2$$



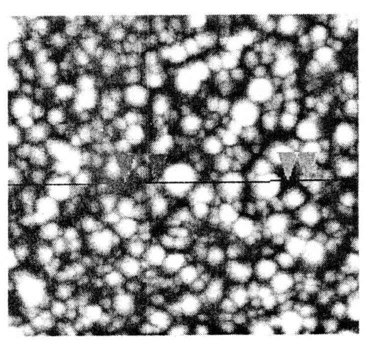
where Ψ_S is the dihedral angle at the triple line, γ_s and γ_b are the surface energy and the relative dimensionless grain boundary energy, respectively. The complete methodology of extracting the values of γ_{rel} from the AFM data was detailed in [1].

The microstructure of polysilicon films was characterized by transmission electron microscope (TEM).

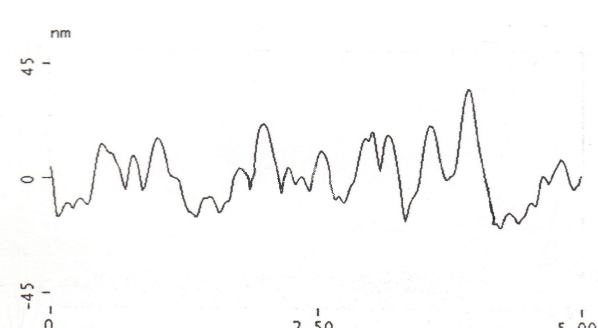
The type of grain boundary (special or general type) was determined by the misorientation angle between the grains. The orientation ratios between the grains were determined by electron diffraction and also by measuring the angle between <112> directions of the microtwins in the grains.

Results

Relative grain-boundary energy measurements



a



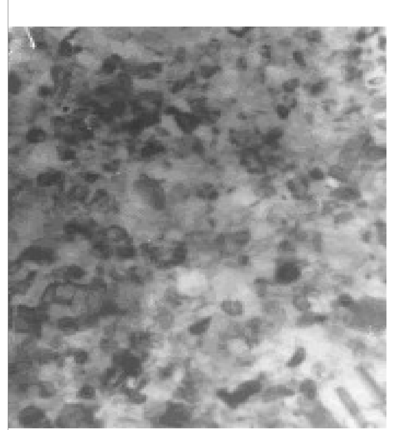
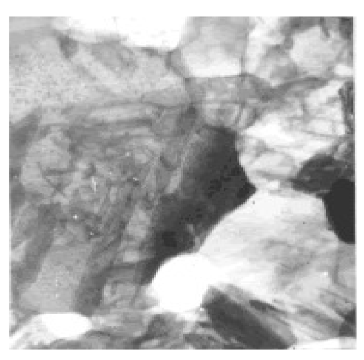
b

Typical AFM image of a silicon film surface (line corresponds to scan line) (a) and AFM-scan (b)

The average values of dihedral angles and relative grain boundary energy

Annealing temperature, ^{0}C	Annealing time, min	Ψ_s, degree	γ_b/γ_s
As deposited	-	176,55	0,60
900	30	154,37	0,44
1150	30	162,31	0,43
1150	180	164,40	0,271

Processes in films during annealing

Grain growth	Changes in grain growth mechanisms from coalescence to grain boundary migration [2]	Grain boundaries faceting
 	 	 100 nm ---------

Analysis of experimentally obtained grain boundary misorientation distribution showed that amount of special boundaries (Σ=3, 9, 11, 27) increases with increasing annealing temperature from 1040 to1200^{0}C. It is suggested that the difference in grain boundary misorientation distribution for variable annealing temperature is caused by different grain growth mechanisms for differ temperatures: coalescence and migration of boundaries.

Conclusion

Thus, upon annealing, a rearrangement of the grain-boundary structure of silicon films occurs, at which the number of special grain boundaries and joints of grain boundaries increases and the value of the relative grain-boundary energy decreases.

A decrease in the relative grain boundary energy is due to such processes as grain growth, an increase in the number of special grain boundaries, and faceting of grain boundaries.

References

1. Y.Amouyal, E. Rabkin, Acta Materialia, vol. 55, pp. 6681- 6689, 2007.
2. N.G. Nakhodkin and T.V. Rodionova, Phys. Status Solidi A,. vol. 123, № 2, pp. 431-439, 1991.

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