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Abstract

EFFECT OF THE UNDOPED SILICON FILMS THICKNESS ON THE RELATIVE GRAIN-BOUNDARY ENERGY
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The relative grain-boundary energy of undoped silicon films with equiaxed and fibrous structure depending on film thickness was determined by the method of grain boundary grooves with the use of atomic force microscopy. It was shown that undoped films with equiaxial structure possess the lowest relative grain-boundary energy; the largest relative energy was observed in fibrous structure. It can be assumed that this is due to the different nature of the grain boundaries in these structural modifications.

Silicon films are the subject of intense fundamental and applied research, due to their wide use in modern microelectronics and solar power. As is known [1], the characteristics of the electronic devices that used silicon films are directly connected with the structural properties of the films, in particular, their grain boundary and grain boundary joints. The stability of the properties of the grain boundaries strongly affects the stability of the element containing silicon films. The most direct indicator of the degree of non-equilibrium is grain-boundary energy [2,3]. The lower it is, the more equilibrium and, therefore, stable is the structure.

The aim of this work is to estimate the relative grain-boundary energy in undoped silicon films in a wide range of thicknesses with be means of atomic force microscopy (AFM).

Nanosilicon films were prepared by low-pressure chemical vapor deposition from a silane/argon mixture. Films were deposited on thermally oxidized (100 nm oxide thickness)(100) single-crystal silicon wafers. The deposition temperature was equal to 6300C. The film thickness was ranged from 10 to 2200 nm.

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:

$\gamma rel = \gamma b/\gamma s = 2\cos(\Psi/2)$,

where Ψ is the dihedral angle at the triple line, γs and γb are the surfase energy and grain boundary energy, respectively. γrel is the relative dimensionless grain boundary energy. The measurement of grain boundaries dihedral angles were performed by AFM. The complete methodology of extracting the values of γrel from the AFM data was detailed in [3]. Since the groove sides have a different inclination, the two-corner angle was defined as the sum of two angles and which were measured separately:

The advantage of ASM research is the ability to receive and process a large amount of data.

Fig. 1. Schematic geometry of the grain boundary groove

It has been shown (Table 1) that as the average values of dihedral angles and relative grain boundary energy of undoped nanosilicon films strongly depend on film thickness. At thicknesses of 85 nm, a sharp increasing of relative grain boundary energy is observed. This behavior correlates with changing of film structure from equiaxial to fibrous (at thickness ≥ 70 nm) and appearance of preferred orientation [110] [4].

Table 1.

Film thickness, nm
ΨS, degree
γb/γs
10
148,22
0,54
50
155,63
0,40
85
71,64
1,62
100
169,08
1,18
1500
141,53
0,66
2200
116,56
1,06

Analysis of the data showed that the largest dihedral angle and the lowest relative grain-boundary energy are observed for undoped silicon films with a equiaxed structure. This is due to the presence in such films of a large number of high-angle grain boundaries with low stresses. The small relative grain boundary energy for films with a thickness of 100 nm is due to the predominance in these films of twin boundaries of the first order with very low energy. In thicker films with a fibrous structure multiple twin boundaries and low-angle grain boundaries predominate. Such boundaries contain dislocations with high stress fields. This leads to an increase in the relative grain boundary energy.

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