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Faceting of twin tips in polysilicon films

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ABSTRACT

The faceting of tips of twin plates in the interior of grains under annealing in phosphorus-doped polysilicon films, produced by low-pressure chemical vapor deposition, has been investigated by transmission electron microscopy. It has been shown that the facet types and number of facets depend on the annealing temperature. The stability diagram for the different facet types has been constructed. Three kinds of faceting transitions that take place on the twin tips have been studied. The transformation of curved grain boundary into a grain boundary facet with increasing temperature has been observed for the first time.

1. Introduction

Polysilicon films are widely used in integrated circuit technology, as a material for solar cells [1,2], and other applications. In terms of reliability and stability of electrical and optical parameters of the films, it is important to study their defect structures, in particular, the internal interfaces (grain boundaries (GB) and twin boundaries in the interior of grains), because their structure determines the structure-sensitive properties of the films [3–8]. It is therefore of particular interest to study grain boundary transformation in films, including twin boundaries inside the grains.

Under post-deposition annealing of polysilicon films in parallel with grain growth, grain boundary structure changes take place, with the resulting formation of GB facets. As is known [9], faceted GB have a low trap density for charge carriers. Thus, the presence of the faceted GB is favorable for polycrystalline electronic devices, such as thin transistors and solar cells.

For silicon, as well as for other materials with low stacking fault energy is typical of the large number of twin boundaries. Studies have shown that there are two types of twin boundaries in polysilicon films: 1—twin misorientation between adjacent grains that is a result of grain growth and 2—twin plates in the interior of grains [10].

Faceting of twin GB in polysilicon films was considered in [11] in detail. At the same time, faceting of tips of twin plates has not been investigated until now. However, their study is of interest because the nature of the defect structure of the grains determines the uniform distribution of doping impurities in the film and creates effective ways to charge carrier transport [3–8].

In this work, the facet transitions of twin tips inside grains of phosphorus-doped polysilicon film under annealing have been investigated by transmission electron microscopy (TEM).

2. Experimental procedure

Polysilicon 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 630 °C. The film thickness was 500 nm. Samples were doped with phosphorus. Doping concentration was 10^{21} cm^{-3}. Polysilicon films were annealed for 30 min in a nitrogen atmosphere at a temperature ranging from 950 °C to 1200 °C. Annealing temperature range was chosen on the basis of previous investigations [10,12].

Experimental measurements were performed by means of TEM combined with electron diffraction. Specimens were prepared by chemical etching.

3. Results and discussion

TEM studies show (Fig. 1) that twin plates are observed in the interior of grains in polysilicon films over all the temperature

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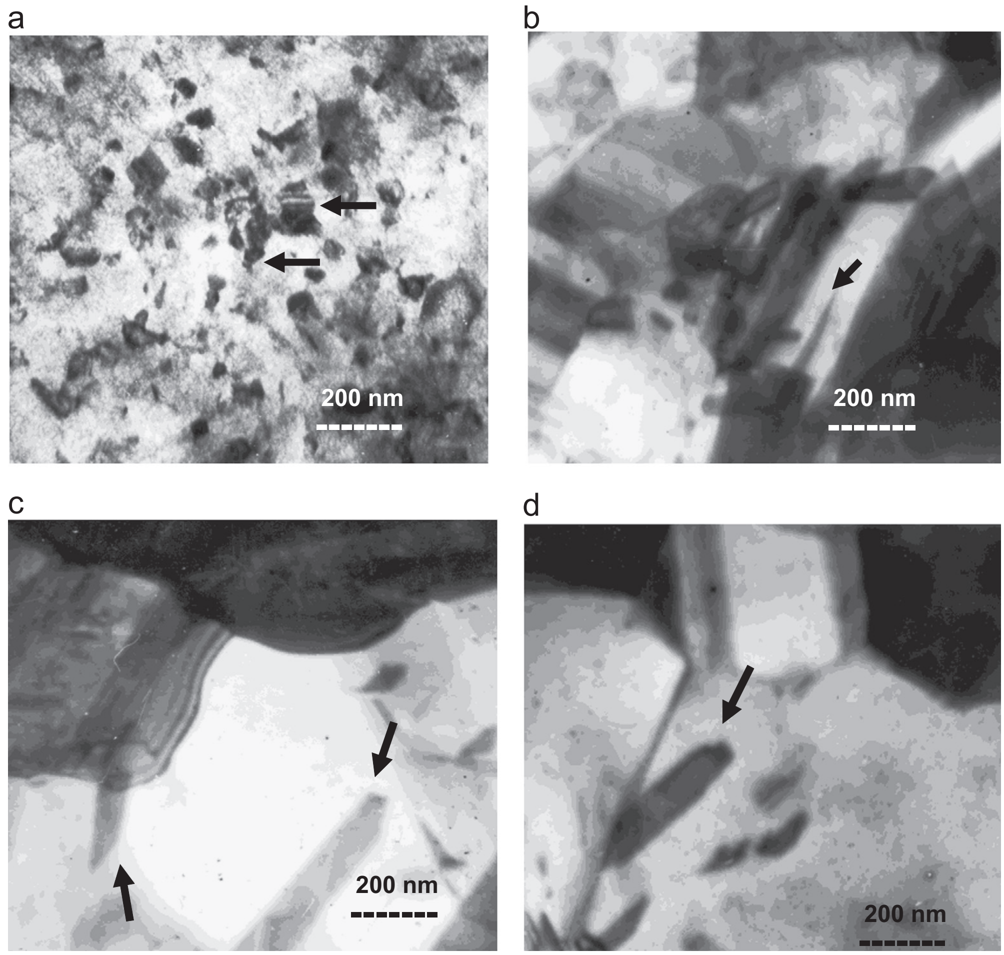

Fig. 1. TEM images of as-deposited (a) and annealed (b), (c), and (d) polysilicon films. Arrows indicate faceted GB (a) and faceted twin tips inside grains (b), (c), and (d). Annealing temperatures 1120 °C (b), and (c) and 1150 °C (d).

range from 630 °C (deposition temperature) to 1200 °C. At temperatures from 630 °C to ≅1120 °C twin plates are extended over all the grains from boundary to boundary (Fig. 1a). Twins, ending inside the grains, are absent. It can be assumed that this film structure is caused by multiple twinning under film formation. At the same time, as Fig. 1b–d shows, at higher annealing temperatures (≥1120 °C) there are many twin plates that are ending inside grains. This is called annealing twins, forming during the grain boundary migration, which is the mechanism that determines the grain growth at these temperatures [10,12].

TEM analysis shows (Fig. 1) that twin plates inside of grains in polysilicon films are perpendicular to the film surface and have a uniform width along the full length. The parallel elongated sides of the twin plates are formed by the coherent symmetric twin GB (STGB) $\{111\}_1/\{111\}_2$ (the subscripts 1 and 2 correspond to the grain 1 and twin plate 2, respectively). This crystallographic relation corresponds to the $(100)_{CSL}$ plane in the coincidence site lattice (CSL) and is denoted by $\Sigma=3$ (Σ is the inverse density of coincidence sites). It is the most closely packed CSL boundary. The energy of symmetric twin boundary is very low [13–15].

The width of the twin plates varies widely, from 25 nm to 200 nm. Twins of small in width are observed at all annealing temperatures. At the same time, a maximal value of twin width increases with increasing temperature. Thus, twins of width up to 200 nm are observed at temperature 1200 °C. STGB are stable at all annealing temperatures. As for tip of the twin plates, their morphology and orientation modify considerably at different annealing temperatures.

TEM studies show that several main types of facets are observed, which differ by their orientation with respect to STGB. Furthermore, the twin tip may contain one or more flat facets.

The micrographs and corresponding schematic drawing in Fig. 2 show the shape of twin tips that contain one flat facet with various angles between STGB and facets. Fig. 2a shows the shape of the twin tips with one flat facet that has an angle of 26° with STGB. Facet orientation corresponds to crystallographic relation $\{522\}_1/\{144\}_2$ or $(130)_{CSL}$ [10]. These facets are observed inside grains of polysilicon films at 1120 °C. Similar facets were observed in [13,14,16] in copper. The next facet type is shown in Fig. 2b. Facet has orientation $\{511\}_1/\{111\}_2$ or $(120)_{CSL}$ and an angle of 35° with STGB and is observed at annealing temperature 1120 °C. The presence of such facets is well documented for Cu [13,14,16] and at low temperatures for Al [17,18]. In the temperature range from 1120 °C to 1200 °C the facets with orientation $\{100\}_1/\{112\}_2$ (or $(110)_{CSL}$) are observed (Fig. 2c). These facets have an angle of approximately 54° with STGB. Similar facets were observed in Cu [13,14,16] and Al [18]. In the polysilicon films, as well as in Al, facets $(110)_{CSL}$ are observed in a wide range of annealing temperatures, in contrast to Cu [13].

TEM-images of twin tips with two facets (facet 1 and facet 2) and corresponding schematic drawing are presented in Fig. 3. Fig. 3a and b shows twin tip in which facet 1 has an angle of 70° with the STGB and facet 2 has an angle of 26° with the STGB. The facet orientations are $\{411\}_1/\{012\}_2$ (or $(210)_{CSL}$) and $\{522\}_1/\{144\}_2$ (or $(130)_{CSL}$), correspondingly. The angle between facets is 90°. In the polysilicon films similar facets are observed at annealing