Effect of twinning on the grain shape of crystallized amorphous Si0.7Ge0.3 thin films on SiO2

Hong Seung Kim and Jeong Yong Lee

Citation: Appl. Phys. Lett. **73**, 2739 (1998); doi: 10.1063/1.122575
View online: http://dx.doi.org/10.1063/1.122575
View Table of Contents: http://apl.aip.org/resource/1/APPLAB/v73/i19
Published by the American Institute of Physics.

Effect of twinning on the grain shape of crystallized amorphous $Si_{0.7}Ge_{0.3}$ thin films on SiO_2

Hong Seung Kim and Jeong Yong Lee
Department of Materials Science and Engineering, KAIST, Taejeon 305-701, Korea

(Received 27 April 1998; accepted for publication 11 September 1998)

The grain morphology of $Si_{0.7}Ge_{0.3}$ depends on the number of the primary noncoplanar twin variants formed at the early stage of solid-phase crystallization. The grain with major twin bands of a single twin variant parallel to a {111} plane develops an elongated shape, owing to the preferential growth in a ⟨112⟩ direction along twins. When the grain has major twin bands of two or more noncoplanar twin variants, the growth front between noncoplanar twin bands develops as fast as the ⟨112⟩ direction along twins propagates, because such a growth front is formed from a {111} ledge. As results, the grain becomes more or less equiaxed due to the increasing number of primary, noncoplanar twin variants. © *1998 American Institute of Physics.* [S0003-6951(98)02945-3]

Recently, polycrystalline $Si_{1-x}Ge_x$ (poly-$Si_{1-x}Ge_x$) alloy materials have become attractive for thin film transistors (TFTs). Since the melting point of $Si_{1-x}Ge_x$ is lower than that of Si, physical phenomena controlling fabrication processes such as deposition, crystallization, grain growth, and dopant activation occur at lower temperatures for $Si_{1-x}Ge_x$ than for Si.[1–4] While some poly-$Si_{1-x}Ge_x$ thin film studies have been performed, the fundamental growth mechanism at the stage of solid-phase crystallization have been scarcely investigated. The $Si_{1-x}Ge_x$ grains formed by solid-phase crystallization were internally twinned.[3,4] In our experiments, the twinning events that occurred in the early stages of solid-phase crystallization were related to the grain shape in the solid-phase crystallized amorphous $Si_{0.7}Ge_{0.3}$ films.

In this work, transmission electron microscopy was used to characterize the various grain shapes during the solid-phase crystallization of amorphous $Si_{0.7}Ge_{0.3}$ alloy films. The results show that the number of primary noncoplanar twin variants formed at the early stage of solid-phase crystallization is crucial for the grain shape. A schematic model, explaining the grain shape change upon increasing the number of the primary noncoplanar twin variants is proposed.

A Riber SIVA45 solid source molecular beam epitaxy (MBE) system with a base pressure in the 1×10^{-10} Torr was used to deposit amorphous $Si_{0.7}Ge_{0.3}$ films on thermally oxidized Si⟨100⟩ wafers at 300 °C. The deposition rate was 0.1 nm/s and the thickness of films was 50 nm. The Ge mole fraction was measured by Rutherford backscattering spectroscopy (RBS). The amorphous $Si_{0.7}Ge_{0.3}$ films were annealed at 550 °C in a dry N_2 ambient. Transmission electron microscope specimens were prepared by the lift-off process,[5] in which a sandwiched SiO_2 layer was etched with HF:H_2O = 1:1 solution. Bright field transmission electron micrographs and selected area electron diffraction patterns were obtained by a JEOL JEM2000EX, operated at 200 kV.

Figure 1(a) is a bright field transmission electron micrograph that shows a grain in the $Si_{0.7}Ge_{0.3}$ thin film annealed at 550 °C in a dry N_2 ambient for 4 h and Fig. 1(b) is a selected area electron diffraction pattern obtained from the grain in Fig. 1(a). The grain has a typical elongated shape. According to the method proposed by Hatalis and Greve,[6] the grain size is about 150 nm. Bright and dark stripes which are exhibited by the narrow twin platelets[7] parallel to the long axis of the elongated grain are observed in the central region of the grain. Indexing of the pattern shows that spots indicated by arrows were diffracted from the (200), (111), (111), and (422) lattice planes, respectively. These lattice planes have the zone axis of the [011] direction. The continuous streaks, indicated by an arrow along a ⟨111⟩ direction are seen in the diffraction pattern and normal to twin bands of the grain in Fig. 1(a). Comparing the diffraction pattern with the grain shows that the direction where the grain grows preferentially corresponds to the ⟨211⟩ direction along twin

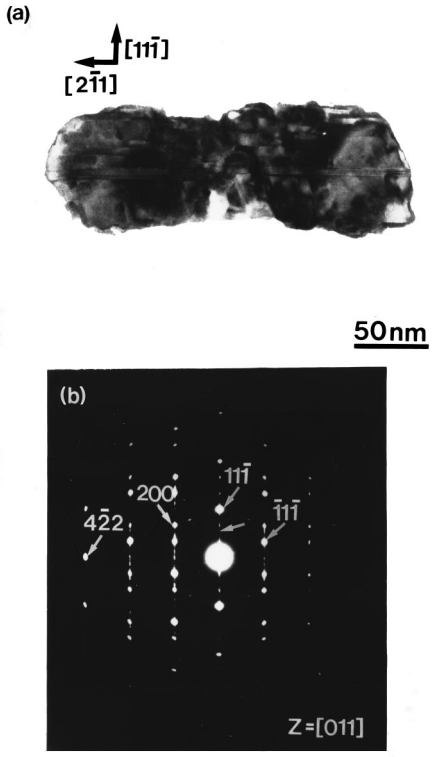

FIG. 1. (a) Bright field TEM micrograph showing an elongated $Si_{0.7}Ge_{0.3}$ grain with one primary twin variant in the film annealed at 550 °C in a dry N_2 ambient for 4 h and (b) corresponding electron diffraction pattern.

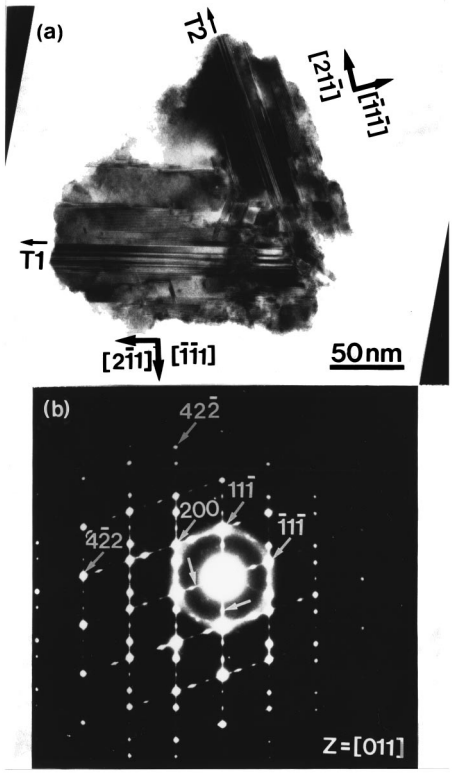

FIG. 2. (a) Bright field TEM micrograph showing another $Si_{0.7}Ge_{0.3}$ grain with two primary nonplanar twin variants in the film annealed at 550 °C in a dry N_2 ambient for 4 h and (b) corresponding electron diffraction pattern.

bands and the growth in the ⟨111⟩ direction is a {111} facet growth and slowest.

Figure 2(a) shows a bright field transmission electron micrograph of another grain in the $Si_{0.7}Ge_{0.3}$ thin film annealed at 550 °C in a dry N_2 ambient for 4 h and Fig. 2(b) is a selected area electron diffraction pattern obtained from the grain in Fig. 2(a). The grain no longer has an elongated shape, but a triangular shape. Major twin bands are observed inside the grain and those are parallel to the two directions indicated by T1 and T2, which have an angle of 70.5° with respect to each other. The diffraction pattern shows that this grain also has a [011] orientation, as did the grain in Fig. 1(a). Amorphous/crystal interfaces in the [111] and [$\bar{1}$11] directions of the grain sustain {111} facet boundaries like that of an elongated grain, however, the outline of the amorphous/crystalline interface between two major noncoplanar twin bands of the grain is rounded and convex. This fact shows that the growth in the [111] and [$\bar{1}$11] directions is {111} facet growth, however, the growth in the [$\bar{1}\bar{1}$1] and [$\bar{1}$1$\bar{1}$] directions is not {111} facet growth, but is limited by the growth in the ⟨211⟩ directions, which are the preferential growth direction along twin bands.

The widely accepted explanation for the anisotropic growth of such an elongated grain is the formation of two or more parallel twin bands leading to the formation of reentrant grooves which can act as a nucleation site for atomic steps.[8–10] In Fig. 3(a), at this twin boundary on a {111} surface, only two atoms are required to establish a nucleus, while three atoms are required for the nucleation of new layer on the {111} surface.[9] Therefore, the grain with several parallel twin bands has to be an elongated elliptical shape.

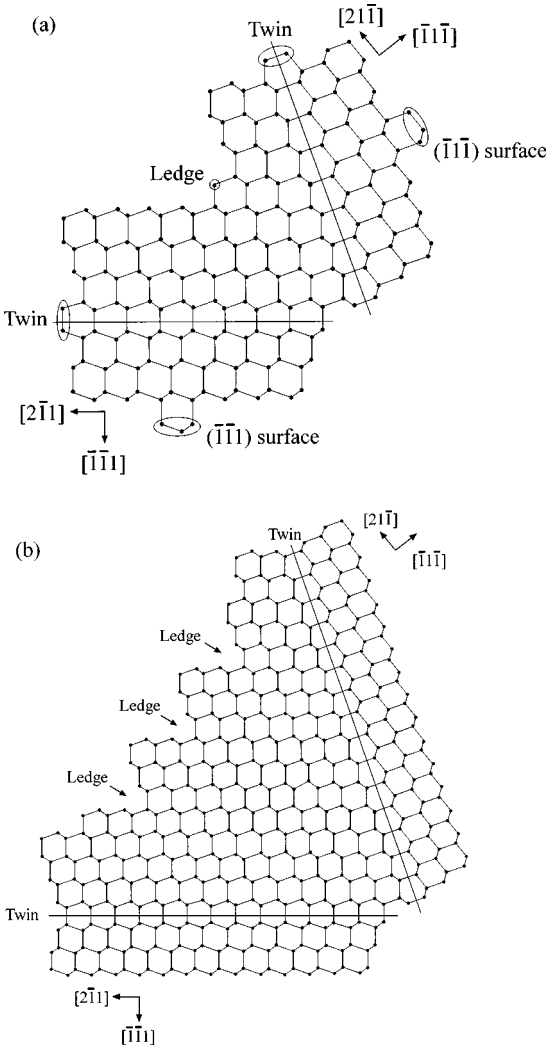

FIG. 3. (a) A schematic drawing of the growth process shows a {111} surface, twins and a ledge. At the atomic ledge, the addition of single atom can nucleate a new layer and at twin boundaries, two atoms are required, however, on the {111} surface, cluster of three atoms is required for nucleation of a new layer and (b) a schematic drawing shows that the ledges form owing to the protruding amorphous/crystal interface at the junction.

Also, the grain with two or more primary non-coplanar twin bands can be a branched elliptical or dendritic shape.

However, in our experiments, when a second (noncoplanar) twin variant which makes an angle of 70.5° with respect to the first twin forms in sequence at an early stage of crystallization, the growth front between two noncoplanar twin bands develops as fast as the ⟨112⟩ directions along twin bands propagate. We suggest that the atomic {111} ledge can form easily at such a growth front.

When two primary noncoplanar twin bands, which make an angle of 70.5° with respect to each other, form in the grain at the early stage of crystallization, the growth fronts of two primary noncoplanar twin bands develop in the ⟨211⟩ directions, respectively, and the surfaces in the ⟨111⟩ directions are bounded by two sets of {111} planes, thus the grain has two noncoplanar elongated arms. However, the contact of these two elongated arms reveals the contact of two sets of {111} planes, which make an angle of 70.5° with respect to each other. So, the junction at the intersection of two noncoplanar elongated arms with the amorphous/crystalline interface forms a {111} atomic ledge in Fig. 3(a). Since this {111}

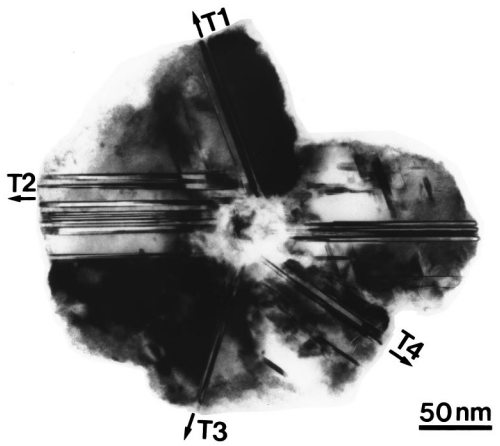

FIG. 4. Bright field TEM micrograph showing an equiaxed $Si_{0.7}Ge_{0.3}$ grain with four primary twin variants in the film annealed at 550 °C in a dry N_2 ambient for 4 h.

ledge requires only a single atom to nucleate a new layer, the ledge accelerates the growth on the adjacent {111} surfaces.[9] Thus, the development of the amorphous/crystalline interface at the junction is as fast as the growth in the ⟨211⟩ direction along twins. While new {111} layers also nucleate directly on the {111} surfaces where are apart from the junction, the amorphous/crystalline interface in the neighborhood of the junction develops so fast owing to the easy nucleation of new layers at the junction that this interface protrudes. This protruding interface should soon be bounded by the growing {111} faces. This leads to the formation of new {111} ledges as in Fig. 3(b). These ledges also provide preferential sites for the nucleation of new layers. Hence, {111} ledges can be formed continuously during grain growth. In addition, the nucleus, which attaches directly on the {111} surface, often reverses the stacking order and this nucleus is thus the beginning of a new twin. Therefore, additional twins can be formed.

While the grain grows, not only additional twins form continuously in two arms, but also {111} ledges form continuously between two arms by above reason. Therefore, the development of amorphous/crystal interface between two arms is as fast as the growth of arms in the ⟨112⟩ direction along twins, so the outline between two arms is rounded and convex.

When more than two primary noncoplanar twin variants are formed at the early stage of solid-phase crystallization, the grain has a more or less equiaxed shape. An observation of such a grain is shown in a bright field transmission electron micrograph in Fig. 4. There are four major noncoplanar twin bands, indicated by T1, T2, T3, and T4. The outlines of the amorphous/crystal interfaces between T1 and T2, T2 and T3, and T3 and T4, which make an angle of 70.5° with respect to each other, are rounded and convex.

In solid-phase crystallized amorphous $Si_{0.7}Ge_{0.3}$ thin films, the grain with major twin bands of a single twin variant parallel to a {111} plane develops an elongated shape owing to the slowest {111} facet growth in the ⟨111⟩ direction and the preferential growth in the ⟨112⟩ direction along major twin bands. However, the grain with two noncoplanar twin variants, that have an angle of 70.5° with respect to each other, is not elongated. The growth front between two noncoplanar twin bands develops as fast as the preferred ⟨112⟩ growth direction along major twins propagates, owing to the easy nucleation at the corner where two arms meet resulting in accelerated {111} ledge growth. As the number of primary, noncoplanar twin variants formed at the early stage of solid-phase crystallization is increased, the grain morphology of the $Si_{0.7}Ge_{0.3}$ alloy becomes increasingly equiaxed.

This work was supported by the Institute of Information Technology Assessment and the Korean Science and Engineering Foundation (KOSEF) through the Center for Interface Science and Engineering of Materials. The authors acknowledge Dr. S. C. Lee at Electronics and Telecommunications Research Institute (ETRI) for the preparation of MBD samples.

[1] T.-J. King, K. C. Saraswat, and J. R. Pfiester, IEEE Electron Device Lett. **12**, 584 (1991).
[2] T.-J. King and K. C. Saraswat, IEEE Trans. Electron Devices **41**, 1581 (1994).
[3] C. W. Hwang, M. K. Ryu, K. B. Kim, S. C. Lee, and C. S. Kim, J. Appl. Phys. **77**, 3042 (1995).
[4] F. Edelman, Y. Komem, S. S. Iyer, J. Heydenreich, and D. Baither. Thin Solid Films **222**, 57 (1992).
[5] R. B. Iverson and R. Reif, J. Appl. Phys. **57**, 5169 (1985).
[6] M. K. Hatalis and D. W. Greve, J. Appl. Phys. **63**, 2260 (1988).
[7] J. P. Hirth and J. Lothe, *Theory of Dislocations,* 2nd ed. (Wiley, New York, 1982), p. 374.
[8] D. R. Hamilton and R. G. Seidensticker, J. Appl. Phys. **31**, 1165 (1960).
[9] R. Drosd and J. Washburn, J. Appl. Phys. **53**, 397 (1982).
[10] J. H. Kim, J. Y. Lee, and K. S. Nam, J. Appl. Phys. **77**, 95 (1995).