Growth speed, growth textures, and twin boundary structures of quartz twinned after Japan twin law

Koichi Momma[1]; Toshiro Nagase[2]; Takahiro Kuribayashi[3]; Yasuhiro Kudoh[3]

[1] Tohoku Univ; [2] Tohoku Univ. Muse.; [3] Tohoku Univ.

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In general, crystal growth is often enhanced at twin boundaries, with a result that sizes and forms of twinned crystals are different from coexisting single crystals. As a model case for the study of growth mechanism of twinned crystals, growth textures and atomic configurations of Japan twin boundaries in quartz were studied by the observation of natural samples and by computational simulations.

In all the samples from Narushima, Nagasaki Prefecture, Japan, narrow regions are found adjacent to Japan twin boundaries to be formed by submicron-scale intergrowths of right- and left-handed quartz, i.e. Brazil twinning. At the bottom of Japan twin, there is no such sector. The hourglass-shaped sector with dense Brazil twin lamellae develops progressively as long as composition plane of Japan twin is smooth and flat plane parallel to {11-22}.

Cathodoluminescence images of the samples revealed that the samples have undergone two distinct growth stages. Rhombohedral faces are bounded by the Japan twin boundary in the early growth stage and prism faces are bounded by the twin boundary in the later stage. Development of the densely concentrated Brazil twin lamellae takes place almost exclusively in growth sector of the rhombohedral faces bounded by the Japan twin boundary. The crystal growth at Japan twin boundary is enhanced only when Brazil twin lamellae develop near the Japan twin boundary. Once prism faces appear at Japan twin boundary, number of Brazil twin lamellae decrease significantly and preferential growth no longer takes place.

Atomic configurations at {11-22} composition planes of Japan twin were simulated by using molecular dynamics (MD) simulations and the energy minimization method. The simulated structures proved that {11-22} or {-1-122} composition planes are the only composition planes that do not introduce unsatisfied bonding between silicon and oxygen atoms. Based on the structures of Japan twin boundaries, structures where the Japan and Brazil twin boundaries intersect each other are successfully determined by MD simulations. It is confirmed that all the silicon atoms in these structures have four nearest oxygen atoms, and all the oxygen atoms have two nearest silicon atoms. The results of MD simulations demonstrate that structural handedness of quartz can be exchanged coherently at Japan twin boundaries when some Brazil twin boundaries intersect with Japan twin boundaries.

An important insight from this study is that preferential growth at twin boundaries takes place only when twin boundaries have structural flexibility to allow more than one type of structures to grow coherently on the substrate crystals. Once twin boundary structures become similar to general incoherent grain boundaries, in which many dangling bonds exist, twin boundaries no longer serve as preferential growth sites.