

Structural relation of Japanese twin boundary and Brazil twin boundary in quartz

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Growth textures of quartz twinned after Japan law were studied by using optical observations of etched figures, and atomic configurations at Japanese twin boundaries were studied by computational simulations. Samples of Japanese twin from Narushima, Nagasaki Prefecture, Japan were polished and etched by conc. HF solutions for several minutes. Then, the samples were coated by evaporated silver and observed by reflection microscopy.

Near the composition plane of Japanese twin, hourglass-shaped sectors are observed to have mosaic textures composed of polysynthetic Brazil twin. Composition plane of Japanese twin is curved or bended near the surface of crystals, whereas in inner part of crystals, composition plane is a very straight $\{11-22\}$ plane. Especially high concentration of Brazil twin is observed in a growth sector where composition plane of Japanese twin is a straight $\{11-22\}$ plane. Some of these Brazil twin lamellae repeat on a scale less than 1 micro meter.

Atomic configurations at $\{11-22\}$ composition plane of Japanese twin were simulated by using molecular dynamics simulations and energy minimization method. Simulations are started from two slabs of the bulk crystals spaced about 2 Angstrom. In order to explore a twin boundary structure with the minimum energy, simulations were performed for a series of initial configurations covering all the different displacements of slabs parallel to the composition plane. From the simulated structures, twin displacement vector was determined for each of 10 subtypes of Japanese twin.

When the composition plane is $(-12-12)$, twin displacement vector of subtypes I(R), II(R), and II(R)a is $[0.5a, -0.45b, 0.3c]$. The two twin individuals of subtypes III IIIa, IV, and IVa are related by simple mirror operations, without any translational components. Twin displacement vector of Brazil twin is known to be a function of orientation of the composition plane. Therefore, screw dislocations are necessarily present where orientation of Brazil twin boundaries changes from one orientation to another. Based on these twin displacement vectors, it is shown that incorporation of a screw dislocation is not required at junction of Japanese twin boundary with Brazil twin boundary.

High concentration of Brazil twin observed near Japanese twin boundary and atomic configurations of these twin boundaries indicate that $\{11-22\}$ composition plane of Japanese twin serve as a source of Brazil twin during the course of growth of Japanese twin.