and 111 surface and the particles size was reduced. The valence of Ce was measured. With decreasing the size of the nanocrystals, valence of Ce was changed from 4 to 3. FTIR analyses revealed that the chemical bond between the surface modifier and 100 surface and 111 surface are different. Ab-initio calculation could successfully explain all of those experimental results.

Keywords: supercritical fluids, hydrothermal synthesis, organic inorganic hybrid materials

P16.12.36

The role of Japanese twin boundary in quartz as a source of Brazil twin

Keiichi Momma, Toshiro Nagase, Yasuhiro Kudoh,
Takahiro Kuribayashi

Tohoku University, Department of Earth and Planetary Materials Science, Aoba, Sendai, Miyagi, 980-8578, Japan, E-mail: mmnakou@ganko.
tohoku.ac.jp

Growth textures and atomic configurations of Japanese twin boundary in quartz were studied by using optical microscopy and computational simulations. Samples from Narushima, Nagasaki Prefecture, Japan were polished, etched by hydro fluoride for several minutes, and coated by evaporated silver. From observations by reflection microscopy, hourglass-shaped sectors are found near the composition plane of Japanese twin to have mosaic textures composed of polysynthetic Brazil twin. Especially high concentration of Brazil twin with a repeat scale less than 1 micro meter is observed in a growth sector where composition plane of Japanese twin is a straight {112} plane. Atomic configurations at {112} composition plane of Japanese twin were simulated by using molecular dynamics simulations and the energy minimization method. The initial atomic configurations are two slabs of the bulk crystals and simulations were performed for all the different displacements of slabs. From the simulated structures, the twin displacement vector was determined for each of 10 subtypes of Japanese twin. In the case of Brazil twin, the twin displacement vector is known to be a function of orientation of the composition plane. Therefore, screw dislocations are necessarily present where orientation of Brazil twin boundary changes from one orientation to another. Based on the twin displacement vectors of 10 subtypes of Japanese twin determined in this study, we found that dislocations are also required at stepped boundary of Japanese twin, whereas dislocations are not required where Japanese twin boundaries intersect with Brazil twin boundaries. Observations in this study indicate that {112} composition plane of Japanese twin serves as a source of Brazil twin during the course of crystal growth.

Keywords: quartz, twin boundary, molecular dynamics

P16.04.39

Synthesis large-scale high purity InP crystal by P-injection method

Sun Niefeng1, Mao Luhong2, Guo Weiliam1, Wu Xiawan2, Zhou Xiaolong1, Sun Tongnian1

1Hebei Semiconductor Research Institute, National Key lab. of ASIC, P. O.Box 179-40, No. 113, Hezuo Road, Shijiazhuang, Hebei, 050051, China, 2School of Electronic Information Engineering, Tianjin University, Tianjin, P. R. China, E-mail: niefung@sohu.com

Polycrystalline InP is the starting material for InP crystal growth by Liquid Encapsulated Czochralski (LEC) and Gradient Freezing (GF) Technique. Hence, polycrystalline must therefore be pre-synthesized prior to crystal growth. A large quantity of high purity InP crystal material has been produced by the phosphorus in-situ injection synthesis and LEC growth process. In the injection method, phosphorus reacts with indium very quickly so that the rapid polycrystalline synthesis is possible. It also has an easiness to increase the production scale, so that the method is very promising for the large-scale production. This method however has a difficulty in obtaining stoichiometric polycrystalline because the cease point of phosphorus injection is difficult to find. For realizing this method as an industrial method, the stoichiometric control is one of the key technologies to be developed. It was found a suitable thermal distribution on injector tube and melt are necessary for the synthesis of stoichiometric InP with such a large quantity. The quartz injector with two or multi-transfer tubes was used to improve the synthesis result. It will avoid quartz injector blast when the melt was indraft into the transfer tube. The injection speed, melt temperature, phosphorus excess, and so on are also important for a successful synthesis method. About 4-6Kg high purity, stoichiometric poly InP is synthesized reproducibly by improved transfer tubes P-injection method in the high-pressure puller in nearly 60-70 minutes. The obtained high mobility and low background concentration as measured from van der Pauw method implies the electrical quality of the synthesized material. Glow discharge mass spectroscopy (GDMS) results confirmed the low background levels of impurities.

Keywords: indium phosphide, growth from melt, liquid encapsulated Czochralski method

P16.06.40

Initial state of VLS-growth of InAs nanorods on GaAs(111), probed by X-ray diffraction and TEM

Ullrich Pietsch1, Anton Davydov1, Andreas Biermann1, Joerg Grenzer2, Jens Bauer1, Volker Gottschalch2

1University of Siegen, Physics, Walter-Flex-Str. 3, Siegen, NRW, 57068,