

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 he 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

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

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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 fluoric acid 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

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Preparation and characterization of cadmium telluride thin films by vacuum evaporation

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Cadmium telluride thin films are prepared by vacuum evaporation of CdTe powder using an Edwards 306 coating unit. Calculated

quantity of copper is evaporated on top of CdTe layer. The whole assembly is then annealed at 400 OC fore 4-6 Minutes. The thin films are characterized optically and electrically using spectrophotometer and measurements of van der pauw & Hall Effect. Characterization of CdTe has shown it to have a band gap of 1.475 eV and a resistivity of 0.132 to 0.002 ohm-cm, depending upon the concentration of copper. As the weight percentage of copper increases the resistivity decreases and the mobility increases up to 3 wt% of copper. The Carrier concentration showed a systematic increase.

Keywords: thin films, deposition, XRD

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

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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 process. 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

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

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