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 0C 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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We studied the initial state of VLS-growth of InAs nanorods onto GaAs[111]B via Au catalyst at growth temperature of 450℃ where the growth was truncated after 20s, 40s, 60s and 300s, respectively. The whole samples have been analyzed at room temperature using out-of plane high-resolution x-ray diffraction in home laboratory and in-plane depth-resolved x-ray grazing-incidence diffraction (GID) with synchrotron radiation. Selected NRs have been inspected by TEM as well. Samples with growth time of 20s and 40s did not show InAs NRs. Instead we identified several Indium rich Au phases at the surface and a strongly enhanced diffuse scattering in vicinity of the GaAs peaks. InAs NRs appeared after 60s growth time crystallized in wurzite phase. At same time small $In_{1-x}Ga_xAs$ components with composition ranging between x=0.05 and 0.22 were observed grown with zinc-blende structure accompanied with large diffuse scattering close to the GaAs. Depth-resolved GID and HR-TEM showed that the $In_{1-x}Ga_xAs$ components are located at the basement of NRs. Additionally we found alloy clusters buried under truncated NRs. Our data suggest a model where InAs NRs grow out of an Indium enriched Au-Ga phase. However, inclusion of indium into Au-Ga (T_e=339℃) first decreases the melting point of Au-Ga-In eutecticum, but for higher Indium content the eutectic melting temperature increases up to 454 ℃ valid for the Au-In system. For a growth temperature between 350 ℃ and 460 ℃ Au alloy droplets remain liquid since the gallium concentration exceeds about 30 to 0 at%, respectively. Therefore Au droplets with low gallium content become solid and cannot act as catalyst anymore. Hence, stable NR growth can be established only if the metallic alloy droplet contains a sufficient concentration of gallium.

Keywords: growth mechanisms, nanocrystals, high-resolution X-ray diffraction

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InGaP/GaAs(001) structural characterization by means of synchrotron radiation Renninger Scan

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Synchrotron radiation Renninger Scan (RS), a high resolution structural probe, is applied in the layer and the substrate simultaneous characterization of the InGaP/GaAs(001) epitaxial structures. Around $\phi = 0^o$ symmetry mirror of the RS, Bragg-Surface reflections (BSD) which are secondary beams propagating along the surface/interface which provide the strain distribution in the layer/substrate interface and around $\phi = 45^o$ the coherent hybrid reflections (CHR) [Morelhão et al, Appl. Phys. Lett., 73(15), 2194 (1998)] allow for the simultaneous characterization of layer and substrate lattices. InGaP layers with composition variation into [1 0 0] and [0 1 0] directions were grown on GaAs(001) by Chemical Beam Epitaxy (CBE). Several (002) rocking curves were measured and plotted as pole figures around [0 0 1] direction to evidence the occurrence of (1 -1 3)(1 -1 -1) CHR. Entrance and exit positions of (1 -1 1), (1 1 1), (-1 -1 1) and (-1 1 1) BSD reflections in the (002) RS of both GaAs and InGaP lattices carried out in the Brazilian synchrotron (LNLS) allowed to figure out the strain in-plane [Morelhão et al, Phys. Stat. Sol (a), 8, 2548 (2007)] along the [1 1 0] and [1 -1 0] directions. The layer value ($25.1(4) \times 10^{-4}$) is one order of magnitude greater than the substrate value ($1.3(4) \times 10^{-4}$) as expected since the layer has a composition variation. (0 -2 2)(0 2 2) and (-2 0 2)(2 0 2) four-beam reflections measured as a negative peak in the (004) substrate RS at $\phi = 45^o$ and 135^o, respectively. Each peak has turned into two three-beam reflections in the layer RS due to the structural tetragonal distortion ($a = b = 5.6539$ Å and $c = 5.6872$ Å obtained from RS simulation). Financial support: CAPES, CNPq and FAPESP.

Keywords: semiconductor epitaxy, X-ray multiple diffraction, strain determination

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High resolution X-ray diffraction study of $Al_xGa_{1-x}Sb$ alloys grown by liquid phase epitaxy

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AlxGa1-xSb epitaxial layers were grown by liquid phase epitaxy at 400 ℃ on (001) and (111) undoped GaSb substrates. The layer composition was measured by energy dispersive x-ray spectroscopy, obtaining composition values between x=0.05 and x=0.36 of Al content. High resolution x-ray diffraction profiles were obtained from the (004) and (444) reflections respectively. In both cases the relative lattice mismatch was of the order of 10^{-3}. From the rocking curves was obtained the out of plane lattice parameter, directly from the symmetrical diffractions for (001) and (111) alloys. It was determined that all the layers are strained, and those grown on (001) GaSb are slightly more strained than the corresponding layers grown on (111) GaSb. This difference is explained by the dependence of the strain ratio on growth direction [1, 2]. The out of plane lattice parameter as a function of Al content is higher than the corresponding bulk lattice parameter of AlxGa1-xSb layers obtained with Vegard's law. Also, the perpendicular lattice parameter expected for pseudomorphic alloys as a function of Al content, was estimated from the strain ratios (001) and (111) [1, 2]. It was observed that almost all the layers for both orientations are fully strained. For other hand, the in-plane lattice parameter, was determined from the strain ratios, assuming an elastic deformation and using the EDX alloy composition to interpolate the elastic constants Cij. The behavior of this parameter with Al content, also shows that almost all the layers are fully strained.

References

[1] E. Anastassakis, J. Appl. Phys. 68 (1990) 4561
[2] A. Navarro-Quezada, A.G. Rodríguez, M.A. Vidal, H. Navarro-Contreras, J. Crystal Growth 291 (2006) 340.

Keywords: liquid phase epitaxy, lattice distortion, high-resolution X-ray diffraction