

GaCl will be shown. The analysis provides us useful information on the growth rate and the deposition composition. Next, HVPE growth of AlN and AlGaIn will be described.

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Keywords: HVPE, Al-related nitrides, thermodynamic analysis

MS.49.3

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Fabrication of InN dot structures by droplet epitaxy using NH₃

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Quantum dots (QDs) of nitride semiconductors have been studied intensively because of their usefulness for device applications. Recently, we have fabricated GaN dots by droplet epitaxy. The droplet epitaxy requires neither any anti-surfactants nor the induction of surface strain for the formation of dot structures, which means the possibility of the QD formation on any substrates. In this study, we investigated fabrication of InN dots by droplet epitaxy with changing substrate temperature. After nitridation of Si(111) substrates, 1 ML of In was deposited on the substrates at 200 °C, leading to the formation of In droplets. Then, NH₃ gas was irradiated on the In droplets for nitriding. AFM observation showed that the average density of dots of 1.1x10¹⁰ cm⁻² at 450°C decreased as the temperature increased. Then, the density increased again up to 4.0x10¹⁰ cm⁻² at 570°C. However, no InN dot was observed on the sample nitridated at 600 °C. In 3d XPS spectra in Fig.1 indicates that In-N component was increased as the temperature increased while In-O component was decreased. Almost all In atoms was found to bind to N atoms at 570°C by the formation of InN crystalline.

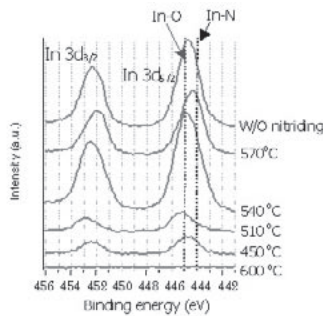


Fig. 1 In 3d XPS spectra of InN dots grown by droplet epitaxy using NH₃.

Keywords: droplet epitaxy, indium nitride, nitriding

MS.49.4

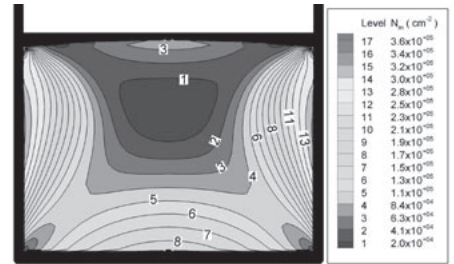
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Dislocation density in silicon ingot during a unidirectional solidification process

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Many dislocations and impurities in the silicon significantly affect the conversion efficiency of solar cells. Thermal stress is one of the major factors responsible for generation of dislocations during the unidirectional solidification process. Therefore, it is necessary to investigate the distribution of thermal stresses and dislocation density in the silicon ingot. A transient global model was used to obtain the solution of thermal field within the entire furnace. And then, based on transient global solution of heat transfer, computations were carried out to investigate the distribution of thermal stresses in silicon ingot. Finally, the dislocation density was also simulated by using Haasen-Alexander-Sumino model. The results on boundary condition to grow a silicon ingot with low thermal stresses and dislocation density. The effects of solidification time on thermal stresses and dislocation density were also studied. The results reveal that long solidification time can reduce thermal stresses and dislocation density in a silicon ingot during the solidification process.



Keywords: solidification, stress, dislocations

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AlN and GaN hetero epitaxy on Si substrate using activity modulation migration enhanced MBE

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In order to control chemical and physical nitrogen activities two discharge modes of E and H modes[1] under a radio frequency inductive coupled (RF-ICP) discharge of nitrogen gas was investigated changing RF-power of nitrogen pressure. The chemical activities of dissociated nitrogen atoms N+N* are much higher than those of excited nitrogen molecules N₂*. However N₂* has small chemical activity but large physical activity, which has large energy to enhance migration of Al or Ga atoms on a growing surface. The E and H modes of the ICP discharge are low brightness (LB) and high brightness (HB) discharges, respectively. Dissociated atomic nitrogen species are created by only the HB mode. The time sequence of the opening of the shutter of a Ga effusion cell was used for the trigger signal to operate the mode change operation of nitrogen ICP-RF discharge. An activity modulation migration enhanced epitaxial growth (AM-MEE) method is proposed as an application of the MEE[2]. In order to grow the high quality layers on a Si substrate the AM-MEE growth method was performed. The sequence of the LB and HB discharges during the AM-MEE the nitrogen flux irradiation plays an important role to control the chemical activity of nitrogen. Activity control of nitrogen is also applied to a fabrication method of beta-Si₃N₄ epitaxial layer on Si(111) as an initial buffer layer for AlN film.

References

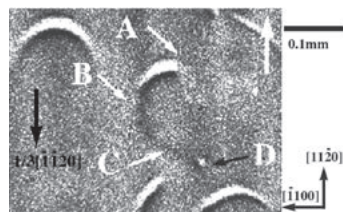
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 [2] Y. Horikoshi, M. Kawashima, and H. Yamaguchi, Jpn. J. Appl.

Phy 27 (1988) 169.

Keywords: activity, MBE, gallium nitrides

MS.49.6*Acta Cryst.* (2008). A64, C89**Contrast of dislocations in 4H-SiC by SR topography in grazing-incidence geometry**Hirofumi Matsuhata¹, Hiroataka Yamaguchi¹, Toshiyuki Ono², Bin Chen³, Takashi Sekiguchi³¹National Institute of Advanced Science and Technology, Laboratory of Energy Semiconductor Electronics, 1-1-1, Umezono, Tsukuba, Ibaraki, 305-0032, Japan, ²Central Research Laboratory, Hitachi Ltd, 1-280 Higashi-Koigakubo, Kokubunji Tokyo 185-8601, Japan, ³National Institute for Materials Science, Namiki, Tsukuba 305-0044, Japan, E-mail: h.matsuhata@aist.go.jp

Dislocations near surface of 4H-SiC were observed using synchrotron radiation topography in the Bragg case with grazing-incidence geometry. Figure is an image of basal-plane dislocation half-loop at $g=11\text{-}28$, $\lambda=0.15\text{nm}$ on Si-face. The (0001) plane is tilted towards the $[-1\text{-}120]$ direction by 8 degrees from the surface. In this condition, lattice defects within 10 μm depth are observed. Along this dislocation line, bright contrast at A, dark and bright asymmetric line at B, and dark contrast at C are observed. Absence of contrast can be seen at B at $g=1\text{-}108$, and so that B is a screw dislocation part. We have observed migrations of dark dislocations in specimens after forward-bias degradation effect, in which Si-core dislocations are known to move. Thus we concluded that C is Si-core, A is C-core edge dislocation, and the Burgers vector is $1/3[-1\text{-}120]$. The observed dark and bright contrast is discussed to be similar effect described by Ando and Kato (1970). By applying this rule we could identify uniquely 6 different Burgers vectors for all basal-plane dislocations and threading edge dislocations at only one diffraction condition. Ando and Kato: *J. Appl. Cryst.* **3** (1970) 74.



Keywords: wide-bandgap semiconductors, dislocations, topography X-ray

MS.50.1*Acta Cryst.* (2008). A64, C89**Decoding homophilic recognition specificity of Dscam, a neuronal receptor with thousands isoforms**

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The Dscam gene gives rise to thousands of diverse cell surface receptors thought to provide homophilic and heterophilic recognition specificity for neural development and immune responses. Mutually exclusive splicing allows for the generation of sequence variability in three immunoglobulin (Ig) ecto-domains (D2, D3, D7). X-ray structures of the N-terminal four Ig domains (D1-D4) of four distinct Dscam isoforms have been determined. The structures

reveal a horseshoe configuration, with variable residues of D2 and D3 constituting two independent surface-epitopes on either side of the receptor. All these four isoforms engage in homo-dimerization coupling variable domains D2 with D2 and D3 with D3 using the same epitope. The recognition specificity has been analyzed to decode how sequence and local conformation of these two variable domains contribute to homophilic interaction. The structure of the third Ig-like domain D7 has also been determined in the form of D7-D8 fragment for several isoforms. A general view of how these variable Ig domains embedded in thousands receptor isoforms offer homophilic recognition for neuronal wiring has been provided.

Keywords: dscam receptor, decoding recognition specificity, thousand isoforms

MS.50.2*Acta Cryst.* (2008). A64, C89**Crystal structure of the [2Fe-2S] transcriptional activator SoxR bound to DNA**Kunio Miki^{1,2}, Satoshi Watanabe¹, Akiko Kita¹, Kazuo Kobayashi³¹Kyoto University, Department of Chemistry, Graduate School of Science, Sakyo-ku, Kyoto, Kyoto, 606-8502, Japan, ²RIKEN Spring-8 center at Harima Institute, Koto 1-1-1, Sayo, Hyogo 679-5148, Japan, ³Osaka University, Mihogaoka 8-1, Ibaraki, Osaka 567-0047, Japan, E-mail: miki@kuchem.kyoto-u.ac.jp

SoxR functions as a sensor of oxidative stress such as superoxide and nitric oxide. It exists as a dimer with each subunit containing a [2Fe-2S] cluster. Reversible oxidation of the [2Fe-2S] cluster activates SoxR to enhance the production of various antioxidant proteins through the *soxRS* regulon. SoxR belongs to the MerR family of transcriptional activators, target promoters of which have an unusual 19 or 20 bp spacer between the -35 and -10 operator elements. In the active state, SoxR and other MerR family proteins activate transcription from unique promoters by distorting the DNA conformation. In order to elucidate structural features of the iron-sulfur cluster of SoxR and the transcriptional activation mechanism, we have determined the crystal structures of SoxR and its complex with DNA in the oxidized (active) state [1]. The overall structure of SoxR consists of a DNA binding domain, a dimerization helix and an Fe-S cluster binding domain. The dimerization helix forms an antiparallel coiled-coil, stabilizing the SoxR dimer. The structures reveal that the [2Fe-2S] cluster of SoxR is unusually solvent-exposed and surrounded by an asymmetric environment, suggesting that the asymmetrically charged environment is a key factor of redox-dependent conformational changes of SoxR and the target promoter. The DNA structure is shown to be sharply bent at the middle and unwound by 3-bp, compared to a B-form DNA. Based on comparison of the target promoter sequences of the MerR family, the present structures shows an activated promoter conformation with a 20-bp spacer in the MerR family.

[1] Watanabe S, Kita A, Kobayashi K, Miki K., *Proc Natl Acad Sci USA*, 2008, 105, 4121.

Keywords: SoxR protein, MerR family, transcription factors

MS.50.3*Acta Cryst.* (2008). A64, C89-90**Hybrid LRR technique and crystal structures of the toll-like receptor complexes**

Jie-Oh Lee