SiC Bulk Single Crystal Growth

Shin-ichi Nishizawa

SiC single crystal is usually grown by sublimation (modified Lely method). There is a lot of remaining issues that should be solved. One is the technical problems of SiC single crystal growth process. And the other is the theoretical problem based on SiC physical properties. As the example of technical issues, in this paper, the example of design optimization for SiC sublimation growth is described. The shape of SiC grown crystal (diameter and length) can be controlled by using modified crucible design. And as the example of the theoretical problem, the author has tried to use atomic scale modeling (DFT calculation) to understand the physics that determine SiC polytype during crystal growth process. By calculating the bulk crystal energy of each polytype, and surface energy of each possible surface during growth, it is pointed out that growing surface itself has effects on the polytype stability of SiC.

First-Principles Investigation for the Polytypism in Semiconductors

Tomonori Ito, Toru Akiyama, and Kohji Nakamura

Polytypism in semiconductors such as SiC and ZnS is systematically investigated using ab initio pseudopotential approach for the total energy calculations in four structures such as 3C (zinc blende), 6H, 4H, and 2H (wurtzite) structures with/without vacancies. Our calculated energy differences $\Delta E$ among four structures without vacancy reveal that SiC favors 3C and 4H while 3C is preferred for ZnS. The $\Delta E$ for SiC with vacancy explicitly elucidates the most stable structures such as 6H with Si-vacancy and 4H with C-vacancy. On the other hand, ZnS with vacancy prefers 2H with S-vacancy. In particular, the calculated vacancy formation energies suggest that C-rich and Si-rich conditions respectively prefer 6H-SiC and 4H-SiC, while 2H-ZnS appears independent of the conditions. These results suggest that the vacancy formation plays an important role in the polytypism in semiconductors. Furthermore, nitrogen substituting for carbon and silicon in SiC respectively stabilizes 3C and 4H. It is found that the polytypism in semiconductors can be systematically interpreted by considering difference in interatomic bond charges between before and after point defect formation.
Effect of the Inclusion of Transparency on the Thermal Field and Interface Shape in Long-term Sublimation Growth of SiC Crystals

Bing Gao 1* and Koichi Kakimoto1

To determine if the transparency of SiC crystals affects the crystal growth during long-term sublimation growth and the difference between the results with and without the inclusion of transparency, a global solver that considers almost all of the effects in the heat and mass transport processes, such as the compressible effect, the convection effect, the buoyancy effect, flow coupling of argon gas and species, and the Stefan effect, was developed. The results indicate that the transparency of SiC crystals affects the temperature field distribution inside the crystal, seed holder and gas chamber, and the shape of the growth interface. Therefore, the transparency of SiC crystals should not be neglected in global simulations of SiC PVT growth.


Commentary

Current Advances in SiC Solution Growth

Shunta Harada 1*, Yuji Yamamoto1, Kazuaki Seki 1, and Toru Ujihara 1

Solution growth has a potential to achieve high quality bulk SiC growth. In this paper we review current advances in SiC solution growth specially focusing on the crystal quality. During the solution growth, threading dislocations tend to be converted to basal plane defects by the step-flow of macrosteps. This phenomenon implies that all dislocations can be excluded from the lateral face of the crystal in principle. Actually, high quality SiC crystal with very low threading dislocation density was obtained applying the dislocation conversion during the solution growth.

Commentary

Analysis of Defect Formation in 4H-SiC Epitaxial Growth and Development of Defect Control Techniques

Hidekazu Tsuchida 1*, Isaho Kamata 1, Tetsuya Miyazawa 1, Masahiko Ito 1, Masahiro Nagano 1, and Ryohei Tanuma 1

This paper reviews recent achievements in defect formation analysis and reduction techniques of extended and point defects for 4H-SiC epilayers. Basal plane dislocations (BPDs) are found to convert to threading edge dislocations (TEDs) by not only epitaxial growth but also simple high-temperature annealing. A very low BPD density of 0.09 cm$^{-2}$ is obtained in the use of a 4º off 4H-SiC substrate. 8H in-grown stacking faults are also reduced to be <0.1 cm$^{-2}$ in 4H-SiC epitaxial growth by controlling the gas system. Elimination of the Zic center and significant improvements in carrier lifetimes are realized by in-diffusion of carbon interstitials from a surface region to a deep region of 4H-SiC epilayers.


Epitaxial Growth and Characterization of 4H-SiC Layers

Anne Henry1* and Erik Janzén1

The growth of thick 4H-SiC epilayers needed for high power applications is described using horizontal hot-wall chemical vapor deposition with both the standard and the chloride based chemistry. The use of various kinds of substrates (various off-axis and nominally on-axis substrates) is compared and advantages and drawbacks are discussed for each case. Low angle off-cut substrates are proposed for further development of the SiC activities. Using the chloride based approach the Cl/Si ratio is a new important parameter and chlorinated precursor as methyltrichlorosilane is shown more efficient than the simple addition of chlorine to the gas mixture.


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