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論 文 要 旨

THESIS SUMMARY

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要旨（英文 800 語程度）
Thesis Summary（approx.800 English Words ）

This thesis presents first-principles theoretical works on group IV and III-V semiconductors. Ever since the polytypism in SiC was discovered, sp3 hybridized polymorphs of group IV and III-V semiconductors have been studied a lot. While the polymorphs of group IV and III-V semiconductors have been studied more than one hundred years, new phases were also still first reported in last few years. Since the differences in electronic properties of various polymorphs have been reported including the variations in the band gap values, the further studies for new production of group IV and III-V semiconductors are of high importance and high interest not only scientifically but also from the viewpoint of the future device applications. Furthermore, sp, sp2, and sp3 hybridizing abilities of carbon has led to the discovery of a lot of new polymorphs with unique properties. Particularly, sp2-sp3 hybridized amorphous carbon, named Q-carbon, with ferromagnetism was synthesized. It was also reported that Q-carbon in B-doped phase shows superconductor with high critical temperature. For future application of these unique carbon materials, a theoretical analysis has been awaited to understand the local structure giving such properties.

We have studied the possibility of chemical vapor deposition (CVD) homoepitaxial growth of the hexagonal polymorphs of group IV and III-V semiconductor on the substrate in 3H(3C) phase by compressive biaxial stress. Firstly, we study electronic properties of C, Si, SiC, and BN polymorphs in 2H, 3H, 4H, and 6H phases. In optimized phases, all semiconductors in 2H, 4H, 6H are found to possess smaller lattice constant a and longer bond length along c-axis than those in 3C phase. From the band gap calculations, the band gap values are found to be different from one another among polymorphs. We further calculate the total energies and free energies as a function of in-plane lattice constant a. As a result, the relative stabilities of 2H, 4H, and 6H phases are found to be enhanced with reducing the lattice constant a. Furthermore, relative stabilities of 2H, 4H, and 6H phases are also found to be enhanced with increasing temperature. We further estimate biaxial stress values to reduce the lattice constant of substrate to a where the polymorphs other than 3H(3C) phase becomes

the most stable. Estimated stress values are small enough to realize in the case of isotropic pressure. Furthermore, from comparison to the enthalpy in isotropic pressure, biaxial compression is found to make the 2H, 4H, and 6H phases the most stable at lower pressure than the isotropic compression. Therefore, biaxial compression are suitable to realize 2H, 4H, and 6H phases. When the value of lattice constant a of substrate becomes controllable by biaxial pressure, one may be able to select the polymorphs to grow semiconductors and even synthesize the superlattice composed of heterostructures. Since the superlattice composed of polymorphs should create the quantum well due to the difference of the band gap, its application to optoelectronics devices may be possible.

For the last four decades, a lot of new carbon allotropes with unique properties were discovered. Recent experimental studies for sp2-sp3 hybridized carbon reported the ferromagnetism. Furthermore, its B-doped phase was reported to have high superconducting transition temperature T_c. We have studied the electronic properties of sp2-sp3 hybridized carbon polymorphs. In this work, we focus on theoretically predicted carbon polymorphs that have been reported by other research group, named C20-sc, C21-sc, and C22-sc. We further propose new carbon polymorphs, named C21-sc', based on the C20-sc. Firstly we calculate the electronic properties of C20-sc, C21-sc, C21-sc', and C22-sc. While the C22-sc is found to be semiconductor, C20-sc, C21-sc', and C22-sc are found to be metallic. Furthermore, C21-sc' is found to exhibit magnetic moment of 0.5 μB/sp2 atom. From the phonon calculation, all of these phases are found to be mechanically stable. We further perform the electron-phonon coupling calculation and estimate superconducting transition temperature T_c. One of the highest T_c of 61.2 K is obtained in C22-sc with 22.7 % boron doping. We have found that the C21-sc' and C22-sc in B-doped phase are expected to exhibit comparatively high T_c. Furthermore, our results in C21-sc' are found to be closer to experimental results of Q-carbon. Therefore, we confirm that C21-sc' is good candidate of local structure of Q-carbon. Present results would be useful for designing carbon and B-doped phase with interesting physical properties.