論文の内容の要旨

論文題目　Materials Design on Electronic and Optical Properties of Nitride by First-Principle Method
（窒素化合物の電子的及び光学的特性の第一原理手法による材料設計）

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The objective of material design is to find out suitable elements and atomic constituents to fabricate new materials with specified characteristics based on available database information and appropriate computational methods. The challenge is to extract the structural essence and unearth the relationships among chemical composition, structure, physical properties. Among many factors that determine the properties of materials, the structural and processing to achieve a certain structure from raw materials play essential roles.

The polymorph formed from elements in Group-IV and Group-V is an interesting and important class of materials. Recently, Silicon nitrides have attracted increasing attention as promising optoelectronic materials. Silicon nitride (Si_3N_4) is a well-known material because of its high fracture toughness, hardness and wears resistance. Three phases, alpha, beta and spinel phases of Si3N4 and Ge3N4 are well known by experiments and theoretically. It has been shown that the spinel-Si3N4 and spinel-Ge3N4 have wide, direct electronic band gaps that are comparable to those of the newly developed solid state promising optoelectronic material such as GaN, InN, AlN. Dong *et al.* indicated by their calculation that a transition to a metastable olivine phase in Ge3N4 could occur under appropriate pressure and temperature, if beta to spinel transition could be bypassed. The spinel structure type is the cubic closest-packed analogue of olivine. But until now there is no evidence in experiment to confirm this prediction. One objective of present research is to investigate the olivine material theoretically, figure out

the possibility of the transition from beta to olivine phase and compare the structural and electronic and optical properties between spinel and olivine structure in nitride. So far the spinel phases of the polymorph in Group-IV and Group-V have been synthesized under an extreme pressure and at a high temperature. Namely the total energies of them are higher than the stable beta phases respectively. For practical pplication, the stable one should be obtained and because of the difficulty of synthesizing the spinel phases, the author investigates them theoretically and obtains the optimum host spinel phase nitride of IVA group. At last, as a promising material for optoelectronic material, the dielectric function is not as efficient as some well-known optical materials such Si, GaAs. And this directly affects the function of optical conductivity and so on. It is apparent to use doping in host material to increase the peak of epsilon2 to increase the optical functions. In order to achieve the objective, a calculation based on the density functional theorem (DFT) and local density approximation (LDA) with generalized gradient approximation (GGA) is performed. The FLAPW method using a scalar relativistic effect without spin-orbit interaction embodied in the WIEN2k code is employed. As for the optical properties, the random phase approximation (RPA) is used.

In this dissertation, the author obtains the following conclusions:

(1) A investigation on the structural, electronic and optical properties of spinel and olivine phase of Si3N4 and Ge3N4 is performed. The calculation results of spinel phases agree well with experimental values. Olivine-Ge3N4 is difficult to observe which is different from the others results while olivine-Si3N4 might be observed under appropriate pressure and temperature because of small energy difference to other stable phases. Olivine-Si3N4 has a very favorable direct band gap of 2.99 eV and a large bulk modulus of 262.9 GPa.

(2) A serial of single and double spinel nitrides of IVA group are calculated and total energy of them are analyzed. The relations among the lattice parameter, the anion parameter and some

other parameters are investigated. The author obtains that the formation energy decreases as the electronegativity of double spinel materials. And as the stablest semiconductor and has good optical property, SiGe2N4 is chosen as the host material for doping to increase the peak of the epsilon2.

(3) Spinel-SiGe2N4 serial materials, spinel-Si3N4, spinel-Ge3N4 and spinel-GeSi2N4, have been investigated and the relation among the peak of epsilon2, percentage of Si in spinel structure formula and energy gap is obtained. Meanwhile, the maximum contributions of the interband transition to the peak of epsilon2 in four materials are given. The author shows that the cations in octahedrally coordinated sites play an important part on the relation. This gives some hints to improve the peak of epsilon2. Hence doping technology is utilized to confirm the hypothesis. The analysis on the result offers significant information to optical application.