論文 / 著書情報
Article / Book Information

題目(和文)	
Title(English)	Electronic properties and relative stabilities of crystalline polymorphs of group IV and III-V semiconductors: A first principles study
著者(和文)	北玲男
Author(English)	Reo Kita
出典(和文)	学位:博士(理学), 学位授与機関:東京工業大学, 報告番号:甲第12311号, 授与年月日:2023年3月26日, 学位の種別:課程博士, 審査員:齋藤 晋,村上 修一,笹本 智弘,三宅 隆,打田 正輝
Citation(English)	Degree:Doctor (Science), Conferring organization: Tokyo Institute of Technology, Report number:甲第12311号, Conferred date:2023/3/26, Degree Type:Course doctor, Examiner:,,,,
学位種別(和文)	博士論文
Category(English)	Doctoral Thesis
種別(和文)	要約
Type(English)	Outline

Electronic properties and relative stabilities of crystalline polymorphs of group IV and III-V semiconductors: A first principles study

Reo Kita

Department of Physics, Tokyo Institute of Technology

In chapter 1, we introduce the background of this study. We explain the history of sp^3 polymorphs of group IV and III-V semiconductors. In present work, we consider the probabilities of homoepitaxial CVD growth of group IV and III-V polymorphs on the substrate compressed by biaxial stress. Thus, in this chapter, we also suggest the biaxially compressed CVD method. In carbon, we further introduce the electronic properties of sp^2-sp^3 hybridized polymorphs including superconducting properties of their B-doped phase.

In chapter. 2, we give detailed explanations for the systems we studied in this work.

In chapter 3, we introduce the first-principles methods we used in our thesis.

In chapter 4, we first present electronic and thermal properties of group IV and group III-V semiconductors in 2H, 3C(3H), 4H and 6H phases. Then we also discuss the reliability of the methods we used from comparison with experimental results.

In chapter 5, we discuss the possibilities of synthesis of group IV and group III-V semiconductors in 2H, 4H, and 6H phases by biaxially compressed CVD method based on the total energy and free energy calculations. Then the biaxial stress values are estimated. Furthermore, we also estimate critical thickness where dislocations occur.

In chapter 6, we explore the carbon polymorphs with unique properties of Q-carbon. Among dozens of sp^2-sp^3 hybridized carbon polymorphs proposed so far, the C21-sc with sp^2 ratio similar to Q-carbon would be good candidate of such polymorphs. We further propose new sp^2-sp^3 hybridized carbon polymorph, named "C21-sc'", with same sp^2 ratio as C21-sc. In this study, we investigate the electronic properties of C21-sc and C21-sc' including related carbon polymorphs previously proposed so far (C20-sc and C22-sc). Especially, we focus on the magnetism since it has been reported in Q-carbon.

In chapter 7, we perform electron-phonon coupling calculation and estimate superconducting transition temperature *T*c of their B-doped phases. We also discuss the relationship between carbon polymorphs we studied and Q-carbon.

In chapter 8, we conclude whole of our studies and provide future view of this work.