論文 / 著書情報
Article / Book Information

題目(和文)	ダイヤモンド同位体超格子での電子-格子相互作用の理論研究
Title(English)	Theoretical Study of Electron-Phonon Interactions in Isotopic Diamond Superlattice
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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11044号, 授与年月日:2019年3月26日, 学位の種別:課程博士, 審査員:齋藤 晋,吉野 淳二,西森 秀稔,村上 修一,西田 祐介,是常 隆,渡邊 幸志
Citation(English)	Degree:Doctor (Science), Conferring organization: Tokyo Institute of Technology, Report number:甲第11044号, Conferred date:2019/3/26, Degree Type:Course doctor, Examiner:,,,,,,
学位種別(和文)	博士論文
Category(English)	Doctoral Thesis
種別(和文)	論文要旨
Type(English)	Summary

（博士課程）
Doctoral Program

論 文 要 旨

THESIS SUMMARY

系・コース： Department of, Graduate major in	物理学　系 物理学　コース	申請学位（専攻分野）： Academic Degree Requested	博士　（理学） Doctor of
学生氏名： Student's Name	坂東　優樹	指導教員（主）： Academic Supervisor(main)	斎藤　晋
		指導教員（副）： Academic Supervisor(sub)	

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

Isotopic diamond superlattice (IDS) where ^{12}C and ^{13}C diamond layers are periodically stacked along the [001] direction has been synthesized by H. Watanabe, et al. (2009). In this system, the confinement of excited charge carriers to ^{12}C diamond layers has been demonstrated from the carrier recombination spectrum by cathodoluminescence. This is the first evidence of the formation of quantum wells in homojunction superlattice. Although isotope effects and electron-phonon interactions (EPIs) are expected to play an important role in this carrier confinement, the details of theoretical backgrounds of this phenomenon have never been established so far because it is theoretically and numerically difficult to correctly treat isotope effects on electron-phonon interactions. In this study, we propose one approach to address these problems and reveal the physical mechanism of the formation of quantum wells due to isotope effects and electron-phonon interactions in IDSs.

We have carried out density functional theory (DFT) and density functional perturbation theory (DFPT) calculations to obtain electronic states and phonon modes of diamond, respectively. By using maximally localized Wannier functions and the force constant model, we have converted real-space physical parameters of a specific unit cell of diamond to those of IDSs. This approach allows us to carry out computations of electronic states and phonon modes in large IDSs while keeping the accuracy of first-principles calculations with much less computational costs. In the calculations of EPIs, we have developed a simple tight-binding (TB) model for diamond. This TB model is based on the Wannier representation of EPIs. Furthermore, we have adopted the quasiparticle self-consistent GW method to correctly include isotope effects on EPIs. As a consequence, we have introduced a new theoretical approach for calculating EPIs which takes the off-diagonal matrix elements of the self-energy operator of EPIs into account. We name this approach as quasiparticle TB model.

We have studied phonon localizations in several IDSs by using the DFPT and the force constant model. We have revealed that phonon localizations are caused by isotope effects when the thickness of each isotopic diamond layer is over 3.1 nm in [001] and [111] IDSs and there are several types of phonon localizations depending partly on the phonon frequencies. Since phonon localizations could strongly influence EPIs, these results are helpful to discuss the formation of quantum wells in IDSs. We have compared zero-point renormalizations (ZPRs) between our quasiparticle TB method and the DFPT in isotopically pure ^{12}C diamond. It has been found that our quasiparticle TB model reproduces the ZPRs obtained from DFPT calculations around the valence-band-top states at the Γ point. In addition, we have revealed that the off-diagonal matrix elements of the self-energy operator of EPIs vanish in isotopically pure ^{12}C diamond. These results indicate that our quasiparticle TB model is theoretically equivalent to the conventional DFPT approach when we consider an isotopically pure system.

To clarify the physical mechanism of the formation of quantum wells in IDSs, we have analyzed the electronic structure at the Γ point in virtual $^{6}C/^{24}C$ [001] IDSs. It has been found that the conventional approach, which considers only the diagonal matrix elements of the self-energy operator of EPIs, cannot provide energy levels corresponding to the valence-band edge of ^{6}C diamond in any IDSs. On the other hand, our quasiparticle TB model shows energy levels approaching the valence-band edge of ^{6}C diamond as a function of the number of stacking ^{6}C and ^{24}C diamond layers. Here, we have confirmed that several energy levels localize either to ^{6}C or ^{24}C diamond layers from the partial density of states in real and energy space. Then, off-diagonal matrix elements of the self-energy operator of EPIs are not zero and we have revealed that they are of high importance when several isotopes are spatially distributed in the system.

We have carried out the same analysis by using our quasiparticle TB model in actual $^{12}C/^{13}C$ [001] IDSs. Here, we have confirmed that several energy levels localize to ^{12}C diamond layers when the thickness of each isotopic diamond layer is about 20 nm. This thickness is consistent with the experimental result reported by H. Watanabe, et al. (2009) and is extremely larger than the thickness of virtual $^{6}C/^{24}C$ IDSs. We therefore have concluded that the difference of the ZPRs between isotopic diamond layers becomes important for the formation of quantum wells.