Web of Science

Clarivate Analytics

Electronic structure of beta-Si3N4 crystals with substitutional icosagen group impurities

By: Kutlu, E (Kutlu, E.)[1]; Narin, P (Narin, P.)[1]; Atmaca, G (Atmaca, G.)[1]; Sarikavak-Lisesivdin, B (Sarikavak-Lisesivdin, B.)[1]; Lisesivdin, SB (Lisesivdin, S. Bora)[1]; Ozbay, E (Ozbay, E.)[2,3,4]

JOURNAL OF OPTOELECTRONICS AND ADVANCED MATERIALS

Volume: 19

Issue: 3-4

Pages: 278-282

Published: MAR-APR 2017

Abstract

The beta-Si3N4 crystals are widely used in industrial and electronics areas. Therefore, beta-Si3N4 has drawn the attention of researchers for many years. In this study, effects of icosagen group impurity atoms in the IIIA group on the electronic properties of the beta-Si3N4 crystal were analyzed by using the density functional theory. As a result of these analyses, it was determined that the electronic properties of the crystal change significantly. Basic electronic characteristics for pure beta-Si3N4 crystal and icosagen group impurity beta-Si3N4 crystals, such as band structures, densities of states, binding energies, and formation energies were investigated. We identified that the band gap of the beta-Si3N4 crystal was affected significantly by the impurity, and this change was varying linearly in line with the formation energy for the impurity cases. As a result of calculations, the Al-impurity was found to be the lowest-energy impurity state.

Keywords

Author Keywords:DFT; beta-Si3N4; Electronic structure; Formation energy; Impurity
KeyWords Plus:SILICON-NITRIDE; OPTICAL-PROPERTIES; 1ST-PRINCIPLES CALCULATIONS; MECHANICAL-PROPERTIES; GAMMA-SI3N4; BETA-C3N4; FIELD

Author Information

Reprint Address: Kutlu, E (reprint author)

+ Gazi Univ, Dept Phys, Fac Sci, TR-06500 Ankara, Turkey.

Addresses:

+ [1] Gazi Univ, Dept Phys, Fac Sci, TR-06500 Ankara, Turkey
+ [2] Bilkent Univ, Nanotechnol Res Ctr, TR-06800 Ankara, Turkey
+ [3] Bilkent Univ, Dept Phys, TR-06800 Ankara, Turkey
+ [4] Bilkent Univ, Dept Elect & Elect Engn, TR-06800 Ankara, Turkey

E-mail Addresses:eciss06@gmail.com

Funding

Funding Agency	Grant Number
TUBITAK Ankara	113F364

View funding text

Publisher

NATL INST OPTOELECTRONICS, 1 ATOMISTILOR ST, PO BOX MG-5, BUCHAREST-MAGURELE 76900, ROMANIA

Categories / Classification

Research Areas: Materials Science; Optics; Physics
Web of Science Categories: Materials Science, Multidisciplinary; Optics; Physics, Applied

Document Information

Document Type: Article

Language: English
Accession Number: WOS:000411913200024
ISSN: 1454-4164
eISSN: 1841-7132

Journal Information

- **Impact Factor:** Journal Citation Reports

Data from the 2016 edition of Journal Citation Reports

Other Information

IDS Number: FI4BB
Cited References in Web of Science Core Collection: 21
Times Cited in Web of Science Core Collection: 1

Electronic structure of beta-Si3N4 crystals with substitutional icosagen group impurities

By: Kutlu, E (Kutlu, E.)[1]; Narin, P (Narin, P.)[1]; Atmaca, G (Atmaca, G.)[1]; Sarikavak-Lisesivdin, B (Sarikavak-Lisesivdin, B.)[1]; Lisesivdin, SB (Lisesivdin, S. Bora)[1]; Ozbay, E (Ozbay, E.)[2,3,4]

JOURNAL OF OPTOELECTRONICS AND ADVANCED MATERIALS
Volume: 19 **Issue:** 3-4 **Pages:** 278-282
Published: MAR-APR 2017
View Journal Impact

Abstract

The beta-Si3N4 crystals are widely used in industrial and electronics areas. Therefore, beta-Si3N4 has drawn the attention of researchers for many years. In this study, effects of icosagen group impurity atoms in the IIIA group on the electronic properties of the beta-Si3N4 crystal were analyzed by using the density functional theory. As a result of these analyses, it was determined that the electronic properties of the crystal change significantly. Basic electronic characteristics for pure beta-Si3N4 crystal and icosagen group impurity beta-Si3N4 crystals, such as band structures, densities of states, binding energies, and formation energies were investigated. We identified that the band gap of the beta-Si3N4 crystal was affected significantly by the impurity, and this change was varying linearly in line with the formation energy for the impurity cases. As a result of calculations, the Al-impurity was found to be the lowest-energy impurity state.

Keywords

Author Keywords: DFT; beta-Si3N4; Electronic structure; Formation energy; Impurity
KeyWords Plus: SILICON-NITRIDE; OPTICAL-PROPERTIES; 1ST-PRINCIPLES CALCULATIONS; MECHANICAL-PROPERTIES; GAMMA-SI3N4; BETA-C3N4; FIELD

Author Information

Reprint Address: Kutlu, E (reprint author)

+ Gazi Univ, Dept Phys, Fac Sci, TR-06500 Ankara, Turkey.

Addresses:

+ [1] Gazi Univ, Dept Phys, Fac Sci, TR-06500 Ankara, Turkey
+ [2] Bilkent Univ, Nanotechnol Res Ctr, TR-06800 Ankara, Turkey
+ [3] Bilkent Univ, Dept Phys, TR-06800 Ankara, Turkey
+ [4] Bilkent Univ, Dept Elect & Elect Engn, TR-06800 Ankara, Turkey

E-mail Addresses: eciss06@gmail.com

Funding

Funding Agency	Grant Number
TUBITAK Ankara	113F364

View funding text

Publisher

NATL INST OPTOELECTRONICS, 1 ATOMISTILOR ST, PO BOX MG-5, BUCHAREST-MAGURELE 76900, ROMANIA

Categories / Classification

Research Areas: Materials Science; Optics; Physics
Web of Science Categories: Materials Science, Multidisciplinary; Optics; Physics, Applied

Document Information

Document Type: Article
Language: English
Accession Number: WOS:000411913200024
ISSN: 1454-4164
eISSN: 1841-7132

Journal Information

Impact Factor: Journal Citation Reports

Other Information

IDS Number: FI4BB
Cited References in Web of Science Core Collection: 21
Times Cited in Web of Science Core Collection: 1