

本期目录 | 下期目录 | 过刊浏览 | 高级检索

[打印本页] [关闭]

论文

C和As共掺杂的 γ -Si₃N₄电子性质的密度泛函理论研究

张玉芬, 程秀凤, 赵显

山东大学晶体材料研究所, 济南 250100

摘要:

采用密度泛函理论研究了C和As共掺杂的 γ -Si₃N₄的电子性质. 当晶体中少量的四配位硅原子被碳原子所取代, 同时用少量的砷原子取代氮原子, 晶体结构的带隙可以被调整; 当 $n(\text{C})/n(\text{Si})\approx 0.063$, $n(\text{As})/n(\text{N})\approx 0.047$ 时, 材料会发生绝缘体到金属的转变. 从态密度图中可以观察到价带顶端的能量明显上升. 讨论了关于这种共掺杂所引起的带隙较大减小的可能原因和潜在的应用.

关键词: 密度泛函理论; 电子性质; C和As共掺杂的 γ -Si₃N₄

Electronic Properties of Codoped Spinel Silicon Nitride with C and As by DFT Method

ZHANG Yu-Fen, CHENG Xiu-Feng, ZHAO Xian*

State Key Lab of Crystal Materials, Shandong University, Jinan 250100, China

Abstract:

Density functional calculations were performed to investigate the electronic properties of codoped spinel silicon nitride with C and As. When very low concentrations of Si was replaced by C at the tetrahedral sites, together with the doping of substitutional As impurity in spinel silicon nitride, the band-gap could be adjusted, and an insulator-to-metal transition would occur at the C/Si ratio ~ 0.063 and As/N ratio ~ 0.047 . Seen from the DOS spectra, it is clearly observed that the TDOS increases at the valence band maximum. Finally, some possible examinations and potential applications for the large band-gap reduction are discussed.

Keywords: Density functional theory; Electronic property; Codoped spinel silicon nitride with C and As

收稿日期 2009-03-02 修回日期 网络版发布日期

DOI:

基金项目:

国家“九七三”重大基础研究前期专项(批准号: 2005CCA00900)资助.

通讯作者: 赵显, 男, 博士, 教授, 博士生导师, 主要从事晶体材料理论研究. E-mail: zhaoxian@sdu.edu.cn

作者简介:

参考文献:

- [1] Zerr A., Miehle G., Serghiou G., et al.. Nature[J], 1999, 400: 340—342
- [2] Sekine T.. J. Am. Ceram. Soc.[J], 2002, 85: 113—116
- [3] Serghiou G., Miehle G., Tschauner O., et al.. J. Chem. Phys.[J], 1999, 111: 4659—4662
- [4] Leinenweber K., O’Keeffe M., Somayazulu M. S., et al.. Chem. Eur. J.[J], 1999, 5: 3076—3078
- [5] Scotti N., Kockelmann W., Senker J., et al.. Anorg. Allg. Chem.[J], 1999, 625: 1435—1439
- [6] Soignard E., McMillan P. F., Leinenweber K.. Chem. Mater.[J], 2004, 16: 5344—5349
- [7] Sekine T., Mitsuhashi T.. Appl. Phys. Lett.[J], 2001, 79: 2719—2721
- [8] Mo S. D., Ouyang L., Ching W. Y., et al.. Phys. Rev. Lett.[J], 1999, 83: 5046—5049
- [9] Dong J., Deslippe J., Sankey O. F., et al.. Phys. Rev. B[J], 2003, 67: 094104-1—094104-7
- [10] Ching W. Y., Mo S. D., Tanaka I., et al.. Phys. Rev. B[J], 2001, 63: 064102-1—064102-4
- [11] Ching W. Y., Mo S. D., Ouyang L., et al.. Phys. Rev. B[J], 2000, 61: 10609—10614

扩展功能

本文信息

Supporting info

PDF(314KB)

[HTML全文]

[\({article.html_WenJianDaXiao}\)
KB](#)

参考文献[PDF]

参考文献

服务与反馈

把本文推荐给朋友

加入我的书架

加入引用管理器

引用本文

Email Alert

文章反馈

浏览反馈信息

本文关键词相关文章

密度泛函理论; 电子性质; C和As共掺杂的 γ -Si₃N₄

本文作者相关文章

PubMed

- [12]Kroll P.. J. Solid State Chem.[J], 2003, 176: 530—537
- [13]Zhang Y. F., Zhao X., Cheng X. F., et al.. J. Solid State Chem.[J], 2008, 181: 2113—2116
- [14]Zerr A., Riedel R., Sekine T., et al.. Adv. Mat.[J], 2006, 18: 2933—2948
- [15]Pankove J. I., Hutchby J. A.. J. Appl. Phys.[J], 1976, 47: 5387
- [16]Bellaiche L., Wei S. H., Zunger A.. Appl. Phys. Lett.[J], 1997, 70: 3558—3560
- [17]Li J. B., Wang L. W.. Phys. Rev. B[J], 2003, 67: 033102-1—033102-4
- [18]Kohn W., Sham L. J.. Phys. Rev.[J], 1965, 140: A1133—A1138
- [19]Payne M. C., Teter M. P., Allan D. C., et al.. Rev. Mod. Phys.[J], 1992, 64: 1045—1097
- [20]Vanderbilt D.. Phys. Rev. B[J], 1990, 41: 7892—7895
- [21]Perdew J. P., Burke K., Ernzerhof M.. Phys. Rev. Lett.[J], 1996, 77: 3865—3868
- [22]Monkhorst H. J., Pack J. D.. Phys. Rev. B[J], 1976, 13: 5188—5192
- [23]Polak E.. Computational Methods in Optimization[M], New York: Academic, 1971: 56
- [24]Zerr A., Schwarz M., Schmechel R., et al.. Acta Crystallogr.[J], 2002, A 58: C47
- [25]Leitch S., Moewes A., Ouyang L., et al.. J. Phys.: Condens. Matter[J], 2004, 16: 6469—6476
- [26]Xua M., Dinga Y. C., Xionga G., et al.. Physica B[J], 2008, 403: 2515—2520
- [27]Lagowski J. J.. Modern Inorganic Chemistry[M], New York: Marcel Dekker, 1973: 806

本刊中的类似文章

文章评论

反馈人	<input type="text"/>	邮箱地址	<input type="text"/>
反馈标题	<input type="text"/>	验证码	<input type="text" value="4729"/>