



吉首大学学报自然科学版 » 2004, Vol. 25 » Issue (1): 71-74 DOI:

[重点学科](#)

[最新目录](#) | [下期目录](#) | [过刊浏览](#) | [高级检索](#)

[◀◀ Previous Articles](#) | [Next Articles ▶▶](#)

## 热膨胀对固体能带结构的影响

( 1. 湘潭大学物理系, 湖南湘潭 411105; 2. 吉首大学物理与电子工程系, 湖南吉首 416000)

### The Influences of the Thermal Expansion on the Energy Band Structure of a Solid

( 1. Department of Physics, Xiangtan University, Xiangtan 411105, Hunan China; 2. Department of Physics and Electronic Engineering, Jishou University, Jishou 416000, Hunan China)

- [摘要](#)
- [参考文献](#)
- [相关文章](#)

**全文:** [PDF \(752 KB\)](#) [HTML \(1 KB\)](#) **输出:** [BibTeX](#) | [EndNote \(RIS\)](#) [背景资料](#)

**摘要** 以体心立方结构为例, 利用紧束缚理论, 讨论了热膨胀对固体能带结构的影响, 具体计算了体心立方晶格的1S能带和2S能带。结果表明: 随着温度的上升, 热膨胀将使固体的晶格常数发生变化, 使得1S和2S的能带中心和能带边缘产生移动, 从而对各能带的宽度和两带之间的禁带宽度都产生影响。所得结论能较好地说明锂金属的部分实验结果。

**关键词:** 热膨胀 能带宽度 禁带宽度

**Abstract:** Using the tight-binding theory, the influences of the thermal expansion on the energy band structure of the solid with a body-centered cubic lattice was discussed, the 1S and 2S energy bands of body-centered cubic lattice were calculated. The results show that with the increase of temperature, the thermal expansion makes lattice constant change, which will result in the shifts of the center of the 1S and 2S energy bands and the energy band edge; therefore, the width of every energy band and the forbidden band-width between two bands will change. These results can explain fairly the partial experimental results of the Li metal.

**Key words:** [thermal expansion](#) [energy band-width](#) [forbidden band-width](#)

#### 服务

- ▶ [把本文推荐给朋友](#)
- ▶ [加入我的书架](#)
- ▶ [加入引用管理器](#)
- ▶ [E-mail Alert](#)
- ▶ [RSS](#)

#### 作者相关文章

- ▶ [李德俊](#)
- ▶ [唐翌](#)
- ▶ [叶伏秋](#)
- ▶ [赵鹤平](#)
- ▶ [周秀文](#)

#### 基金资助:

湖南省自然科学基金资助项目( 03JJY6008) ; 湖南省教育厅自然科学基金资助项目( 00C189)

**作者简介:** 李德俊( 1956- ), 男, 湖南省澧县人, 吉首大学物理与电子工程系副教授, 主要从事凝聚态物理研究。

#### 引用本文:

李德俊, 唐翌, 叶伏秋等. 热膨胀对固体能带结构的影响[J]. 吉首大学学报自然科学版, 2004, 25(1): 71-74.

LI De-Jun, TANG Yi, YE Fu-Qiu et al. The Influences of the Thermal Expansion on the Energy Band Structure of a Solid[J]. Journal of Jishou University ( Natural Sciences Edit), 2004, 25(1): 71-74.

- [1] 沈学础. 半导体的光学性质[M]. 北京: 科学出版社, 1992. 131- 140.
- [2] FAN H Y. Temperature Dependence of the Energy Gap in Semiconductors[ J]. Phys. Rev. , 1951, 82: 900.
- [3] COHEN M L, TSANG Y W. Calculation of the Temperature Dependence of the Energy Gaps in PbTe and SnTe[ J]. Phys. Rev. , 1971, B3: 1 254.
- [4] SCHLUTER M, MARTINZE G, COHEN M L. Pressure and Temperature Dependence of Electronic Energy Levels in PbSe and PbTe[ J]. Phys. Rev. , 1975, B12: 650.

- [5] ALLEN P B, HEINE V. Theory of the Temperature Dependence of Electronic Band Structures[ J] . J. Phys. , 1976, C9: 2 305.
- [6] CHADIAND D J, COHEN M L. Electronic Structure of Hg<sub>1-x</sub>Cd<sub>x</sub>Te Alloys and Charge- Density Calculations Using Representative k Points [ J] . Phys. Rev. , 1973, B7: 692.
- [7] GUENZER C S, BIENENSTOCK A. Temperature Dependence of the Energy Gap in Semiconductors[ J] . Phys. Rev. , 1973, B8: 4 655.
- [8] HEINE V, VAN VECHTEN J A. Effect of Electron- Hole Pairs on Phonon Frequencies in Si Related to Temperature Dependence of Band Gaps [ J] . Phys. Rev. , 1976, B3: 1 622.
- [9] 祇圣麟. 原子物理学[M]. 北京: 人民教育出版社, 1979. 115- 120.

没有找到本文相关文献

版权所有 © 2012 《吉首大学学报(自然科学版)》编辑部  
通讯地址: 湖南省吉首市人民南路120号《吉首大学学报》编辑部 邮编: 416000  
电话传真: 0743-8563684 E-mail: xb8563684@163.com 办公QQ: 1944107525  
本系统由北京玛格泰克科技发展有限公司设计开发 技术支持: support@magtech.com.cn