

论文

自由能展开式中点群的不可约表示的基函数

周国香, 何文辰, 郭革新, 李佳

河北工业大学理学院, 河北师范大学

摘要:

一个群的基函数的选择并非唯一, 不同的基函数对应不同的表示矩阵。即使相同的表示矩阵, 基函数也可以有不同的选择。在相变的宏观唯象理论中, 自由能展开式可由同一个表示矩阵的基函数来构造, 因而给出不可约表示的基函数表就非常有意义。现有文献给出的32点群不可约表示的基函数只写到二次幂, 而且有些文献中的同一个不可约表示所选取的不同的基函数却对应不同的表示矩阵, 这样在构造群变换不变式时, 就会出错。该文将基函数表写至三次幂, 这有助于准确、迅速地写出到六次幂群变换不变的自由能表达式。由新的基函数表发现十八种点群有三次幂的群操作不变式, 高温相属这些点群铁电体, 发生的本征铁电相变为一二级相变。

关键词: 点群 不可约表示 基函数 不变式 自由能展开式 Landau 理论

分类号:

20C35

The Base Function of the Irreducible Representation for Point Groups in the Expansion of Free Energy

ZHOU Guo-Xiang, HE Wen-Chen, GUO Ge-Xin, LI Jia-

Abstract:

There are many choices for the selection of the base functions (BF) of the irreducible representations for point groups. The different BF corresponds to the different representative matrix. Although under the same matrix, there are different choices for BF. The expansion of the free energy can be constructed by BF when the phenomenological phase transition theory is used. So the table of the BF of the irreducible representations is significant. In the literatures before, the BF is up to the second order. Furthermore, in some literature, the different BF for the same irreducible representations corresponds to different representative matrix. It is wrong by using such BF to obtain the invariant. The third order BF was supplemented in this paper. The table of BF given in this paper is very helpful for obtaining the expansion of the free energy correctly and rapidly. Eighteen kinds of point groups were found having third order invariant. If the group of the high temperature crystal structure is one of these points groups, then the ferroelectrics undertake the first order phase transition when temperature is lowered.

Keywords: Irreducible representation, Base function Invariant, Expansion of free energy, Landau theory

收稿日期 修回日期 网络版发布日期

DOI:

基金项目:

河北省高校重点学科建设项目资助

通讯作者:

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