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论文

# 金属缺陷能量学基础及掺杂晶界电子结构

王崇愚

冶金工业部钢铁研究总院;北京,100081

摘要： 本文综述了我们发展建立的第一原理原子间相工作用势及原子间相互作用能的理论计算方法同时报告了在金属缺陷、掺杂晶界电子结构及晶体基本性质的研究中，能量函数作为理论基础的里要应用另一方面、基于第一原理及Green函数方法研究了具有重要应用潜势的金属间化合物的电子结构及掺杂效应，揭示了杂质-晶界复合的量子效应及其与合金特性及位错反应的相关机制；指出B，N等元素具有强化晶界作用，P，S为脆化元素，MI影响Ti—AI合金形变机制

关键词： 原子间相互作用 掺杂晶界 电子结构

## ENERGETICS OF METALLIC DEFECT AND ELECTRONIC STRUCTURE OF DOPED GRAIN BOUNDARY

WANG Chongyu (Central Iron and Steel Research Institute, Ministry of Metallurgical Industry, Beijing 100081)

Abstract: In this paper, we reviewed that a first principles interatomic potential and the theoretical calculation method of interaction energy between atoms, which are developed by us. Meanwhile, the important role of the energetic functions in the studies of the electronic structure of the impurity-grain boundary complexes and the basic properties of the crystal are reported. On the other hand, the electronic structure and the doping effect of intermetallic compound are studied by the use of first principles method and Green function method. The quantum effect of impurity-grain boundary complexes and the correlation mechanism between the electronic structure with the property of a1loy and dislocation reaction are explored.We find that Boron and Nitrogen have strengthening effect for the cohesion of grain boundary, and the phosphorous and sulphur are embrittle exements in the grain boundary of Ni-base alloy. Molybdemum influence the deformation mechanism of Ti-Al intermetallic compound.

Keywords: interaction of atoms doped grain boundary electronic structure

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通讯作者:

作者简介:

作者Email:

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