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H和B原子在有序态 Ni_3Fe 表面的吸附

刘婧颖, 谢耀平, 陈业新, 黄晓君, 赵世金

上海大学 微结构重点实验室，上海 200072

Effect of Electronic Structure on Adsorption of H and B Atoms on Ordered Ni-3Fe Surface

LIU Jing-ying, XIE Yao-ping, CHEN Ye-xin, HUANG Xiao-jun, ZHAO Shi-jin

Laboratory for Microstructures, Shanghai University, Shanghai 200072, China

- 摘要
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摘要 采用基于密度泛函理论(density functional theory, DFT)的第一性原理方法，对H和B原子在有序态 Ni_3Fe 合金(111)表面的吸附进行研究.结果表明，B原子在有序态 Ni_3Fe 合金(111)表面的吸附能远低于H原子，从而更容易被有序态 Ni_3Fe 合金(111)表面吸附，形成稳定结构.这导致H原子在有序态Ni-3Fe合金表面的吸附机会大大减少，降低了有序态 Ni_3Fe 合金在氢气中的环境氢脆.进一步的电子结构分析表明，H原子的表面吸附能高于B原子是由于H原子在有序态 Ni_3Fe 合金(111)表面吸附时，H原子的反键态被推到了费米面以上所引起的.

关键词： Ni-3Fe 环境氢脆 硼（B）

Abstract: This paper performs first-principles calculations based on the density functional theory (DFT) to investigate the interaction of H and B atoms with ordered Ni_3Fe (111) surface. The results showed that the B atom can be strongly absorbed onto the surface, and absorption energies of B atoms are much lower than that of H atoms. It indicates that the B atom can be easily bound by the ordered Ni_3Fe surface, which occupies the suitable site and inhibits the access of H into the matrix. Furthermore, electronic structure analysis is presented to understand that the adsorption energy of H atom higher than that of B atom is accrediting to its anti-bonding state being pushed up to the Fermi level when an H atom is absorbed on the (111) surface of the ordered Ni_3Fe

Keywords: Ni_3Fe, environmental hydrogen embrittlement, boron (B)

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作者简介: 陈业新（1958—），男，研究员，博士生导师，博士，研究方向为材料中的扩散与相变. E-mail：yxchen@shu.edu.cn

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