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Ni-B非晶态合金局域结构和电荷转移性质的理论研究

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摘要 根据非晶态合金结构的短程有序、Ni和B间存在较强的化学作用、
结构中存在B－B键直接相连的实验事实，选择Ni~mB~2(m=1,2,4)
原子簇作为非晶态局域结构的计算模型。考虑原子簇间的相互作用，又对[Ni~4B~2]~n(n=1,2,5,7)
簇团进行了系统计算。结果表明在所选Ni-Br的簇模型中，都是B原子提供电荷给Ni原子，
这些均与非晶态合金实验结果和一些理论计算结果相符。簇团的计算结果还表明，小原子簇Ni~4B~2
内原子间存在较强的化学键作用，而簇间的相互作用相对较弱，很容易造成对称性破缺而导致产生长程无序，
因此Ni-B非晶态可以被看成是由大量i上原子簇无序堆砌成的，
这一点也同实验事实相吻合。计算结果也表明我们前面工作中所取的和最常见的Ni-B非晶态合金Ni~6~4B~3~6
有相似组成的Ni~4B~2原子簇模型能在一定程度上反映Ni-B非晶态合金的局域结构特征。

关键词 镍合金 硼合金 电荷转移 原子簇 非晶

分类号 0641

Theoretical study on the local structure and properties of electron transfer of Ni-b amorphous alloy

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Abstract The electron-transfer between Ni and B is an open issue in the study of Ni-B amorphous alloy. This problem is very important in the understanding of its catalytic behavior and other related properties. According to the experimental facts of the presence of direct B-B contact, a very strong interaction between Ni and B and short-range- ordering in the amorphous alloy, Ni~mB~2(m=1,2,4) cluster models were chosen as the models of local structure of amorphous alloy Ni-B, and they were calculated for examining their structure and electronic properties. Considering the interaction between the clusters, we also performed the calculation of the group of clusters [Ni~4B~2]~n(n=1,2, 5,7). The results of the calculations show that boron is a electron- donor in the Ni-B amorphous alloy, while nickel is a electron-acceptor, which agrees well with the experimental results and previous theoretical result. Meanwhile, the results also show that there exists quite strong interaction of chemical bond in the cluster, while the interactions between the clusters is relatively weak. Thus, it could be concluded that the Ni~4B~2 cluster model is able to reflect the character of local structure of Ni-B (Ni~6~4B~3~6) amorphous alloy partly.

Key words NICKEL ALLOYS BORON ALLOY CHARGE TRANSFER AMORPHOUS

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