MgB_2(001)面超导结构的电子浓度第一原理分析

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摘要 采用密度范函理论计算了金属化合物MgB_2(001)薄膜结构的电子能带结构和状态密度，计算的交换相关能分别采用LDA和GGA。规范保守赝势的计算结果表明，晶格常数与实验值误差在很小的范围内，分析了引起MgB_2(001)面结构超导转变时电子浓度和偏态密度的变化情况，发现构成该超导体结构的成键有3种，着重从结构的电子浓度变化分析了其超导特性，六角蜂窝状结构中硼原子间相互作用为sp2杂化的共价键，镁原子和硼原子之间是离子键结合，镁原子层是金属键结合，镁原子的价电子部分转移到硼原子的pz轨道，部分电子为镁原子层共用。MgB_2(001)的超导机制为强烈的电子-声子耦合，为B原子间强烈的共价作用形成，是传统S波超导体。对Mg元素同一主族的其它硼化物进行布居分析，发现MgB_2中Mg原子电子转移明显强于BeB_2和CaB_2，说明电子浓度是引起超导转变的一个重要因素。

关键词 耐热镁合金 ZC62 ZC63 显微组织

First Principles Analysis of Electronic Concentration of Superconducting

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Abstract Both GGA and LDA are applied to calculate the band structure and DOS of MgB_2 (001). The ionic “core” is represented by Pseudo potential. Crystal lattice constants are close to other experiment results. Three kinds of chemical bonds exist among Mg and B atoms, between magnesium and boride is ionic bond and metallic bond is the predominant interaction in the layer formed by magnesium atoms. A strong covalent bond in the form of sp2 hybrid between boride atoms is the most important factors which can affect the transition temperature of MgB_2. Population analysis clearly shows that electrons are transferred from Mg to B, as a result, the electron-phonon coupling in the layer of B is very strong. The electron populations of BeB_2 and CaB_2 are also clarified and the results among them are compared. The electron transfer between metallic atom and B is mostly obvious in MgB_2.

Keywords High-T_C superconductors, density functional theory, electronic structure, DOS, electron-phonon coupling

责任编辑：
2008年3月第2期