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氢氧化铝表面性质的CASTEP计算及其晶面叠合分析

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摘 要：用剑桥连续总能量软件包(CASTEP)程序，对氢氧化铝的各个经常显露面族的(001)、(100)、(010)、(011)、(110)、(101)和(112)面进行理论计算，分析氢氧化铝晶体的晶面显露特征与表面化学键力的关系。对氢氧化铝晶体的径向长大、附聚长大的机制和晶体生长中晶面叠合方式以及同类面族、非同类面族间的叠合进行研究。计算结果表明，对于长大后的氢氧化铝晶体，当(001)，(101)和(100)面为主要显露面时，能量状态较为稳定；若(010)面显露较多，长大后的晶体的能量稳定性较差。氢氧化铝的(001)面的前线价电子较为活跃，其晶面可能存在与铝酸钠溶液中不同形态的铝酸根离子或者是晶体生长基元发生键合的“活性点”。键布居分析结果表明，整体上氢氧化铝的(001)面的Al—O键的结合力不强，(011)和(110)面的Al—O键的平均键布居数较高，结合力较强；若小幅度降低(001)面的显露比例，并使(110)和(011)面较多显露，就有可能提高氢氧化铝表面的Al—O键的结合力。

关键字：氢氧化铝；表面性质；晶面叠合；机制

CASTEP calculation of surface property of gibbsite and analysis of crystal surface combination

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Abstract: Based on the theoretic calculation of crystal faces (001), (100), (010), (011), (110), (101) and (112) of gibbsite by CASTEP program, the relationship between unfold character of crystal face and chemical bond strength of surface of gibbsite was investigated. The mechanism of precipitation and growth of sodium aluminate solution and crystal surface combination mode were studied. The combinations of same faces and different faces of gibbsite were investigated. The results show that the energy state of gibbsite is more stable when faces (001), (101) and (100) are mainly unfold faces, while the energy state would be instable when face (010) is mainly unfolded. Whereas the calculation result of electric structure shows that the front valence electron of face (001) of gibbsite is active correspondingly. That is there may be some activity points on this face. It is found that from bond population calculation results, the bonding strength of Al—O bond of faces (011) and (011) of gibbsite are stronger than that of face (001). If the proportion of unfold of (001) surface is decreased and

the proportion of unfold of (011) and (011) surfaces is increased to same possible extend, the bonding strength of Al—O bond of gibbsite would be more strong.

Key words: gibbsite; surface property; crystal surface combination; mechanism

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