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含硅杂质对铝酸钠溶液分解过程的影响及相互作用机理

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摘 要：研究了二氧化硅对铝酸钠溶液分解过程的分解率、产品粒度及形貌的影响。根据实验结果用基于密度泛函的Dmol3程序计算SiO_3^{2-}以各种不同方式位于氢氧化铝(001)和(100)面时的总能量和电子结构等，用晶体生长习性计算程序Morphology分析各体系的平衡形态及生长习性。实验结果表明：在一定的分解时间范围内，硅能抑制铝酸钠溶液种分分解，对分解产物氢氧化铝的晶体形貌有影响，其(100)面的显露有所增加。理论计算结果表明：SiO_3^{2-}的存在明显改变氢氧化铝(001)和(100)表面的电子结构，SiO_3^{2-}在氢氧化铝(001)和(100)表面上时，靠近(001)面的O原子多的体系稳定性低。平衡形态及生长习性计算结果表明：SiO_3^{2-}在氢氧化铝(001)表面上时，各体系长大晶粒的体积均小于无SiO_3^{2-}体系中(001)的晶粒体积；而SiO_3^{2-}在氢氧化铝(100)表面上时，各体系长大晶粒的体积比均大于SiO_3^{2-}体系中(100)的晶粒体积。

关键字：铝酸钠溶液；含硅杂质；微观机制；结晶习性

Effect of silicon-containing impurity on precipitation of sodium aluminate solution and interaction mechanism

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Abstract: By analyzing the changes of precipitation ratio, particle size and morphology, the effect of the impurity ingredient contained silicon on the process of precipitation of sodium aluminate was studied. According to these experimental results, the total energy and electronic structure of SiO_3^{2-} located on gibbsite (001) and (100) face with some different modes were calculated by using Dmol3 program based on DFT, and the equilibrium and growth morphology of systems were analyzed by using crystal growth habit program morphology. The experimental results show that the silicon dioxide influences the precipitation rate and morphology of gibbsite, and the (100) face of gibbsite is easier to unfold. The theoretic calculation results indicate that the electronic structures of (001) and (100) surface change obviously when SiO_3^{2-} is located on the

surface, and the stability of the system with more oxygen atom is lower. The calculation results of equilibrium morphology and growth habit show that the volume of growth crystal is smaller when SiO_3^{2-} is located on gibbsite (001) surface, while the volume is larger when SiO_3^{2-} is located on gibbsite (100) surface, compared with the systems without SiO_3^{2-}.

Key words: sodium aluminate; silicon-containing impurity; microcosmic mechanism; crystal habit

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