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氢氧化铝晶体生长习性的Morphology分析

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摘要: 对氢氧化铝晶体生长习性进行Morphology理论研究, 明确氢氧化铝晶粒长大后的晶粒形态特征及氢氧化铝的理论晶体生长习性。首先, 用BFDH法说明了生长过程中最重要的面; 其次, 采用晶体平衡形态(Equilibrium morphology)法, 用Morphology程序对氢氧化铝 $3 \times 4 \times 2$ 超晶胞及其(001), (100), (010), (011), (110), (101)和(112)面真空slab模型进行平衡形态计算, 计算结果与实验结果吻合, 很好地预测了各显露面族(001), (100), (010), (011), (110), (101)和(112)面族。理论生长习性计算结果表明, 氢氧化铝 $3 \times 4 \times 2$ 超晶胞及其各表面真空slab模型的生长习性差异显著; 氢氧化铝(gibbsite)超晶胞趋向于生长为准六棱柱或厚的准六角板状晶体; (001), (100)和(010)面slab基本上是生长为楔板状晶体; (110), (101)和(112) slab的晶体形态则趋向于生长为较细长的棒状晶体; (011) slab的生长形态介于楔板状和棒状之间, 很可能生长为较薄的片状晶体。

关键字: 氢氧化铝; 超晶胞; 生长习性; 晶体形态

Morphology analysis on crystal growth habit of gibbsite

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Abstract: By analyzing the crystal growth habit of gibbsite theoretically using Morphology program, the morphology character of crystal grain and the theoretic habit of gibbsite were studied. Firstly, the important faces of the process of precipitation of sodium aluminate were calculated preparatory using Bravais-Friedel Donnay Harker (BFDH) method. Secondly, the equilibrium morphology calculations were processed on gibbsite $3 \times 4 \times 2$ super cell and its (001), (100), (010), (011), (110), (101) and (112) slab models. The calculation results are coincident with experimental results, and the theoretic estimation about unfold faces such as (001), (100), (010), (011), (110), (101) and (112) faces is quite good. The theoretic habit calculation indicates that gibbsite super cell is inclined to form crystal with quasi hexagonal prism or thick hexagonal angle slab shapes. (001), (100) and (010) slab models are inclined to form wedge slab shape, (110), (101) and (112) slab models are likely to form slim stick shape.

Key words: gibbsite; super cell; growth habit; crystal morphology

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