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研究论文

高岭土/二甲亚砜插层复合物脱嵌反应热动力学

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摘要 采用TG和XRD研究了高岭土/二甲亚砜插层复合物的脱嵌反应过程, 提出了一种新的动力学计算方法. 首先用迭代的等转化率法求得反应的活化能E_a, 然后用Malek法拟合得到最可能的机理函数$G(\alpha)$和$f(\alpha)$, 最后用多升温速率-等温法求得了指前因子A. 研究结果表明, 高岭土/二甲亚砜的插层物脱嵌反应的活化能E_a=86.65 kJ/mol, 指前因子A位于1.6050×10^8~3.6151×10^8 s^{-1}之间. 其反应机理为n级的化学反应, 机理函数是$G(\alpha)=[1-(1-\alpha)^{1-n}]/(1-n)$, $f(\alpha)=(1-\alpha)^n$. n值和升温速率有一定的关系, 当升温速率较大(30 ℃/min)或较小(5 ℃/min)时, n=1.5, 当升温速率为7~25 ℃/min时, n=1.6.

关键词 高岭土/二甲亚砜 迭代法 Malek法 多升温速率-等温法 热分析动力学

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Thermokinetics Study on the Deintercalation Reaction of Intercalating Composite Kaolinite/Dimethyl Sulphoxide

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Abstract

The de-intercalation processes occurring in the solid state Kaolinite/Dimethyl sulphoxide were stu-died by using TG and XRD techniques, and a new method of how to calculate the kinetic triplet was proposed on the thermokinetics study: Firstly, the activation energy E_a is calculated by interative procedure; secondly, the optimized methanism and the corresponding function $G(\alpha)$, $f(\alpha)$ is derived from the regression of Malek method; lastly, the pre-exponential factor A is estimated by multiple rates-isotemperature method. The apparent activation energy E_a of the decomposition of Kaolinite/Dimethyl sulphoxide is about 86.65 kJ/mol, and the pre-exponential factor A is 1.6050×10^8—3.6151×10^8 s^{-1}, the optimized methanism is nth-order chemical reaction, the corresponding functions are $G(\alpha)=[1-(1-\alpha)^{1-n}]/(1-n)$ and $f(\alpha)=(1-\alpha)^n$. But the value of n has a relationship with the heating rate to a certain extent: when heating rate is rather quick(30 ℃/min)or rather slow(5 ℃/min), n is equal to 1.5, but when heating rate is between 7 and 25 ℃/min, n is equal to 1.6.

Key words Kaolinite/dimethyl sulphoxide Interative procedure Malek method Multiple rates-isotemperature method Thermokinetics

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