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焙烧过程晶粒生长的Monte Carlo模拟

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摘 要: 基于Monte Carlo(MC)方法, 根据晶粒生长机理建立改进的转换概率模型, 在不同焙烧温度、焙烧时间和激活能条件下可实现晶粒生长过程结构演化的计算机模拟, 对模拟和实验数据进行分析, 结果表明: 当晶粒生长指数为2.17时, 模拟与实验具有较好的一致性, 从而得出焙烧过程晶粒的生长动力学模型; 该模型能够较好地解释焙烧过程晶粒的生长过程, 对晶粒生长动力学研究等具有一定的指导意义。

关键字: 晶粒生长; 焙烧; Monte Carlo模拟

Monte Carlo simulation of grain growth in calcination process

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Abstract: A new Monte Carlo model was presented according to the grain growth theory. Using this model the computer simulation of microstructure evolution of grain growth was carried out under the condition of different calcinating temperatures, calcinating time and activation energies, and the dynamic model of grain growth in calcination process was obtained. The statistical analysis reveals that the simulated results are in good agreement with the experiment ones when the grain growth exponent is 2.17. It indicates that the grain growth in calcinations progress can be well explained using this model, so the model is valuable to the experiment about grain growth kinetics.

Key words: grain growth; calcinations; Monte Carlo simulation

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