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晶粒长大的Monte Carlo模拟方法——递归统计法测定晶粒度

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摘要: 应用Monte Carlo(MC)法模拟在周期性边界条件下的晶粒长大行为。利用MC法模拟时, 晶界处格点的迁移引起晶粒的长大, 根据这一主要特征提出一种精确快速的测定晶粒度的新方法——递归统计法, 然后采用递归统计方法测量晶粒度。结果表明, 递归统计法测得的晶粒度比截点法的更精确, 而且测量精确度不受模型的格点类型以及晶粒的尺寸、形状等的影响, 测量速度比其他统计方法要快。

关键字: 递归统计; 晶粒度; Monte Carlo方法; 晶粒长大

Monte Carlo simulation of grain growth—Recursive statistics method of grain size

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Abstract: Monte Carlo method was used to simulate grain growth process under periodic boundary condition. A new improved measurement method of grain size named recursive statistics method was introduced according to the fact that grain growth induced by displacement of single lattice around the grain boundary, and then the recursive statistics method was used to measure grain size. The results show that the grain size measured by the recursive statistics method is more accurate than the one measured by intercept method; the lattice types of method, sizes and shapes of grains cannot affect the measurement accuracy of the recursive statistics method; and the measuring speed of statistics method is faster than those of other statistics methods.

Key words: recursive statistics method; grain size; Monte Carlo method; grain growth

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