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论文

相场方法研究硬质颗粒钉扎的两相晶粒长大过程

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摘要:

采用相场方法模拟第三相颗粒钉扎的两相耦合的晶粒长大过程, 系统地研究了第三相颗粒体积分数和尺寸大小对两相晶粒长大 过程的影响. 模拟结果表明, 第三相颗粒体积分数越大, 对晶界的钉扎作用越强, 且极限晶粒尺寸越小. 单个第三相颗粒尺寸越大, 对晶界钉扎作用越强. 但当体积分数一定时第三相颗粒尺寸越小时, 颗粒数目会越多, 此时总的钉扎效果会越好, 晶粒极限尺寸也越小. 若晶粒长大系统同时引入两种不同大小的第三相钉扎颗粒, 且两种颗粒所占比例相同时, 钉扎效果最好. 相场方法模拟所得到的二相多晶材料晶粒组织演化规律和晶粒生长指数、晶粒形态、生长动力学和拓扑结构特征与已有实验和理论结果相符合

关键词: 相场模拟 晶粒长大 硬质颗粒 Zener钉扎

PHASE-FIELD SIMULATION OF TWO-PHASE GRAIN GROWTH WITH HARD PARTICLES

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Abstract:

Grain growth, due to its importance in controlling the physical properties of a wide variety of materials, has been extensively investigated. Second–phase particles have the capacity to "pin" grain boundaries and therefore affect the grain growth behavior of polycrystalline materials profoundly. They reduce the mobility of grain boundaries and eventually, when a critical grain size is reached, arrest grain growth. Based on a diffuse–interface description, a computer simulation model for studying the microstructural evolution in two–phase solid has been developed. For a grain system with hard particles, the kinetics of two–phase grain growth with the third hard particles was investigated by phase field model with a continuum diffuse–interface field. A polycrystalline microstructure of temporal and spatial evolution of the three–phase–solid system was obtained by solving three kinetics equations. It is found that the pinning effect is enhanced with the increase of the size and the volume fraction of third–phase particles. The greater the volume fraction and size of third–phase particles are, the smaller the limited sizes of grain growth are. If the volume fraction of third–phase particle maintains a constant and the size of third–phase particles is smaller, then the pinning effect of third–phase particles is stronger. When third particles with two different sizes under the same volume fraction are introduced in the system of grain growth, the pinning effect of the particles is the best. The power growth law, grain morphology, critical grain size, grain growth dynamics and topology structure of two–phase polycrystalline materials simuated by phase–fielmodel are in well accordnce with the experimental results and theoretical results of other simulations.

Keywords: phase-field simulation grain growth hard particle Zener pinning

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