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用分子动力学方法模拟零温下铜及其掺银或铋的晶界结构

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摘要 本文采用五参数对势和固定体积的假定, 应用分子动力学方法模拟了零温下纯Cu、Cu-Ag和Cu-Bi合金的晶界弛豫结构, 计算结果表明, 在上述情况下, 原子分布在平行晶界面的两个方向是周期性的, 在垂直晶界面的方向是镜面对称的。两种合金弛豫结构与纯铜的结构差别不大, 铋原子周围的铜原子离铋原子较近, 而银原子周围的铜原子离银原子较远。

关键词 分子动力学 晶界 铜 合金

分类号

MOLECULAR DYNAMICS SIMULATIONS OF GRAIN BOUNDARY STRUCTURES AT 0°K IN COPPER WITH SUBSTITUTIONAL IMPURITIES

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Abstract

The 0°K relaxed structures of grain boundaries in Cu and its alloys (Cu-Ag, Cu-Bi) were simulated with molecular dynamics method by using a five-parameter potential and constant volume assumption.In these cases, the results showed that the atomic distribution was periodic in the two directions paralled to the grain boundary and it was mirror-symmetric in the direction perpendicular to the boundary. The difference between relaxed structures of Cu and its alloys was small, nevertheless, the host atoms were cl...

Key words molecular dynamics grain boundary copper alloy

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