

论文

马氏体在位错偶上形核长大的分子动力学模拟研究

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摘要: 应用分子动力学方法和NiAl合金的嵌入原子势(EAM);模拟研究了位错偶上马氏体形核长大的过程和微观机理. 计算结果表明,马氏体形核的位置与位错应力场的分布有关. 马氏体总是在位错偶应力场中的一些特殊位置优先形核,因为这些位置的应力状态有利于完成从奥氏体向马氏体转变的点阵畸变. 在马氏体长大过程中,在相变应变的驱动下,其中一根位错逐渐向下滑移,起到了塑性协调的作用

关键词: 马氏体相变 位错偶 位错应力场 分子动力学 嵌入原子势

MOLECULAR DYNAMICS SIMULATION ON MARTENSITIC NUCLEATION AND GROWTH AT AN EDGE DISLOCATION DIPOLE

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Abstract: Molecular dynamics simulation has been performed to investigate martensite nucleation and growth at an edge dislocation dipole employing embedded atom method (EAM) type interatomic potential. The results indicate that the stress field of the dislocation dipole has important effect on the martensite nucleation and growth. The calculation of the stress distribution of the dislocation dipole shows that martensitic nucleation was preferentially initiated at the sites in the stress field where the stress state assists the lattice deformation of martensitic transformation. The two dislocations moved apart gradually, driven by transformation strain during the growing process of the martensite. The slip of the dislocation plays a role of plastic accommodation.

Keywords: molecular dynamics simulation edge dislocation dipole EAM potential martensitic nucleation and growth stress field

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