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论文

NiAl合金相变伪弹性的分子动力学模拟

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摘要： 利用NiAl合金的嵌入原子势，进行了B2结构NiAl单晶中相变伪弹性的分子动力学模拟模拟过程中系统的径向分布函数和键连线原子分布图的变化表明，在外加拉应力的作用下，B2结构的奥氏体向L10结构的马氏体转变，马氏体在长大过程中发生了变体间的转化与合并，不同取向的变体之间由于自协调效应形成共格的孪晶界面.当外加拉应力释放以后，首先沿着变体间的孪晶界面，马氏体逐渐收缩随着马氏体－奥氏体界面的不断迁移，系统又逆转变成为初始B2结构的奥氏体

关键词： 相变伪弹性 分子动力学模拟 嵌入原子势 NiAl合金

MOLECULAR DYNAMICS SIMULATION ON TRANSFORMATION PSEUDOELASTICITY IN NiAl ALLOY

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Abstract: Molecular dynamics simulation was carried out to study transformation pseudoelasticity in NiAl alloy with a initial B2 structure, using EAM (embedded atom method) type interatomic potential for NiAl. The evolution of the RDFs and bonded atomic patterns indicate that martensitic transformation took place when external tensile force increased to a certain level.During the transformation, variants could integrate each other under the action of the external force, coherent twinning interfaces were formed between misoriented variants. A reverse process initiated at the coherent interfaces occurred when the external force was withdrawn. With the migration of martensite-austenite interfaces the stress induced martensites transformed back into austenite.

Keywords: transformation pseudoelasticity molecular dynamics simulation EAM potential NiAl alloy

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280)

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