

论文

分子动力学模拟研究单个刃型位错对NiAl马氏体相变的影响

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摘要: 利用嵌入原子类型的势函数,通过分子动力学模拟方法研究了单个刃型位错对NiAl热诱发和应力诱发马氏体相变的影响,不受外力时,单个刃型位错的应变区不能诱发马氏体形核;位错在马氏体的长大过程中被继承,并可在相变的驱动下逐渐运动拉应力作用下,3R结构的应力诱发马氏体首先在位错芯附近形核,长大过程中先形成蝶状马氏体,随后位错多余半原子面的中部也发生了马氏体形核.刃型位错降低了应力诱发马氏体形核的激活能,并在相变中起到了塑性协调作用.

关键词: 马氏体相变 刃型位错 分子动力学模拟 嵌入原子势 NiAl

MOLECULAR DYNAMICS STUDY ON THE INFLUENCE OF SINGLE EDGE DISLOCATION ON MARTENSITIC TRANSFORMATIONS IN NiAl

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Abstract: Via embedded atom type potential, molecular dynamics simulation has been performed to study the influence of single edge dislocation on both thermally and stress induced martensitic transformations in a stoichiometric NiAl B2 alloy. If no external force is applied to the system, the strain field of single edge dislocation can not nucleate martensites. Edge dislocation can be inherited during the growth processes of thermally induced martensite, and can also migrate toward the surface with the help of the transformation. When a tensile force is applied, stress induced martensite with 3R structure can initially nucleate near the dislocation core. Butterfly martensite appeared first during the growth process, and then another martensitic variant nucleated in the middle of the dislocation.Edge dislocation can reduce the activation energy for stress induced martensitic nucleation, and it also plays a role of plastic accommodation in the transformation processes.

Keywords: martensitic transformation edge dislocation molecular dynamics simulation embedded atom type potential NiAl

收稿日期 1997-11-18 修回日期 1997-11-18 网络版发布日期

DOI:

基金项目:

国家自然科学基金!59271019

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参考文献:

1MageeCL.MetallTrans,1971;2:2419
2OlsonGB,CohenM.MetallTrans,1976;7A:1897,1905,1915
3KajiwaraS.MetallTrans,1986;17A:1701
4SuezawaM,CookHE.ActaMetall,1980;28:423
5EasterlingKE,TholenAR.ActaMetall,1976;24:333
6YuZZ,ClappPC.MetallTrans,1989;20A:1617

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8SchryversD.PhilosMag,1993;A68:1017

9MartynovVY,EnamiK,KhandrosLG,NennoS,TkachenkoAV.PhysMetMetallogr,1983;55:136

10沙宪伟,张修睦,李依依.钢铁研究学报,1997;9(6):

11DawMS,BaskesMI.PhysRev,1984;B29:6443

12RoseJH,SmithJR,GuineaF,FerranteJ.PhvsRev,1984;B29:2963

13ChenSP,SrolovitzDJ,VoterAF.JMaterRes,1989;4:62

14沙宪伟,张修睦,陈魁英,李依依.金属学报,1996;32:1184

15HeermannDW.ComputerSimulationMethodsInTheoreticalPhysics.2nded,Berlin:Springer-Verlag,1990:147

16ClappPC.PhysStatusSolidi,1973;B57:561

17ShaoY.PhD Thesis,UniversityofConnecticut,1993

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1. 孟庆平,戎咏华,徐祖耀.马氏体相变的形核问题[J].金属学报,2004,40(4):337-341
2. 郭世海,张羊换,李健靓,祁焱,王新林.Ni₅₂Mn_{21+x}Ga_{27-x}(x=0—5)磁性形状记忆合金的相变[J].金属学报,2004,40(9):972-974
3. 陈浩,高克玮,褚武扬,王燕斌,乔利杰.304不锈钢应力腐蚀促进马氏体相变[J].金属学报,2002,38(8):857-860
4. 林成新,谷南驹,刘庆锁,温春生,赵连城.Fe-Mn-Si形状记忆合金低温松弛机理[J].金属学报,2002,38(8):825-828
5. 许峰云,徐雪霞,白秉哲,方鸿生.粒状组织的相变残余应力[J].金属学报,2008,44(9):1063-1068
6. 赵新清,黎业生.Fe(N)纳米微粒的马氏体相变[J].金属学报,2002,38(1):11-16
7. 王宝奇,谷南驹,郭素珍,马晓莉.Bain对应和K-S模型的数学描述[J].金属学报,2002,38(5):474-478
8. 张华力,刘卫,苏金瑞,丁锦文,陈初升.La₂NiO₄.147体系相变的低频内耗[J].金属学报,2003,39(11):1157-1159
9. 饶光斌,王俭秋,韩恩厚,柯伟.应力诱发马氏体相变对TiNi形状记忆合金疲劳过程影响的原位实验观察[J].金属学报,2002,38(6):575-582
10. 谷臣清,付萍,贾建军.马氏体相变的弹性波诱发形核[J].金属学报,2001,37(8):791-794