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论文

NiTi形状记忆合金中共格Ni_4Ti_3沉淀相生长动力学行为的相场法模拟

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摘要：

采用基于扩散场理论的宏观相场模型对NiTi形状记忆合金中具有菱方结构的共格Ni_4Ti_3相的析出及长大过程进行了模拟研究; 沉淀相的形貌演化通过求解非守恒参量场Ginzburg-Landau控制方程和守恒浓度场Cahn-Hilliard扩散方程获得. 与二维模型相比, 本研究采用了准确的晶体学参数及改进的数学模型, 获得了更为直观及合理的三维盘状变体及二维透镜状变体; Ni_4Ti_3沉淀相的长度、宽度和面积分数随时间的变化分别遵循指数、线性和对数关系; 且其长度与宽度的比值并非恒定值, 在生长初期该比值有较大的增速而随后逐渐减慢, 能很好地解释沉淀相盘状及透镜状形貌特征形成的原因并与相关实验结果吻合.

关键词： NiTi形状记忆合金 共格沉淀相 生长动力学 相场法 形貌演化

PHASE FIELD SIMULATION OF GROWTH KINETICS OF COHERENT Ni_4Ti_3 PRECIPITATE IN NiTi SHAPE MEMORY ALLOY

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Abstract:

The precipitation of metastable Ni_4Ti_3 particles and their distribution feature in Ni-rich NiTi shape memory alloys have significant influence on the subsequent martensitic transformation behavior and shape memory effect as well as superelasticity. The Ni_4Ti_3 particles with the space group *R*3 precipitate coherently along four {111} planes of the B2 matrix and form four pairs of conjugate variants. The diffusion-interface phase field model was used to simulate the nucleation and growth of the Ni_4Ti_3 precipitate in NiTi shape memory alloy, and its morphological evolution was characterized by solving Ginzburg-Landau equation for non-conserved field variables and Cahn-Hilliard diffusion equation for conserved field variables. More accurate crystallographic parameters and improved mathematical model were used in simulating the formations of 3D plate-shaped or 2D lenticular-shaped Ni_4Ti_3 variants. The time dependences of length, width and area fraction of Ni_4Ti_3 precipitate obey a power law, a linear and a logarithmic equation, respectively. The length-to-width ratio of the precipitate is not a constant value, but increases rapidly in the early stage of precipitation and slows down in later stage, which is corresponding to the plate- or lenticular-shaped morphologies and coincident with the experimental observations reported.

Keywords: NiTi shape memory alloy coherent precipitate growth kinetics phase field method morphology evolution

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