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论文

多晶沉积薄膜生长过程中织构演变的模拟研究

王沿东;刘沿东;徐家桢;梁志德

东北大学材料科学与工程系;沈阳,110006;东北大学材料科学与工程系;沈阳,110006;东北大学材料科学与工程系;沈阳,110006;东北大学材料科学与工程系;沈阳,110006

摘要: 将织构组态熵的概念应用于沉积多晶薄膜织构演变的模拟研究,考虑薄膜沉积过程中晶体表面能各向异性及应变能各向异性的变化,建立了沉积薄膜晶体择优生长的定量模型;模拟了Al多晶薄膜沉积过程中晶体的生长规律,分析了织构演变的主要微观物理因素.

关键词: 多晶薄膜 织构演变 组态熵

COMPUTER SIMULATION ON TEXTURE EVOLUTION OF POLYCRYSTALLINE THIN FILMS DURING GRAIN GROWTH

WANG Yandong; LIU Yandong; XU Jiachen; LIANG Zhide(Department of Materials Science and Engineering, Northeastern University, Shenyang 110006)

Abstract: The concept of texture configuration entropy is introduced into the computer simulation on texture evolution of polycrystalline films. The grain orientation distribution in thin films is quantitatively determined by a new simple model. As an example, inverse pole figures of polycrystalline aluminum thin films are simulated by considering the change of texture configuration entropy and another orientation dependent driving forces during grain growth, such as surface energy and strain energy. The physical mechanisms affecting the texture evolution of polycrystalline thin films are discussed.

Keywords: polycrystalline thin film texture evolution configuration entropy

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通讯作者:

作者简介:

作者Email:

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