入射能量对外延生长 Cr 薄膜表面粗糙度和膜基结合强度的影响:分子动力学模拟 *

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摘 要:过渡层是改善膜基关系,提升薄膜质量的关键因素。本文针对常见过渡层材料 Cr 的外延生长过程进行了分子动力学模拟。通过对沉积过程中薄膜的表面形貌、粗糙度、径向分布函数以及膜基结合强度进行分析,研究了入射能量对薄膜质量的影响。结果表明:沉积初期,膜基界面相互作用是影响薄膜生长方式的主要因素;随入射能量升高,表面粗糙度上升,薄膜由层状生长转变为岛状生长;随沉积过程进行,低能沉积(15~50eV)时薄膜表面粗糙度逐渐升高,而高能沉积(75eV)时在刻蚀作用下表现出相反趋势,表面粗糙度逐渐降低;同时,较低能量范围沉积时膜基界面在浅注入作用下被破坏,削弱了膜基结合强度;进一步提高沉积可通过形成成分梯度层,改善膜基结合效果。本文的研究结果对于薄膜沉积过程具有重要指导意义:镀膜过程中提高入射能量并不一定能起到积极效果,沉积粒子能量必须控制在合适的范围。

关 键 词:入射能量;生长模式;表面粗糙度;结合强度;分子动力学

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Influence of Incident Energy on the Surface Roughness and Film/Substrate Adhesion Strength of Epitaxially Grown Cr Films: Molecular Dynamics Simulation

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Abstract: Transition layer is a key factor to improve the film/substrate relationship and increase the quality of the film. In this paper, the epitaxially grown process of Cr, which is a common transition layer material, was simulated using molecular dynamics method. Surface topography, roughness, radial distribution function and adhesion strength was analyzed to study the effect of incident energy on the film quality. The results show that at the initial stage of deposition, the film/substrate interfacial interaction was the main factor affecting the growth mode of the film. As the incident energy increased, the growth mode changed from Frank-Vander Merve to Volmer-Weber. As the deposition process progressed, the film surface roughness gradually raised during low-energy deposition (15-50eV). However, the opposite trend exhibited during high-energy deposition (75eV) because of the etching effect, and the surface roughness decreased gradually. Meanwhile, the film/substrate interface was destroyed by the shallow injection in the lower energy range, which weakened the film/substrate adhesive strength. Further improving the deposition could improve the film/substrate adhesive effect by forming a composition gradient layer. The research results in this paper shows important guiding significance for the thin film deposition process: increasing the incident energy during the deposition process does not meaning a positive effect, and it must be controlled in a suitable energy range.

Key words: incident energy; growth mode; surface roughness; adhesion strength; molecular dynamics

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