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论文

动力学晶格蒙特卡洛方法模拟Cu薄膜生长

吴子若,程鑫彬,王占山

上海市同济大学

摘要：

本文利用动力学晶格蒙特卡洛方法模拟了Cu薄膜在Cu(100)面上的三维生长过程。模型中考虑了四个动力学过程：原子沉积、增原子迁移、双原子迁移和台阶边缘原子迁移，各动力学过程发生的概率由多体势函数确定。主要讨论了基底温度、沉积速率及原子覆盖率对Cu原子迁移、成核和表面岛生长等微观生长机制的影响；获得了Cu薄膜的表面形貌图并计算了表面粗糙度。模拟结果表明，随基底温度升高或沉积速率下降，岛的平均尺寸增大，数目减少，形状更加规则。低温时，Cu薄膜表现为分形的离散生长，高温时，Cu原子迁移能力增强形成密集的岛。Cu薄膜表面粗糙度随着基底温度的升高而迅速减小；当基底温度低于某一临界温度时，表面粗糙度随原子覆盖率或沉积速率的增大而增大；当基底温度超过临界温度时，表面粗糙度随原子覆盖率或沉积速率的变化很小，基本趋于稳定。

关键词： 薄膜生长 原子迁移 KLMC模拟 沉积速率 基底温度 原子覆盖率 表面粗糙度

Kinetic lattice Monte Carlo simulation of Cu thin film growth

Zi-ruo Wu,Xin-bin Cheng,Zhan-shan Wang

Abstract:

The Cu thin film growth process on Cu (100) metal substrate is investigated using a three-dimensional kinetic lattice Monte Carlo (KLMC) method. Four kinetic processes are included in our model: deposition, adatom diffusion, dimer diffusion and ledge adatom diffusion. The activation energies for these three diffusion events are calculated using the embedded-atom method. The dependence of the Cu thin film growth on process parameters, including substrate temperature, deposition rate and coverage, is discussed using the KLMC model. The results show that, as the substrate temperature increases or the deposition rate decreases, the average size of the islands becomes bigger and the number of the islands decreases. As the temperature is low, the film shows fractal growth; at higher temperature, the island becomes compact and more regular in shape. And the higher the temperature, the smaller the Cu thin film surface roughness. When the substrate temperature is lower than the transion temperature, the surface roughness increases as the deposition rate and (or) the coverage increases. At higher temperature, the surface roughness is almost the same for different deposition rates or the coverage.

Keywords: Thin film growth Surface diffusion KLMC simulation Deposition rate Substrate temperature Atom coverage Surface roughness

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通讯作者: 程鑫彬

作者简介:

参考文献：

参考文献：

[1]?YAN Guo-jun, CHENG Guang-de, QIU Fu-sheng, et al. The optical properties of AIN film[J].? Acta Photonica Sinica, 2006,35(2)：221-223.
颜国君，陈光德，邱复生等. 氮化铝薄膜的光学性能[J]. 光子学报. 2006,35(2) :221-223.

[2]?FANG Xiao-lin, GAO Fei, LIU Wei, et al. Optical properties of amorphous silicon film by spectrophotometry[J].Acta Photonica Sinica, 2008, 37(9):1825-1828.
方晓玲，高斐，刘伟等. SiO2薄膜中咔唑的发光特性[J]. 光子学报. 2008, 37(9):1825-1828.
[3]?? Zhang Z Y, Lagally M G. Atomistic Processes in the Early Stages of Thin-Film Growth[J]. Science, 1997, 276(5311):377-383.
[4]?Lagally M G, Zhang Z Y. Thin-film cliffhanger[J]. Nature, 2002, 417(6892):907-910.
[5]?? Wang L G, Clancy P. Kinetic Monte Carlo simulation of the growth of polycrystalline Cu films[J]. Surface Science, 2001, 473(1-2): 25-38.
[6]?? Hwang R Q, Schroder J, Gunther C, Behm R J. Fractal growth of two-dimensional islands: Au on Ru(0001)[J]. Phys RevLett, 1991, 67(23):3279-3282.
[7]?? Parschau M, Schlatterbeck D, Christmann K. Nucleation and growth of silver films on a rhenium (0001) surface: a combined STM and LEED study[J]. Surf Sci, 1997, 376(1-3):133-150.
[8]?? Michely T, Hohage M, Bott M, et al. Inversion of growth speed anisotropy in two dimensions[J]. Phys Rev Lett, 1993, 70(25):3943-3946.
[9]?? Witten T A, Sander L M. Diffusion-Limited Aggregation, a Kinetic Critical Phenomenon[J]. Phys Rev Lett, 1981, 47(19):1400-1403.
[10] Salik J. Monte Carlo study of reversible growth of clusters on a surface[J]. Phys Rev B, 1985, 32(3):1824-1826.
[11] Zhang Z Y, Chen X, Lagally M G. Bonding-Geometry Dependence of Fractal Growth on Metal Surfaces[J]. Phys Rev Lett, 1994, 73(13):1829-1832.
[12] Corbett C. Battaile. The Kinetic Monte Carlo method: Foundation, implementation, and application[J]. Comput. Methods Appl. Mech. Engrg.2008,197(41-42): 3386-3398.
[13] Takano J, Takai O, Kogure Y, et al. Molecular dynamics, Monte Carlo and their hybrid methods: applications to thin film growth dynamics[J]. Thin Solid Film, 1998, 334(1-2):209-213.
[14] Ratsch C, Zangwill A, Smilauer P, et al. Saturation and scaling of epitaxial island densities [J]. Phys Rev Lett, 1994, 72(20):3194-3197.
[15] Huang H C, T.Diaz de la Rubia, Gilmer G H. An atomistic simulator for thin film deposition in three dimensions [J]. J.Appl.Phys. , 1998, 84(7):3636-3649.
[16] Wang Z Y, Li Y H, Adams J B. Kinetic lattice Monte Carlo simulation of facet growth rate[J]. Surface Science, 2000, 450(1-2):51-63.
[17] Adams J B, Wang Z Y, Li Y H. Modeling Cu thin film growth[J]. Thin Solid Films, 2000, 365 (2):201-210.
[18] Adams J B, Foiles S M , Wolfer W G, Self-diffusion and impurity diffusion of fee metals using the five-frequency model and the Embedded Atom Method [J].J. Mater. Res., 1989, 4 (1):102-112.
[19] ZHENG XiaoPing et al.Kinetic Monte Carlo simulation of film morphologies at the initial stages[J]. Sci China Ser G-Phys Mech Astron,2008,51(1): 56-63.
[20] ZHENG XiaoPing et al. Kinetic Monte Carlo simulation of Cu thin film growth[J]. Vacuum,2004,72 (4): 405–410.

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2．张玉虹;康利军;胡宝文;王丽莉;李同海;李育林.用按需滴定技术制备聚合物微透镜阵列[J]. 光子学报, 2005,34 (11): 1639-1642
3．潘永强 吴振森.透明基底表面双向反射分布函数及粗糙度特性研究[J]. 光子学报, 2008,37(6): 1246-1249
4．陈勇 张晋宽 王宇.超光滑基片等离子体表面处理研究[J]. 光子学报, 2009,38(1): 194-198
5．汪震 洪津 叶松 张冬英 王峰.金属表面粗糙度对热红外偏振特性影响研究[J]. 光子学报, 2007,36(8): 1500-1503
6．潘震 赵青南 刘本锋 赵修建.氢化非晶硅薄膜的磁控溅射制备及性能研究[J]. 光子学报, 2008,37(Sup1): 128-130

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