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论文

# TiN/$Si_3N_4$纳米晶复合膜的微结构和强化机制

孔明, 赵文济, 乌晓燕, 魏仑, 李戈扬

上海交通大学金属基复合材料国家重点实验室 上海 200030

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摘要 采用高分辨透射电子显微镜对高硬度的TiN/Si3N4纳米晶复合膜的观察发现, 这类薄膜的微结构与Veprek提出的nc-TiN/a-$Si_3N_4$模型有很大不同: 复合膜中的TiN晶粒为平均直径约10nm的柱状晶, 存在于柱晶之间的$Si_3N_4$界面相厚度为0.5～0.7nm, 呈现晶体态, 并与TiN形成共格界面. 进一步采用二维结构的TiN/$Si_3N_4$纳米多层膜的模拟研究表明,$Si_3N_4$层在厚度约<0.7nm时因TiN层晶体结构的模板作用而晶化, 并与TiN层形成共格外延生长结构, 多层膜相应产生硬度升高的超硬效应. 由于TiN晶体层模板效应的短程性, $Si_3N_4$层随厚度微小增加到1.0nm后即转变为非晶态, 其与TiN的共格界面因而遭到破坏, 多层膜的硬度也随之迅速降低. 基于以上结果, 本文对TiN/$Si_3N_4$纳米晶复合膜的强化机制提出了一种不同于nc-TiN/a-$Si_3N_4$模型的新解释.

关键词 TiN/Si3N4纳米晶复合膜 纳米多层膜 界面相 晶体化 超硬效应

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## Microstructure and Mechanical Properties of TiN/$Si_3N_4$ Nanocomposites

KONG Ming, ZHAO Wen-Ji, WU Xiao-Yan, WEI Lun, LI Ge-Yang

State Key Laboratory of Metal Matrix Composites, Shanghai Jiaotong University, Shanghai 200030, China

**Abstract** A microstructure investigation of TiN/$Si_3N_4$ nanocomposite films with high hardness was performed by means of high-resolution transmission electron microscope, and a result far from the nc-TiN/a-Si3N4 model was presented. Instead of the isotropic one, TiN was pronounced nanocrystalline columnar grains with dimensions of <10nm in width and >100nm in length. Immiscible $Si_3N_4$ interfacial phases between TiN nanocolumns with a thickness of about 0.5--0.7nm existed in nanocrystalline structure and formed coherent interfaces with adjacent TiN nanocrystals. A succedent simulation employing two-dimensional TiN/$Si_3N_4$ nanomultilayers also implied that due to the template effect of crystalline TiN layers, sputter-deposited amorphous $Si_3N_4$ was forced to crystallize and grow epitaxially with TiN layers when its thickness was less than 0.7nm, accompanied by a significant enhancement in film's hardness. Due to the short-range nature of the template effect of TiN layers, the crystalline Si3N4 gradually transformed into amorphous when its thickness exceeded 1.0nm and the coherent interfaces were destroyed as a consequence, with a simultaneous film's hardness decline. By comparing the microstructure and corresponding hardness response of TiN/$Si_3N_4$ nanocomposite films with that of the nanomultilayered ones, a new explanation on hardening mechanism of TiN/$Si_3N_4$ nanocomposites was proposed.

**Key words** TiN/Si3N4 nanocomposites TiN/Si3N4 nanomultilayers interfacial phase crystallization superhardness effect

DOI:

通讯作者 李戈扬 gyli@sjtu.edu.cn