# 薄膜的材料特征*

张 爽[1],董 闯[1,2],马艳平[2,3],丁万昱[1]

(1.大连交通大学,材料科学与工程学院,辽宁省高等学校光电材料与器件工程技术研究中心,大连 116028;
2.大连理工大学,三束材料改性教育部重点实验室,大连 116024;
3.海南大学,海南省特种玻璃重点实验室,海口 570228)

**摘 要**:PVD、CVD 涂层行业发展了多年,出现了多种等离子体和高能束辅助技术,但常用的工业涂层却集中在少数几种材料上,如金属氮化物、碳膜等。本文从材料的成分宽容性、结构稳定性、导电性三个基本原则出发,解释了薄膜材料的选材问题,并以氮化钛、非晶硼化物、金属掺杂类金刚石涂层为例,说明薄膜材料的选择源自工艺特性和材料性能二者的平衡,且以工艺性为主导。材料成分需要进行精确调控,以达到最佳的工艺性与性能的匹配,而成分根源是化学近程序结构,通过引入本课题组所提出并发展的团簇加连接原子模型,构建出类似于分子式的局域结构单元和相应成分式,进而对薄膜材料进行成分设计。

**关 键 词**:薄膜材料;成分设计;氮化钛;非晶硼化物;金属掺杂类金刚石;团簇加连接原子模型
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## Material Characteristics of Thin Films

ZHANG Shuang[1], DONG Chuang[1,2], MA Yan-ping[2,3], DING Wan-yu[1]

(*1.Engineering Research Center of Optoelectronic Materials and Devices, School of Materials Science and Engineering, Dalian Jiaotong University, Dalian 116028, China; 2.Key Laboratory of Materials Modification by Laser, Ion and Electron Beams, Dalian University of Technology, Ministry of Education, Dalian 116024, China; 3.State Key Laboratory of Marine Resource Utilization in South China Sea & Special Glass Key Laboratory of Hainan Province, School of Materials and Chemical Engineering, Hainan University, Haikou 570228, China*)

**Abstract**: There are a variety of PVD and CVD coating techniques using plasma and energetic beams. However, commonly used industrial coatings involve only a few materials, such as metal nitrides and amorphous carbon. To address such a phenomenon, this paper proposes three basic principles of thin film material selection, i.e., composition tolerance, structural stability and electrical conductivity. Three kinds of typical coating materials are then explained based on the principles, namely titanium nitride representative of solid solution materials, amorphous boride, and Cr-doped diamond-like carbon, stressing that the selection of thin film materials is derived from the balance between process characteristics and material performance, and is dominated by processability. It is pointed out that the material compositions must be precisely regulated to achieve the best matching of processability and performance, while material compositions are rooted in chemical short-range-order structures. By introducing the cluster-plus-glue-atom model developed by our research group, molecule-like local structural units and the corresponding composition formulas are constructed and they explain the compositions of thin film materials in use. The perspective of using this method as thin film composition design is envisaged.

**Key words**: thin films; composition design; titanium nitride; amorphous boride; metal-doped diamond-like carbon; cluster-plus-glue-atom model

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**作者简介**:张爽(1990-),女,吉林省吉林市人,博士,讲师。 **通讯作者**:董闯,教授,博导。

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