先进材料及其流变特性教育部重点实验室
(湘潭大学)

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先进材料及其流变特性教育部重点实验室(湘潭大学)

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“先进材料及其流变特性教育部重点实验室(湘潭大学)”第一届学术委员会

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前　言

湘潭大学“先进材料及其流变特性实验室”于2003年11月12日被批准确定为省部共建教育部重点实验室。2004年4月23日，教育部重点实验室建设计划论证专家组，对本实验室的建设计划进行了现场论证、考察、讨论、交流和指导。2005年7月10日，实验室召开了“先进材料及其流变特性教育部重点实验室(湘潭大学)第一次学术委员会”。2005年是实验室快速发展的一年，在基本建设、科学研究、人才培养和学术交流等方面均取得了显著成绩。

与2004年相比，实验室2005年在软件和硬件方面都加大了建设力度：实验室新增了两名湖南省“芙蓉学者计划”特聘教授，购买了材料微纳米力学测试系统、英国输力强电化学测试系统、铁电分析仪等一批先进的仪器设备。这为以后的科研教学工作打下了坚实的基础。

科研工作取得显著成绩。实验室1人获得国家杰出青年基金，在研项目包括国家自然科学基金10项、国家863项目1项。实验室固定人员、博士和硕士研究生在Applied Physics Letters 等杂志上共发表学术论文82篇。获得湖南省科技进步二等奖2项、第五届湖南省青年科技奖1项。

人才培养工作取得长足进展。实验室新招收博士研究生18人、硕士研究生47人，毕业博士研究生1名和硕士研究生17名。1篇博士学位论文被评为湖南省优秀博士论文，1篇博士学位论文获得全国优秀博士学位论文提名奖；1人获得湘潭大学研究生校长奖特等奖；2篇硕士学位论文被评为湖南省优秀硕士论文；3人分别获得第九届“挑战杯”全国大学生课外学术科技作品竞赛一、二、三等奖；一门课程被评为国家级精品课程；获高等教育国家级教学成果奖二等奖1项；出版高校教材1部。

实验室在学术交流方面也取得了较好成绩。2005年，实验室共派出40多人次出国(境)访问交流；邀请了10位国(境)内外知名专家学者前来讲学；承办了“中国青年科学家论坛第96次活动”；举办了实验室2005年度学术研讨会。频繁的学术交流，对于我们开阔学术视野、更好地跟踪国际学术前沿、促进实验室的科学研究与人才培养发挥了重要作用。

所有成绩的取得，离不开各级领导的关心和支持；离不开实验室学术委员会的正确指引；离不开实验室海内外同行与友人的大力支持；离不开实验室全体师生的勤奋工作与团结协作。在此，我谨代表“先进材料及其流变特性教育部重点实验室(湘潭大学)”向各级领导，向实验室学术委员会的各位委员，向一直关心、支持我们事业发展的海内外同行和友人，向实验室的全体师生，表示崇高的敬意与诚挚的感谢！

科学研究，需要耐心与毅力；人才培养，需要爱心与奉献。只要我们紧跟国际学术前沿，忠于党的教育事业，博学笃行、盛德日新，就一定能拓展我们的事业，使我们的工作更好地服务于社会。让我们团结一致、努力工作，力争在2006年的图纸上画上更新更美的图画！

先进材料及其流变特性教育部重点实验室(湘潭大学)主任 周益春

二〇〇六年三月

目　录

一、概况

湘潭大学“先进材料及其流变特性实验室”于 2003 年 11 月 12 日被批准确定为省部共建教育部重点实验室。2004 年 4 月 23 日，根据教育部教技司[2003]250 号文件的要求，湖南省教育厅组织专家组，对本实验室的建设计划进行了现场论证，专家组一致认为本实验室具备建设成为教育部重点实验室的基础和能力，并建议实验室以低维材料研究为特色，注重相关领域的人才引进，建设成在国内外有一定影响的实验室。2005 年 7 月 10 日，在湘潭大学召开了实验室的第一次学术委员会全体会议，会议进一步明确了实验室的发展方向。

本实验室的主要任务是：以有重大应用背景的结构型、功能型和智能型的低维材料为主要研究对象，对其制备、结构和宏微观性能及其跨尺度模拟和实际应用过程中的关键技术进行研究，注重基础研究与应用研究相结合，宏观与微观相结合，服务地方经济建设与提升学术地位相结合。

“先进材料及其流变特性教育部重点实验室(湘潭大学)”行政管理上隶属湘潭大学，实验室的各项工作由室主任全面主持和负责，副主任协助展开。现任实验室主任为周益春教授，副主任为张海良教授和郑学军教授。日常事务由室务委员会处理，较重要的事务由扩大的室务委员会讨论处理。实验室的第一届学术委员会主任为薛群基院士，副主任为丁文江教授和周益春教授，学术委员为崔俊芝院士等 16 名专家学者。李恒德院士、潘际銮院士、师昌绪院士为实验室学术委员会的名誉委员。

以低维材料为主要研究对象，实验室现有“电沉积镀层材料及跨尺度模拟”、“人工微结构及其跨尺度模拟”、“高温涂层材料及其流变特性”、“压电与光电薄膜材料”，“纳米颗粒、纳米线和纳米复合材料”五个研究方向。实验室现有 X 射线衍射仪、扫描电子显微镜、透射电子显微镜、核磁共振波谱仪、覆镍深冲钢带中试生产线、原子外延激光镀膜仪、真空镀膜仪、高温金相显微镜、金相显微镜、偏光显微镜、JM-HRI 型高功率激光器、真空感应中频电炉、磁控电弧炉、摩擦磨损实验机、差热分析仪、分子量测定仪、元素分析仪、红外光谱仪、红外分光光度计、紫外分光光度计、色谱质谱联用仪、反应注射成型机、英国输力强电化学测试系统、材料微纳米力学测试系统、微机控制电子万能试验机、XBL 数显悬臂梁冲击试验机、铁电分析仪等一批先进的材料制备及性能表征设备。

实验室现已形成了一支人员配备较为合理的学术梯队。目前，实验室共有博士生导师 16 人，教授 20 人，博士 30 余人，其中国家杰出青年科学基金获得者 1 人，湖南省“芙蓉学者计划”特聘教授 3 人，教育部(新)跨世纪人才基金获得者 3 人，国家百千万工程人才 1 人，湖南省优秀中青年专家 5 人，享受政府特殊津贴人员 8 人，湖南省“青年科技奖”获得者 3 人，湖南省“杰出青年科技创新奖”获得者 5 人。他们所在的学科领域包括材料、物理、力学、化学等。

科学研究工作取得显著成绩。2005 年，周益春教授获得国家杰出青年基金，张海良教授获得教育部新世纪优秀人才基金。实验室各类在研项目共 52 项，其中国家自然科学基金项目 10 项、国家 863 项目 1 项。实验室固定人员、博士和硕士研究生在 Applied Physics Letters 等杂志上发表各类论文共 82 篇。钟建新教授等的科研成果“奇异量子动力学研究”和谭援强教授等的科研成果“润滑剂结构与性能关系研究”获得湖南省科技进步二等奖；

丁建文教授获得第五届湖南省“青年科技奖”。

在人才培养方面，实验室取得了长足发展。2005 年，实验室招收博士研究生 18 人、硕士研究生 47 人，毕业博士研究生 1 名和硕士研究生 17 名。丁建文教授的博士学位论文被评为湖南省优秀博士学位论文，并被推荐参评全国优秀博士学位论文；郑学军教授的博士学位论文获得全国优秀博士学位论文提名奖；博士研究生钟向丽获得湘潭大学研究生校长奖特等奖；博士研究生毛宇亮和张建军的硕士学位论文被评为湖南省优秀硕士论文；3 人分别获得第九届“挑战杯”全国大学生课外学术科技作品竞赛一、二、三等奖。周益春教授、郑学军教授、李江宇教授和罗文波教授等的《材料的宏微观力学性能》被评为国家级精品课程。周益春教授等的《地方综合性大学材料学科硕士研究生“综合交叉、跨学科”培养模式的实践》获得 2005 年高等教育国家级教学成果奖二等奖。出版高校教材 1 部：《材料固体力学》(上、下册)，周益春，科学出版社，2005 年。

实验室的学术交流活动频繁，参加和承办了一系列高级别的学术会议。审批了实验室的第一批开放课题共 9 项；实验室共派出了 40 多人次出国(境)访问、讲学、合作研究或参加国际学术会议；邀请了 10 位国(境)内外知名专家学者前来讲学；在湘潭承办了“中国青年科学家论坛第 96 次活动－材料学科的迅速发展对固体力学提出的挑战”；罗迎社教授作为组织委员会主席组织了在上海召开的“第四届泛太平洋地区流变学会议”；在湘潭大学举办了“先进材料及其流变特性教育部重点实验室(湘潭大学)2005 年度学术研讨会”。

二、运行管理

2.1 学术委员会

2005 年 7 月 10 日，“先进材料及其流变特性教育部重点实验室(湘潭大学)”第一次学术委员会全体会议成功召开。参加本次会议的学术委员有：薛群基院士、陈启元教授(尹周澜代)、丁文江教授、傅正义教授、黄云清教授、罗迎社教授、肖加余教授、邢定钰教授、徐坚教授、杨奇斌教授、袁建民教授、张海良教授、钟建新教授、周益春教授。湘潭大学党委书记彭国甫、湖南省教育厅副厅长申纪云及部分实验室学术带头人也参加本次会议。会议的第一阶段，实验室主任周益春教授向学术委员会汇报了实验室的整体工作。会议的第二阶段，苏旭平教授汇报了“电沉积镀层材料及跨尺度模拟”方向的研究进展；钟建新教授汇报了“人工微结构及其跨尺度模拟”方向的研究进展；罗迎社教授汇报了“高温涂层材料及其流变特性”方向的研究进展；李江宇教授汇报了“压电与光电薄膜材料”方向的研究进展；王先友教授汇报了“纳米颗粒、纳米线和纳米复合材料”方向的研究进展。会议的第三阶段，学术委员会审批了实验室的第一批开放课题共九项。会议的第四阶段，学术委员会成员参观了重点实验室的部分科研仪器设备。会议的第五阶段，学术委员们就实验室的研究方向、实验室建设等问题各抒己见，展开了广泛的讨论。

2.2 研究方向

实验室目前设有五个研究室：

(1) 电沉积镀层材料及跨尺度模拟研究室

学术带头人：

周益春教授、黄云清教授、苏旭平教授

研究内容：

覆镍深冲钢带电沉积镍镀层材料；纳米晶及纳米晶与纳米线复合镍镀层；热镀锌工艺；耐磨耐蚀合金镀层材料的设计；电沉积机理的数值模拟和分子反应动力学研究；电沉积性能的跨尺度数值模拟；

(2) 人工微结构及其跨尺度模拟研究室

学术带头人：

钟建新教授、唐壁玉教授、杨奇斌教授、唐翌教授

研究内容：

低维材料的性能模拟；准晶材料性能计算与模拟；纳米碳管的结构形态、性能及其模拟；外延生长原子动力学模拟；原子团簇及其电子结构。

(3) 高温涂层材料及其流变特性研究室

学术带头人：

林建国教授、谭援强教授

研究内容：

热障涂层的破坏机理；高温合金的表面流变成形；高温合金涂层的蠕变；激光表面熔覆。

(4) 压电与光电薄膜材料研究室

学术带头人：

李江宇教授、张海良教授、郑学军教授、刘政威教授

研究内容：

压电薄膜材料的制备及相关物理力学性能；稀土发光薄膜和红外多重数码防伪标记；纳米功能薄膜及沉积机理；高分子液晶。

(5) 纳米颗粒、纳米线和纳米复合材料研究室

学术带头人：

王先友教授、张平教授、丁建文教授

研究内容：

金刚石及相关材料纳米晶的脉冲激光制备；纳米晶金刚石 PLIIR 形成中的结构相变；立方氮化硼纳米晶的 PLIIR 热力学相变及 E 相的制备；PLIIR 纳米相成核的热力学理论；半导体(硅)/金属复合纳米线；纳米钠离子电池正极材料；尼龙 6-二氧化硅纳米复合材料及其直接制备新技术。

2.3 实验室建设

2005 年，实验室新购买了英国输力强电化学测试系统、材料微纳米力学测试系统、微机控制电子万能试验机、XBL 数显悬臂梁冲击试验机、铁电分析仪。

2.3.1 英国输力强电化学测试系统

仪器型号：1260+1287+1296；厂家：英国输力强公司

用途：进行材料的电化学性能研究、腐蚀研究及阻抗分析

主要性能参数：

	恒电位仪 1260	频响分析仪 1287	阻抗测试仪 1296
频率范围	10μHz-32MHz	10μHz-1MHz	10μHz-10MHz
测量阻抗最大值	>100MΩ	>10GΩ	>100TΩ(10^{14}Ω)
电压范围	$\pm 46V$	$\pm 14.5V$	$\pm 40V$
电流范围	$\pm 100mA$	$\pm 2A$	$\pm 2A$
测量精度	0.1%, 0.1°	0.2%+测量间隔的 0.1%	0.2%　+1%测量单位
工作温度	0-50℃	0-50℃	10-30℃
工作电极		2-4	

2.3.2 材料微纳米力学测试系统

仪器型号：Triboindenter；厂家：HYSITRON Inc., (美国)

用途：对材料进行纳米压痕测试(包括随着连续的压入深度的变化获得硬度和弹性模量的分布)、纳米划痕测试、纳米摩擦磨损测试；对材料进行高载荷的压痕、划痕测试(微米压痕 5N、划痕 5N)；在压痕、划痕和磨损(微载荷)前后原位探针扫描成像。

主要性能参数：

	纳米压痕 纵向载荷/位移	纳米划痕 横向载荷/位移	高载荷压划系统 可同时获得任意方向上数据
载荷力分辨率	3 nN (1 μN load)	0.5 μN	0.65 μN (横向); 0.75 μN (纵向)
可实现的最小接触力	100 μN	<5 μN	50 μN (横向); 35 μN (纵向);
可实现的最大载荷	10 mN	2 mN	5 N (横向，纵向)
位移分辨率	0.0004 nm	2 nm	500 nm (横向); 0.0004 nm (纵向)
可实现的最小位移	0.2 nm	5 nm	2 nm (横向); 2.5 nm (纵向)
可实现的最大位移	20 μm	15 μm	25 mm (横向); 80 μm
热漂移	<0.05nm/s(室温下)		

2.3.3 微机控制电子万能试验机

仪器型号：$WDTI-5$；生产厂家：深圳市凯强利试验仪器有限公司

用途：对材料进行拉伸、压缩、弯曲等常规实验；测试抗张、弯曲、压缩和剪切性能；用于材料的评价、应用开发和质量控制。

主要性能参数：

系列	*WDTI*
型号	500
最大负荷	5000N
精度等级	0.5 级
有效测力范围	0.4%-100%
测力精度	示值的±1%以内/示值的±0.5%以内
试验机分辨率	最大负荷/100000 码，内外不分档，且全程分辨率不变
负荷传感器	基本配置: 拉，压传感器(最大负荷)一只 扩展配置: 可加配多个传感器
有效试验宽度	330mm
有效拉伸空间	700mm
试验速度范围	0.005-500mm/min
位移测量精度	示值的±0.5%以内/示值的±0.2%以内
变形测量系统	标准配置(大变形: 最小标距 10mm; 变形范围: 800mm) 扩展配置(小变形: 标距 25mm, 50mm, 100mm; 变形范围: 5mm, 10mm, 25mm)
变形测量精度	示值的±0.5%以内 可根据要求选配大变形或小变形）
试台安全装置	电子限位保护
试台升降装置	快/慢两种速度自动控制，可点动
试台返回功能	手动或自动两种选择，试验结束后自动或手动以最高速度返回试验初始位置
超载保护	超过最大负荷 10%，机器自动保护
夹具配置	拉伸夹具一套
主机尺寸	625×380×1550mm
电机	220V±10% 0.4KW、0.75KW
主机重量	(约)130 Kg

2.3.4 XBL 数显悬臂梁冲击试验机

仪器型号：XBL-22；生产厂家：深圳市凯强利试验仪器有限公司

仪器用途：主要用于硬质塑料、增强尼龙、玻璃钢、陶瓷、铸石、电绝缘材料等非金属材料冲击韧性的测定。

主要性能参数：

<table>
<tr><td>冲击速度</td><td>3.5m/s</td><td>摆锤扬角</td><td>160°</td><td>冲击刀刃至钳口上面距离</td><td>22±0.2mm</td></tr>
<tr><td>摆锤能量</td><td>5.5J, 11J, 22J</td><td>分辨率</td><td>0.1°</td><td>刀刃圆角半径</td><td>R=0.8±0.2mm</td></tr>
<tr><td>打击中心距</td><td>0.322m</td><td>重量</td><td>60kg</td><td>使用温度</td><td>15-35℃</td></tr>
<tr><td colspan="2" rowspan="2">摆锤力矩</td><td colspan="2" rowspan="2">pd5.5=2.8354Nm;
pd11=5.6708Nm;
pd22=11.3417Nm</td><td>电源</td><td>220V/50HZ</td></tr>
<tr><td>外形尺寸(长×宽×高)</td><td>420×320×705(mm)</td></tr>
</table>

2.3.5 铁电分析仪

仪器型号：RT66A；生产厂家：Radiant Technologies, Inc., (美国)

用途：主要用于铁电材料的电滞回线测试、记忆特性测试、单脉冲测试、漏电流测试、小信号电容测试、疲劳测试。

主要性能参数：

测试硬件参数	驱动: ±100V@25Ω; 电压范围: ±100V; 外接高压源: ±4KV 最大电流: 50mA(小于±10V); 70mA(±10V - ±100V) 时间精确度: 5mS; 测试分辨率: 12FC; 频率: >1MHZ
传感器	电压范围: ±10V; 输入阻抗: 10 -12 Ohms; 输入频率: up to 1MHz
电滞回线测试	电压(V): ±100V; 周期: 400μs到30s; 测量频率: 33mHz-2.5kHz之间的任意频率; 测量精度: 测量值的0.5%; 测量电压波形: 可任意编辑; 对1pF-50μF电容自动选择量程; 回线之间可以设定300μs到30秒的延迟; 电滞回线的点数可调
记忆特性测	脉冲宽度: 5μs -1s; 0V上升到5V的时间: 1μs-4ms; 5个脉冲的电压, 宽度, 预设直流偏压和偏置时间可以任意设定; 脉冲之间可以设定300μs到30s的延迟
单脉冲测试	执行一个用户定义的测量脉冲或写脉冲; 脉冲的电压, 宽度, 预设直流偏压和偏置时间可以由用户设定; 多个单脉冲可以连起来执行用户定义的残留试验和印痕试验
漏电流测试	漏电流－偏置电压测试; 漏电流－时间测试; 分辨率: 250fA; 最大漏电流测试: 100mA
小信号电容测试	用户可以设定测量信号的直流偏压, 测量振幅, 脉冲宽度 最大测量频率: 100kHz
疲劳测试	最大疲劳测量频率: 1MHz; 最小脉冲宽度: 1μs 测量电压波形: 可任意编辑

三、科学研究

3.1 发表论文

2005 年，实验室的固定人员和实验室的博士、硕士研究生共发表论文 82 篇。发表论文统计如下。

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19. 廖力, 王先友, 罗旭芳, 卓海涛, Mg-F共掺杂对$Li_{1.1}[Ni_{1/3}Co_{1/3}Mn_{1/3}]O_2$电化学性能的影响, 第十三届全国电化学大会论文集(上), (2005), 339 - 340
20. 唐安平, 王先友, 卓海涛, 刘志明, 锂离子电池正极材料$VOPO_4$的研究进展, 第十三届全国电化学大会论文集(上), (2005), 400 - 401
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22. 黄庆华, 王先友, 李俊, 超级电容器电极材料－MnO_2的电化学制备及其应用研究, 第十三届全国电化学大会论文集(下), (2005), 58 - 59
23. 卓海涛, 王先友, 唐安平, 刘志明, 钠离子电池正极材料$NaVPO_4F$的合成, 第十三届全国电化学大会论文集(下), (2005), 116 -117
24. 罗旭芳, 王先友, 廖力, 王希敏, 氢氧化物共沉淀法制备的锂离子电池阴极材料$Li[Ni_{1/3}Co_{1/3}Mn_{1/3}]O_2$及其性能, 第十三届全国电化学大会论文集(上), (2005), 252 - 253

3.2 在研项目

2005 年，实验室共有各类在研项目 52 项，其中国家自然科学基金项目 10 项、国家 863 项目 1 项。

序号	项目名称	项目编号	负责人	项目来源	起止时间	备注
1.	碳纳米管及其分子器件的物理性能研究	10447129	丁建文	国家自然科学基金	2005-2005	
2.	钠离子电池新型正极材料的制备及性能研究	50472080	王先友	国家自然科学基金	2005-2007	
3.	连续镀锌中富铝抑制层和合金体系相平衡的研究	50471064	苏旭平	国家自然科学基金	2005-2005	
4.	铋层状钙钛矿铁电薄膜的制备及其热冲击下断裂失效行为	10472099	郑学军	国家自然科学基金	2005-2007	
5.	TiAl 合金与 Ti 合金的超塑扩散连接及其焊件的高温蠕变性能研究	50371072	林建国	国家自然科学基金	2004-2006	
6.	旋光性嵌段共聚物的设计、合成与性能研究	20374042	张海良	国家自然科学基金	2004-2006	
7.	辐射流体网格自适应技术和并行代数多重网格法研究	10376031	舒　适	国家自然科学基金	2004-2006	黄云清
8.	病毒三维重构的高精度图象处理	10374077	杨奇斌	国家自然科学基金	2004-2006	
9.	聚合物-无机纳米复合材料的微结构与力学行为的研究	10372087	张　平	国家自然科学基金	2004-2006	
10.	覆镊深冲钢带产业化生产中的关键技术研究	2003AA331090	周益春	国家 863 项目	2003-2006	
11.	z 相-FeSi 化合物相平衡和热浸镀锌中硅反应性的研究	50271059	苏旭平	国家自然科学基金	2003-2005	
12.	电沉积镍涂层冲压成形机理及应用	04JJ40035	周里群	省自科基金	2004-2006	
13.	教育部新世纪人才支持计划基金	NCET-04-0778	苏旭平	教育部新世纪	2005-2007	
14.	教育部新世纪人才支持计划基金	NCET-04-0779	颜晓红	教育部新世纪	2005-2007	

15.	ABC 三嵌段共聚物的设计合成、结构调控及性能研究	20040530002	张海良	教育部博士点基金	2005-2007	
16.	求解偏微分方程的移动粒子法研究	20040530001	黄云清	教育部博士点基金	2005-2007	
17.	教育部跨世纪优秀人才资助计划基金项目	教技函[2002]48 号	周益春	教育部跨世纪	2002-2005	
18.	教育部跨世纪优秀人才资助计划基金项目	教技函[2002]48 号	黄云清	教育部跨世纪	2002-2005	
19.	能量上转换稀土纳米薄膜的制备及性能研究	04JJ3041	丁建文	省自科基金	2004-2006	
20.	钠离子电池用氟磷酸盐正极材料的制备及性能研究	04JJ3040	王先友	省自科基金	2004-2006	
21.	聚酰胺-有机纳米复合材料原位直接制备技术应用研究(滚动资助)	04FJ2005	张　平	省科技厅	2004-2006	
22.	陶瓷材料超精密加工的机械-化学耦合模型研究	04JJ1010	谭援强	省杰出青年基金	2004-2006	
23.	碳纳米管的物理性能及其应用研究	204099	颜晓红	教育部重点项目	2004-2005	丁建文
24.	陶瓷材料超精密加工中界面摩擦学行为研究	教外司留[2004]176 号	谭援强	教育部留学基金	2004-2005	
25.	固体金属材料的流变力学特性及其本构模型研究	03JJY3007	罗迎社	省自科基金	2004-2005	
26.	一维原子和分子体系中的极化子和孤立子	03JJY1001	唐　翌	省中青年科学基金	2004-2006	
27.	聚酰胺-有机纳米复合材料原位直接制备技术应用研究	03JZY1002	张　平	省科技厅	2003-2006	
28.	国防机密项目	51479040103 QT5001	黄云清	国防预研基金	2003-2005	
29.	大块金属玻璃基纳米复合材料的制备和性能研究	02JJYB010	林建国	省中青年科学基金	2003-2005	
30.	非线性光学媒质中的孤立波	04A058	唐　翌	省教育厅重点项目	2004-2008	

31.	高性能层状锰酸锂的制备及性能研究	04A054	王先友	省教育厅重点项目	2004-2006	
32.	反应性热浸镀镀层生长动力学研究	04B063	李　智	省教育厅青年项目	2004-2006	苏旭平
33.	BLT 和 BNT 薄膜的制备及相关物理性能	04B061	王金斌	省教育厅青年项目	2004-2006	
34.	RSCVn 型食双星黑子活动研究	04C683	向福元	省教育厅划块项目	2004-2006	
35.	稀土掺杂上转换薄膜的制备及其发光机理研究	04C663	阳效良	省教育厅划块项目	2004-2006	刘政威
36.	玻色-爱因斯坦凝聚中的孤子研究及应用	04C662	王凤姣	省教育厅划块项目	2004-2006	唐翌
37.	数字散斑技术及其在涂层界面断裂韧性测量中的应用	04C655	杨　穗	省教育厅划块项目	2004-2006	周益春
38.	钛氧化物团簇的结构与性质	04C647	毛宇亮	省教育厅划块项目	2004-2006	丁建文
39.	Ni 基块体亚稳材料的制备与性能研究	04C643	喻更生	省教育厅划块项目	2004-2006	林建国
40.	耐液锌腐蚀材料的研究	04C642	赵满秀	省教育厅划块项目	2004-2006	苏旭平
41.	弧面凸轮的廓面修形研究	04C641	张高峰	省教育厅划块项目	2004-2006	谭援强
42.	多羧化改性海藻酸钠的合成及其净化重金属废水的应用研究	04C640	钟超凡	省教育厅划块项目	2004-2006	张海良
43.	碳纳米管的物理性能及其应用研究	03A046	颜晓红	省教育厅重点项目	2003-2005	丁建文
44.	Sandelin 效应机理及控制的研究	03B040	尹付成	省教育厅青年项目	2003-2005	苏旭平
45.	脉冲激光沉积稀土纳米薄膜及上转换发光机理研究	03B039	丁建文	省教育厅青年项目	2003-2005	刘政威
46.	无铅压电薄膜的化学溶液法制备及其相关力学性能	03B038	郑学军	省教育厅青年项目	2003-2005	周益春
47.	钠离子电池电极材料的制备及性能研究	03C491	王先友	省教育厅划块项目	2003-2005	

48.	金属-氧化物界面及薄膜材料的电子显微镜研究	03C487	刘红荣	省教育厅划块项目	2003-2005	杨奇斌
49.	脉冲激光沉积法制备无铅压电薄膜	03C486	钟向丽	省教育厅划块项目	2003-2005	周益春
50.	实用 LP 范分布及其在 GPS 测量平差中的应用	03C483	刘正才	省教育厅划块项目	2003-2005	罗迎社
51.	玻色-爱因斯坦凝聚体的基态特性	03C466	王登龙	省教育厅划块项目	2003-2005	唐翌
52.	陶瓷器件在力和化学环境中的磨损失效行为研究	KFJJ0303	谭援强	湖南省重点实验室	2003-2005	

3.3 专著与获奖

1. 出版教材，《材料固体力学》(上、下册)，周益春，科学出版社，2005 年。
2. 钟建新教授等的“奇异量子动力学研究”获得湖南省科技进步二等奖；
3. 谭援强教授等的科研成果“润滑剂结构与性能关系研究”获得湖南省科技进步二等奖；
4. 丁建文教授获得第五届湖南省青年科技奖。

四、人才培养

2005 年，实验室招收博士研究生 18 人、硕士研究生 47 人，毕业博士研究生 1 人和硕士研究生 17 人。截止 2005 年底，实验室有在册博士研究生 43 人、硕士研究生 131 人。

4.1 在读博士研究生

序号	姓　名	性别	入学时间	导　师
1.	胡　柯	男	2005	唐　翌
2.	胡和平	男	2005	周益春
3.	黄跃宇	男	2005	周益春
4.	刘　亚	女	2005	苏旭平
5.	刘超飞	男	2005	唐　翌
6.	马　蓦	男	2005	林建国
7.	毛宇亮	男	2005	钟建新
8.	秦衡峰	男	2005	黄云清
9.	唐　超	男	2005	钟建新
10.	涂　浩	男	2005	苏旭平
11.	万梅秀	女	2005	张　平
12.	王子菡	女	2005	周益春
13.	肖化平	男	2005	钟建新
14.	肖启振	男	2005	张海良
15.	易　捷	男	2005	张海良
16.	喻更生	男	2005	林建国
17.	张凯望	男	2005	钟建新
18.	钟冠群	男	2005	张海良
19.	蔡灿英	女	2004	杨奇斌
20.	冯建军	男	2004	周益春
21.	胡增顺	男	2004	周益春
22.	江　山	男	2004	黄云清
23.	姜　勇	女	2004	张　平
24.	毛卫国	男	2004	周益春
25.	唐安平	男	2004	王先友
26.	唐明华	男	2004	周益春

27.	王行柱	男	2004	张海良
28.	向福元	男	2004	周益春
29.	肖良红	男	2004	周益春
30.	杨　丽	女	2004	周益春
31.	喻更生	男	2004	林建国
32.	钟向丽	女	2004	周益春
33.	邓　康	男	2003	黄云清
34.	邓旭辉	男	2003	张　平
35.	李　慰	女	2003	黄云清
36.	刘红荣	男	2003	杨奇斌
37.	唐松花	女	2003	罗迎社 罗文波
38.	王奇生	男	2003	黄云清
39.	王智超	男	2003	罗迎社 钟新谷
40.	尹久仁	男	2002	张　平
41.	肖映雄	男	2001	张　平
42.	谢桂兰	女	2001	张　平
43.	张为民	男	2001	张　平

4.2 在读硕士研究生

序号	姓　名	性别	入学时间	导　师
1.	曹俊琪	男	2005	王先友
2.	陈宏波	男	2005	丁建文
3.	戴春岭	男	2005	王先友
4.	桂　贵	女	2005	钟建新
5.	何　猛	男	2005	苏旭平
6.	贺　涛	男	2005	张海良
7.	胡　涛	男	2005	唐　翌
8.	胡　涛	男	2005	王先友
9.	胡天辉	男	2005	张海良
10.	胡新广	男	2005	唐　翌
11.	蒋科兵	男	2005	黄云清

12.	蒋丽梅	女	2005	周益春
13.	金　国	男	2005	李江宇
14.	李　金	男	2005	钟建新
15.	李　朋	男	2005	黄云清
16.	李爱华	男	2005	钟建新
17.	李东海	男	2005	郑学军
18.	李秀琴	女	2005	王先友
19.	刘　洋	男	2005	唐　翌
20.	刘永雄	男	2005	苏旭平
21.	刘运牙	男	2005	李江宇
22.	卢　佳	女	2005	郑学军
23.	罗　联	男	2005	林建国
24.	马增胜	男	2005	龙士国
25.	欧阳明辉	男	2005	苏旭平
26.	彭冰川	男	2005	周益春
27.	邱先念	男	2005	杨奇斌
28.	舒海波	男	2005	周益春
29.	唐俊雄	男	2005	唐明华
30.	王宝华	男	2005	潘　勇
31.	王锋华	男	2005	林建国
32.	王孝广	男	2005	潘　勇
33.	王宇飞	男	2005	唐璧玉
34.	王志中	男	2005	唐璧玉
35.	伍　杰	男	2005	周益春
36.	项　炬	男	2005	唐　翌
37.	肖　斌	男	2005	苏旭平
38.	徐　宁	男	2005	丁建文
39.	徐群星	男	2005	张海良
40.	闫仕宇	男	2005	黄云清
41.	杨　锋	男	2005	唐明华

42.	杨长安	男	2005	张海良
43.	于　娜	女	2005	唐璧玉
44.	曾凡清	男	2005	杨奇斌
45.	翟甲友	男	2005	林建国
46.	张俊杰	男	2005	郑学军
47.	张小兵	男	2005	龙士国
48.	曹　铮	女	2004	罗迎社
49.	陈明星	男	2004	颜晓红
50.	程桃祖	男	2004	苏旭平
51.	郭志新	男	2004	丁建文
52.	胡玉林	男	2004	唐璧玉
53.	黄贵军	男	2004	王金斌
54.	黄庆华	女	2004	王先友
55.	金　晶	男	2004	唐　翌
56.	瞿　军	男	2004	潘　勇
57.	李　俊	男	2004	钟建新
58.	李　俊	女	2004	王先友
59.	李海欧	女	2004	苏旭平
60.	梁　琴	女	2004	黄云清
61.	廖艳果	男	2004	周益春
62.	刘婵娟	女	2004	张海良
63.	刘超飞	男	2004	唐　翌
64.	刘文斌	男	2004	罗迎社
65.	刘文亮	男	2004	钟建新
66.	刘小根	男	2004	张　平
67.	刘学斌	男	2004	林建国
68.	刘云新	男	2004	杨奇斌
69.	刘志明	男	2004	王先友
70.	吕业刚	男	2004	郑学军
71.	孟利军	男	2004	钟建新

72.	钱　峰	男	2004	潘　勇
73.	阮　斌	男	2004	张　平
74.	邵志美	女	2004	张海良
75.	檀朝桂	男	2004	林建国
76.	唐立平	男	2004	郑学军
77.	田智鲲	女	2004	黄云清
78.	王希敏	男	2004	王先友
79.	吴　群	女	2004	杨奇斌
80.	吴学庆	男	2004	林建国
81.	谢鹤楼	男	2004	张海良
82.	杨　红	男	2004	唐　翌
83.	杨成英	女	2004	丁建文
84.	杨治国	男	2004	龙士国
85.	易文明	男	2004	郑学军
86.	殷水平	男	2004	罗迎社
87.	张　影	男	2004	曹觉先
88.	张　勇	男	2004	杨奇斌
89.	张卫兵	男	2004	唐壁玉
90.	赵海花	女	2004	王先友
91.	周建伟	男	2004	黄云清
92.	丁庆磊	男	2003	刘政威
93.	何　林	女	2003	郑学军
94.	贺　军	男	2003	潘　勇
95.	贺齐群	女	2003	张海良
96.	黄勇力	女	2003	周益春
97.	黄跃宇	男	2003	周益春
98.	蒋　波	男	2003	黄云清
99.	蒋　波	男	2003	黄云清
100.	蒋文娟	女	2003	林建国
101.	李倩妹	女	2003	罗迎社

102.	廖　力	女	2003	王先友
103.	刘超平	男	2003	丁建文
104.	罗旭芳	女	2003	王先友
105.	罗致春	男	2003	林建国
106.	权伟龙	男	2003	唐壁玉
107.	孙美龄	女	2003	黄云清
108.	谭　铮	男	2003	苏旭平
109.	唐　甜	女	2003	潘　勇
110.	唐平英	女	2003	唐壁玉
111.	吴　煜	男	2003	苏旭平
112.	夏艳琴	女	2003	刘政威
113.	肖化平	男	2003	钟建新
114.	谢月娥	女	2003	颜晓红
115.	徐海清	男	2003	唐　翌
116.	宣　凯	男	2003	颜晓红
117.	杨　银	女	2003	黄云清
118.	杨建桃	女	2003	郑学军
119.	杨润年	男	2003	张　平
120.	杨玉荣	男	2003	颜晓红
121.	于海林	男	2003	杨国伟
122.	余　敏	女	2003	罗迎社
123.	虞学红	女	2003	周益春
124.	袁　军	男	2003	张　平
125.	袁健美	女	2003	黄云清
126.	曾松军	男	2003	杨奇斌
127.	张向华	女	2003	刘政威
128.	章　莎	女	2003	周益春
129.	郑荣杰	男	2003	唐　翌
130.	钟红伟	男	2003	唐　翌
131.	卓海涛	女	2003	王先友

4.3 研究生毕业论文

序号	论文题目	学生姓名	学位	答辩时间	导　师
1.	硫酸盐电沉积锌铁合金及腐蚀、力学性能	龙志林	博士	2005.6	周益春
2.	纳米晶镍镀层的微观结构分析及纳米微孔模板的制备	戴翠英	硕士	2005.6	周益春
3.	热障涂层氧化与蠕变的交互作用	吴　丹	硕士	2005.6	周益春
4.	薄膜 PLD 生长的 Monte-Carlo 模拟	谭　歆	硕士	2005.6	周益春
5.	液体薄膜排液过程的无网格径向基函数数值模拟	汤　健	硕士	2005.6	黄云清
6.	基于局部多项式近似空间的单位分解方法及其误差分析	苏　芳	硕士	2005.6	黄云清
7.	热浸镀锌中锡的作用和相关相平衡研究	王鑫铭	硕士	2005.6	苏旭平
8.	量子波包方法研究O+ HBr和H^++ D_2反应	左国平	硕士	2005.6	唐壁玉
9.	复杂网络模型及其统计性质的研究	唐　超	硕士	2005.6	唐　翌
10.	γ-TiAl 合金超塑扩散连接的理论与实验研究	王秀锋	硕士	2005.6	林建国
11.	两种超分子作用在梯形聚硅氧烷合成中的应用	钟冠群	硕士	2005.6	张海良
12.	ABC 三嵌段共聚物的设计合成	孙晓毅	硕士	2005.6	张海良
13.	基于 PCL 和 PS 构筑的新型嵌段共聚的合成与表征	陈　建	硕士	2005.6	张海良
14.	上转换荧光效率与基质材料相关性研究	闫　磊	硕士	2005.6	刘政威
15.	Er^{3+}-Ho-Tm^{3+}掺杂化合物上转换效率与特征荧光研究	雷军辉	硕士	2005.6	刘政威
16.	锌-空气电池阴极催化剂的研究	黄伟国	硕士	2005.6	王先友
17.	纳米二氧化锰的制备、表征及其在超级电容器中的应用研究	汪形艳	硕士	2005.6	王先友
18.	PA6/PTT 合金相关力学性能的研究	许　福	硕士	2005.6	张平

4.4 获奖

1. 周益春教授等的《地方综合性大学材料学科硕士研究生“综合交叉、跨学科”培养模式的实践》获得 2005 年高等教育国家级教学成果奖二等奖；
2. 周益春教授、郑学军教授、李江宇教授和罗文波教授等组成的课程组的《材料的宏微观力学性能》被评为国家级精品课程。
3. 丁建文教授的博士学位论文“低维纳米结构体系的电性质和应力效应”被评为湖南省优秀博士论文，并被推荐为全国优秀博士论文，导师：颜晓红；
4. 郑学军教授的博士学位论文“压电薄膜的断裂韧性与激光作用下的破坏机制”获得全国优秀博士学位论文提名奖，导师：周益春；
5. 毛宇亮的硕士学位论文“碳纳米管的第一性原理研究”被评为湖南省优秀硕士论文，导师：颜晓红；
6. 张建军的硕士学位论文“半导体量子点体系钟应变调制的自组装”被评为湖南省优秀硕士论文，导师：钟建新；
7. 钟向丽获得湘潭大学研究生校长奖特等奖，导师：周益春；
8. 袁灿、屈岳波、黄俊、尹力、龚海、周文军、李安强同学的“旋转电弧传感轮式移动机器人焊缝跟踪系统”获第九届“挑战杯”飞利浦全国大学生课外学术科技作品竞赛终审决赛一等奖，指导老师：洪波；
9. 唐甜、钱峰同学的“纳米晶镍连续脉冲喷射电沉积装置”获第九届“挑战杯”飞利浦全国大学生课外学术科技作品竞赛终审决赛二等将，指导导师：潘勇、王先友；
10. 谢成荫、陈文林、唐稳庄、孔马斌、王北战、李东星同学的“基于连续分度弧面凸轮机构的大扭矩高性能数控转台”获第九届“挑战杯”飞利浦全国大学生课外学术科技作品竞赛终审决赛三等奖，指导老师：胡自化、杨湘军。

五、合作交流

5.1 开放课题

2005 年共收到 15 项开放课题申请，经“先进材料及其流变特性教育部重点实验室(湘潭大学)”第一次学术委员会的评审，其中 9 项被批准为本实验室开放课题。本批开放课题的执行年限为 2006 年 1 月至 2007 年 12 月。

先进材料及其流变特性教育部重点实验室(湘潭大学)2005 年度批准开放课题清单

序号	课题名称	申请人	职称	所在单位	批准经费	项目编号
1	基于纳米材料修饰的神经递质电化学探针	费俊杰	讲师	湘潭大学	1 万元	KF0501
2	高分子固体材料的非线性流变特性及其应用	罗文波	教授	湘潭大学	1 万元	KF0502
3	高温下热障涂层界面断裂韧性的实验和理论研究	毛卫国	博士生	湘潭大学	1 万元	KF0503
4	简单金属表面典型物理化学过程研究	唐壁玉	教授	湘潭大学	1.5 万元	KF0504
5	纳米TiO_2复合薄膜的合成机理及性质研究	万　隆	教授	湖南大学	2 万元	KF0505
6	镍掺杂 ZnO 稀磁半导体的溶胶－凝胶法制备及其性能研究	王金斌	副教授	湘潭大学	1 万元	KF0506
7	用压痕方法研究块体非晶合金的流变行为	魏炳忱	副研究员	中科院力学所	2 万元	KF0507
8	梯度硬质合金三元系 Ti-Ta-X (X=Co,Ni,Fe)相图研究	徐洪辉	副教授	中南大学	2 万元	KF0508
9	炭/炭材料表面涂层改进与金属的连接性	张福勤	教授	中南大学	2 万元	KF0509

5.2 参加会议、访问研究

2005 年，实验室共派出了 40 多人次出国(境)访问、讲学、合作研究或参加国际学术会议，在湘潭承办了“中国青年科学家论坛第 96 次活动”。实验室的罗迎社教授作为组织委员会主席组织了在上海召开的“第四届泛太平洋地区流变学会议”。

参加会议、访问研究：

序号	会议时间	会议名称	主办单位	会议地点	参加人员
1.	3.19 - 26	第 11 届国防断裂力学会议	意大利力学学会	意大利	毛卫国
2.	4.17 - 20	17 届集成铁电国际研讨会	复旦大学	上海	唐明华
3.	5.23 - 25	中国青年科学家论坛第 96 次活动--材料学科的迅速发展对固体力学提出的挑战	中国科协	湘潭	周益春、李江宇、林建国、谭援强及部分研究生
4.	6.13 - 25	电子结构计算与应用研讨会	中国科学院交叉学科理论研究中心	北京	毛宇亮
5.	8.07 - 11	4th Pacific Rim Conference on Rheology (PRCR4)	中国力学学会、化学学会、流变学专业委员会	上海	罗迎社、王智超、唐立平、杨建桃等
6.	8.25 - 27	第十三届全国凝聚态理论和统计物理会议	宁夏大学	银川	张建军
7.	8.26 - 28	中国力学学会学术大会'2005	中国力学学会	北京	周益春、罗迎社、龙士国
8.	9.18 - 20	中国物理学会 2005 年秋季学术会议	中国物理学会	武昌	唐超、毛宇亮 胡柯、刘超飞
9.	9.25 - 30	56th Annual Meeting of Electrochemistry	国际电化学会	Busan Korea	王先友
10.	10.8 -13	高分子全国学术会议	北京大学	北京	张海良
11.	10.15-16	第十届全国青年材料科学技术研讨会	中国材料研究学会青年委员会	长沙	周益春、钟向丽等部分实验室人员
12.	11.24 - 28	第十三次全国电化学学术会议	中国化学会	广州	王先友
13.	3 月	唐壁玉教授结束在美国马萨诸塞大学的为期两年的访问研究回国			
14.	7 月	龙士国副教授结束在日本东京大学为期一年的访问研究回国			
15.	8 月-12 月	喻更生博士生在 Deakin University(Australia)合作研究			
16.	11 月	郑学军教授结束在美国匹兹堡大学为期一年的访问研究回国			
17.	11 月	张建军博士生前往德国马普研究所进行为期一年的科研合作			
18.	2005 年	钟建新教授在美国橡树岭国家实验室访问研究			

5.3 邀请讲学

2005 年，实验室共邀请了 10 位国内(境)外知名专家学者前来讲学。

序号	时间	报告人	职称(职务)	所属单位	报告题目
1.	3.2	徐　坚	教授	中科院化学所	仿生材料研究进展
2.	5.14	李求长	副厅长	湖南省科技厅	当代高新技术及产业发展态势
3.	5.25	文翠娥	博士	Deakin University (Australia)	金属泡沫材料的制备与性能
4.	6.24	王清明	教授	University of Pittsburgh (America)	Integrated thin film bulk acoustic wave resonator
5.	7.12	邢定钰	教授	南京大学	自旋输运和巨磁电阻
6.	7.12	卢仲毅	研究员	中国科学院理论物理研究所	第一性原理的计算/大规模并行计算与物理学
7.	8.10	龚正虎	教授	国防科技大学	新一代互联网的发展
8.	10.26	闵乃本	院士	南京大学	和平崛起与能源、新世纪面临的科技挑战
9.	10.26.	邹志刚	教授	南京大学	光催化清洁能量转换和环境净化材料
10.	11.17	阳年发	教授	湘潭大学	核磁共振的原理及其应用

5.4 年度学术研讨会

为活跃学术气氛，促进各学科间的学术交流，2006 年 1 月 16-17 日，“先进材料及其流变特性教育部重点实验室 2005 年年度学术研讨会”在湘潭大学逸夫教学楼召开。蔡远利教授等 29 人作了学术报告。参加学术研讨会的有相关院系的老师和研究生共 100 余人。

学术报告人及报告题目如下：

序号	报告人	职称	所属单位	报告题目
1.	蔡远利	教授	湘潭大学	紫外光活化室温可逆加成断裂链转移自由基聚合
2.	杜　勇	教授	中南大学	Al 基体系稳定及亚稳相平衡的精细研究及其应用
3.	费俊杰	博士生	湘潭大学	碳纳米管在电分析化学中的应用
4.	龚曙光	教授	湘潭大学	无网格 Galerkin 法在结构形状优化中的应用研究

5.	李　智	副教授	湘潭大学	TeZnP450 度等温截面的测定
6.	阳年发	教授	湘潭大学	Preparation and Application of Dendrimer-bound Catalytic Material
7.	林建国	教授	湘潭大学	TiAl 合金超塑扩散连接的理论与实验研究
8.	龙士国	副教授	湘潭大学	镍镀层的变形织构生成机理
9.	徐洪辉	副教授	中南大学	采用扩散偶技术和关键合金法高效测定三元合金相图
10.	毛卫国	博士生	湘潭大学	热力耦合下热障涂层界面屈曲破坏实验分析
11.	毛宇亮	博士生	湘潭大学	碳纳米管的第一性原理研究
12.	潘　勇	副教授	湘潭大学	预镀电池钢壳材料的研制
13.	苏旭平	教授	湘潭大学	Interpretation of Si Reactivity in General Galvanizing
14.	孙立忠	副教授	湘潭大学	Hg 空位缺陷对红外光电子材料碲镉汞结构和电学性能影响的第一性原理研究
15.	谭松庭	教授	湘潭大学	无机—聚合物杂化纳米纤维和纳米管
16.	谭援强	教授	湘潭大学	水在氮化硅表面吸附的密度泛函研究
17.	唐壁玉	教授	湘潭大学	量子波包方法在材料科学中的应用
18.	唐明华	副教授	湘潭大学	Fabrication and Characteristics of MFIS Structure Ferroelectric Memory
19.	唐　翌	教授	湘潭大学	Heat Conduction in 1D Systems: Molecular Dynamics Simulation
20.	王金斌	副教授	湘潭大学	稀磁掺杂纳米 ZnO 的制备与磁性能研究
21.	王先友	教授	湘潭大学	高性能组合能源系统的设计、制备及其在军事上的应用研究
22.	曾以成	教授	湘潭大学	分数傅立叶变换及应用
23.	张海良	教授	湘潭大学	ABC 三嵌段高聚物的合成与表征
24.	张俊彦	教授	湘潭大学	金属多孔材料的研究进展及其应用
25.	郑学军	教授	湘潭大学	Measurement of Residual Stress in Ferroelectric Thin Films Based on Statistic Average of Micro-mechanics
26.	钟向丽	博士生	湘潭大学	NvFRAM 用掺杂钛酸铋铁电薄膜的研究
27.	丁建文	教授	湘潭大学	Accurate Energy Spectrum and Spin-Modulated Conductance of a Gated Rashba Ring of Finite Width
28.	周益春	教授	湘潭大学	涂层与薄膜的界面结合性能
29.	朱卫国	教授	湘潭大学	含特殊功能基的有机电致磷光材料及其电磷光性能

六、附录

实验室部分获奖证书

实验室部分论文摘要

Effective electromechanical moduli of ferroelectric ceramics with fiber textures

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In this letter, we report the predictions on the effective piezoelectric coefficients and electromechanical coupling factors of ferroelectric ceramics $BaTiO_3$ and $Pb(Mg_{1/3}Nb_{2/3})O_3-PbTiO_3$ (PMN-PT) with various fiber textures, including [001], [011], and [111], using a two-scale micromechanical model that accounts for microstructural phenomena at both domain and grain levels. It was observed that for $BaTiO_3$ the [011] texture is optimal with highest d_{31} and d_{33}, while for PMN-PT [001] texture is optimal despite the fact that [011]-oriented single-crystalline PMN-PT has higher d_{32} than that of [001]-oriented PMN-PT single crystal. In fact, [011]-textured PMN-PT ceramics have much smaller piezoelectric coefficients d_{32} and d_{33} than does [011]-oriented PMN-PT single crystal. It is also noted that [001]-textured $BaTiO_3$ and PMN-PT ceramics have even higher electromechanical coupling factor k_{31} than that of [001]-oriented single crystals. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1952584]

Ever since the discovery of ultrahigh strain and piezoelectric behavior in relaxor-based [001]-oriented rhombohedral single crystals $Pb(Mg_{1/3}Nb_{2/3})O_3-PbTiO_3$ (PMN-PT) and $Pb(Zn_{1/3}Nb_{2/3})O_3-PbTiO_3$ (PZN-PT),[1,2] there have been efforts devoted to accomplishing similar electromechanical properties in textured polycrystalline ceramics,[3–5] which are relatively cheaper to produce. Texture levels up to 90% and piezoelectric coefficients as high as 90% of single-crystal values have been demonstrated in the resulting ceramics,[6] which are very attractive for transducer applications. However, most of these investigations focused on [001]-textured PMN-PT ceramics, and other textures have rarely been studied. On the other hand, there is compelling experimental and theoretical evidence suggesting that single-crystalline PMN-PT and PZN-PT oriented along other directions, such as [011] axis, may have even higher electromechanical coupling. For example, much higher piezoelectric coefficient d_{32} and electromechanical coupling factor k_{32} were observed in [011]-oriented PZN-PT crystal,[7,8] consistent with theoretical predictions.[9,10] Motivated by these studies, it is natural to ask whether the [001] fiber texture is optimal for PMN-PT and PZN-PT ceramics, as far as electromechanical coupling is concerned. We intend to answer this question from a theoretical point of view in this letter.

Compared with their single-crystalline counterpart, polycrystalline ferroelectric ceramics have much more complicated microstructure. They consist of numerous grains, with each grain having its own domain pattern. As such, microstructural phenomena at both grain and domain levels have to be accounted for in order to model the ferroelectric ceramic accurately, and there are recent theoretical developments in the modeling of ferroelectric single crystals and ceramics that make this possible. In particular, an energy minimization approach has been applied to construct the engineered domain configuration in a ferroelectric single crystal poled along a nonpolar axis using multirank lamination,[9–11] allowing the calculation of the electromechanical moduli of a single-crystalline ferroelectrics using lamination theory. Combining this energy minimization-based lamination theory with an effective medium type self-consistent model that accounts for the intergranular interactions in ferroelectric ceramics,[12,13] it is possible to develop a two-scale micromechanical model to calculate the effective electromechanical moduli of textured polycrystalline ferroelectric ceramics, which we report here.

First, let us consider a ferroelectric grain poled along a nonpolar axis by an electric field $\mathbf{E}_0$, which favors those variants that minimize $-\mathbf{E}_0\cdot\mathbf{p}^{(i)}$, where $\mathbf{p}^{(i)}$ and $\mathbf{e}^{(i)}$ are spontaneous polarization and transformation strain of ferroelectric variants. When those variants are pairwise compatible, laminated domain configurations will be resulted in the grains to minimize their potential energy.[10] The effective electromechanical moduli of a grain having such a laminated domain configuration is given by[10,11]

$$\bar{\mathbf{L}} = \langle \mathbf{L}^{-1}\rangle^{-1},$$

$$\bar{\mathbf{M}} = \langle \mathbf{L}^{-1}\rangle^{-1}\langle \mathbf{L}^{-1}\mathbf{M}\rangle, \tag{1}$$

$$\bar{\mathbf{N}} = \langle \mathbf{M}^t\mathbf{L}^{-1}\rangle\langle \mathbf{L}^{-1}\rangle^{-1}\langle \mathbf{L}^{-1}\mathbf{M}\rangle + \langle \mathbf{N}\rangle - \langle \mathbf{M}^t\mathbf{L}^{-1}\mathbf{M}\rangle,$$

with

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First-principles study of transition-metal-doped single-walled carbon nanotubes

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Abstract
We study the effect of doping transition metals (TMs) into single-wall carbon nanotubes by using first-principles calculations. For metallic isolated (3, 3) single-wall carbon nanotubes, doping of Mn, Fe and Co makes them semi-metallic, while Ni doping leads to semiconductors. For (3, 3) nanotube bundles, a Co atom in the unit cell makes it exhibit semiconductor character. With two or three Co and Ni atoms doped into the bundle, the impurity atoms change the nanotube to semi-metal. In particular, the Mn_2C_{12} and Mn_3C_{12} bundle have comparable large magnetic moments, suggesting that such TM-doped nanotubes could be useful as nanomagnets.

Single-wall carbon nanotubes (SWCNTs) are among the most promising candidates for the construction of nanoscale electronic devices owing to their special properties and intriguing applications in many fields [1–6]. Depending on their chirality, SWCNTs may be semiconducting or metallic and they can thus be used as transistors and interconnects in electronic circuits [1]. However, one could modify the structure and electronic properties by doping. For example, by alkali-metal-atom doping, such as in Li-intercalated carbon nanotube ropes [4] and K-doped individual small carbon nanotubes [7, 8], a similar charge transfer is seen between the alkali-metal atoms and the carbon host. In these cases, the points of interest are the influence of hybridization between the alkali-metal atoms and carbon, and whether they introduce some new states on the valence or conduction band. However, besides the similar aspects with metal doping, there is an important influence in the aspect of magnetism on the nanotube by TM doping, especially the contribution of the d orbital of the TM atom when considering the hybridization.

In experiments, the three most common methods of producing SWCNTs are arc discharge [9], laser ablation [10], and catalyst chemical vapour deposition (CCVD) [11, 12]. A common feature of these methods is the presence of catalytic transition-metal (TM) particles (e.g., Mn, Fe, Co, Ni or their alloys). Study of the interaction of such TM particles with the nanotubes is essential in understanding their potential applications, including nanowires, high-strength composites, metal-coated structures, and nanoelectronic devices [13, 14]. It also provides an opportunity to investigate the magnetism of low-dimensional systems. The interaction between TM particles (Mn, Fe, Co, and Ni) and nanotubes could lead to semi-metallic systems that are of interest for spintronics devices [15] as well as nanomagnets. Moreover, quantitive evaluation of the band structure of SWCNTs doped with TM particles is important for possible electronic applications. However, to our knowledge, a complete understanding of the interaction between TMs (Mn, Fe, Co, or Ni) and CNTs or especially nanotube bundles has not yet been achieved. For instance, how do the TM particles affect the electronic structures of SWCNTs? To what extent do the changes in properties depend on the concentration of TM particles? In this paper, we perform a systematic theoretical study of TM (Mn, Fe, Co, and Ni) atom doping in the (3, 3) SWCNT and its bundles.

We use first-principles plane-wave pseudo-potential density functional theory as implemented in the CASTEP code [16]. For the exchange and correlation terms, the generalized gradient approximation (GGA) is used as proposed

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Band structure and optical properties of single-bonded cubic nitrogen: A first-principle study

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Abstract

The band structure of a single-bonded cubic phase of nitrogen has been investigated by the ab initio calculations of the pseudopotential density functional method. The basic optical constants including the dielectric function, the refractive index, the absorption, the electron energy-loss spectrum, the optical conductivity and the reflectivity of the single-bond cubic nitrogen and their dispersion properties were calculated. These theoretical results suggested that the single-bond cubic nitrogen could be a wide-gap optical material with unique properties.

Nitrogen usually consists of molecules where two atoms are strongly triple-bonded. In the recent decades, the nature of nitrogen at the high pressure has been intensively studied and many progresses have been made in both experimental and theoretical. In experimental, the shock-wave experiments by Nellis et al. [1] showed that the fluid nitrogen undergoes a transition at the modest pressures of 300 kbar and the high temperature of 6000 K, which appears to be the dissociation of the N_2 molecular to form monatomic. Similarly, other high-pressure experiments demonstrated that the nonmolecular solid phase of nitrogen is metastable at the ambient pressure [2–4]. On the other hand, the theoretical predictions showed that the raising pressure destabilizes the triple molecular bond of nitrogen and leads to various nonmolecular structures, in which each atom is bounded by single bond to three neighbors [5–8]. In these constructed phases, the 'cubic gauche' structure proposed by Mailhiot et al. [7] is energetically preferable. Since the cubic gauche phase (cg-N) of nitrogen was proposed, much interest has been paid to the stability of cg-N at the high pressure [8–10]. Recently, the cg-N phase of nitrogen have been synthesized by the high-pressure and high-temperature method [11]. The study showed that the cubic phase of nitrogen is a stiff substance with bulk modulus $\geqslant 300$ GPa, characteristic of strong covalent solids [8]. Therefore, the cg-N represents a new class of single-bonded nitrogen materials with unique properties such as the energy capacity being more five times than that of the currently most powerfully energetic materials. However, a complete understanding of the basically physical properties of cg-N still remains a challenging issue. In this contribution, we present the systemic investigation of the optical properties of cg-N by the first-principle method. To our knowledge, few studies involved in the optical properties of cg-N have been reported in the literatures [8–11].

In this study, we focus on the optical properties of the cg-N phase of nitrogen using the ab initio pseudopotentials density functional method. The ab initio calculations described here are performed with the CASTEP code, based on density functional theory (DFT) using ultrasoft pseudopotentials and a plan-wave expansion of the wave function [12]. We use the generalized gradient approximation (GGA) in the scheme of Perdew–Burke–Eruzerhof

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Lattice dynamics of single-bonded cubic nitrogen

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Abstract

The first principle calculations of the lattice dynamical properties of the single-bonded cubic nitrogen were performed using the density-functional perturbation theory together with plane-wave expansion and nonlocal pseudopotentials. The equilibrium structure of the single-bonded cubic nitrogen was first evaluated via the minimization of the total energy. Then, the harmonic phonon dispersion curves and the density of phonon states of the single-bonded cubic nitrogen have been evaluated within the linear-response framework. Furthermore, the heat capacity, enthalpy, free energy, entropy and velocity of sound of the single-bonded cubic nitrogen were calculated.

Nitrogen usually consists of molecules where two atoms are strongly triple-bonded. In the recent decades, the nature of nitrogen at the high pressure has been intensively studied and many important progresses have been made in both experimental and theoretical. In experimental, the shock-wave experiments by Nellis et al. [1] showed that the fluid nitrogen undergoes a transition at the modest pressures of 300 kbar and the high temperature of 6000 K that appears to be the dissociation of the N_2 molecular to form monatomic. Similarly, other high-pressure experiments demonstrated that the nonmolecular solid phase of nitrogen is metastable at the ambient pressure [2–4]. Theoretical predictions showed that the raising pressure destabilizes the triple molecular bond of nitrogen and leads to various nonmolecular structures, in which each atom is bounded by single bond to three neighbors [5–8]. Note that, among these phases, the 'cubic gauche' structure proposed by Mailhiot, Yang, and McMahan [7] is energetically preferable. Since the cubic gauche phase of nitrogen (cg-N) had been proposed in theoretical, much interest has been paid to the stability of cg-N at the high pressure [8–10]. Very recently, the cg-N phase has been synthesized by the high-pressure and high-temperature method [11]. The cubic phase of nitrogen is a stiff substance with bulk modulus $\geqslant 300$ GPa, characteristic of strong covalent solids [8]. Therefore, the cg-N represents a new class of single-bonded nitrogen materials with unique properties such as the energy capacity being more five times than that of the currently most powerfully energetic materials. However, a complete understanding of the basically physical properties of cg-N still remains a challenging issue. In this contribution, we present the systemical investigation of the thermal properties of cg-N by the first-principle method. To our knowledge, most of previously researches such as [9,10] are only concerned the phase transition of the cubic nitrogen at the high pressure, and few studies involved in the lattice dynamic properties of cg-N have been reported in the literatures [8–11].

In this case, we present the extensive first-principle studies of the structural and lattice dynamical properties of the single bonded cubic nitrogen. First, we briefly review the underlying theoretical methods, and then perform and discuss the theoretical results such as the geometry parameters, phonon dispersion curves, density of phonon states, and heat capacity. The calculations are performed using the plane-wave pesudopotential approach within the framework of density functional theory (DFT) as imple-

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Dependence of morphology of pulsed-laser deposited coatings on temperature: a kinetic Monte Carlo simulation

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Abstract

Considering deposition, dissociation, and diffusion of adatoms on the surface of substrates with hexagonal structure, we performed a kinetic Monte Carlo modelling to explore aspects of the thin film growth via pulsed laser deposition (PLD) within the submonolayer regime. First- and second-nearest-neighbor interactions calculated by the Morse potential are taken into account. The simulations show that the behavior of PLD at a relatively low substrate temperature is similar to that of molecular-beam epitaxy (MBE). However, with increasing temperature, there would be a crossover to PLD characterized by an increase of the island density with the pulse duration decreasing. Moreover, we show that the scaling function of the island size distribution for PLD and MBE at the temperatures T=250 and 550 K. Similarly, the scaling function for PLD resembles that of MBE at the relatively low temperature, and then, it is markedly different from MBE at the higher temperature. The physical origins involved in the growth behaviors above are proposed.

Keywords: Kinetic Monte-Carlo simulation; Pulsed laser deposition; Molecular-beam epitaxy; Film growth

1. Introduction

Thin films are used extensively for electronic devices and optical components, and thin film growth techniques have then become very important in the development of new materials and devices [1–4]. Pulsed-laser deposition is a convention growth technique, in which target materials are ablated by a pulsed-laser and then deposited in pulses on a substrate surface. Note that the technique could improve layer-by-layer growth [5], and is especially suited for the growth of complex multicomponent thin films, e.g., high-temperature superconductors [6], polymers [7], biomaterials [8], or ferroelectric films [9]. It is well known that a great advantage of PLD is the conservation of the stoichiometry of virtually any target material in the deposition [10]. Therefore, it is essential to understand basic physical processes involved in PLD. Recently, Hinnemann et al. [11] proposed a simple model for PLD. In this model, the duration of a pulse is assumed to be zero and the transient enhancement of the mobility of freshly deposited atoms is neglected. Moreover, the PLD process is controlled by three parameters, namely, the intensity I of the pulses, the diffusion constant D, and the average flux density of incident particles F. In detail, the atoms are instantaneously deposited in pulses of intensity I onto a surface. Between two pulses the adatoms diffuse to neighboring sites with rate D until they meet another adatom, in which case they form a stable and immobile nucleus of a 2D island, or until they attach irreversibly to edge of an already existing island. Importantly, these simulations show that thin films growth by PLD can differ markedly from that by MBE, which is consistent with the study by Combe [12] using a model with a finite pulse length. However, these studies have primarily focused on the effect of pulse intensity, while somewhat less

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Pulsed-laser deposition of polycrystalline Ni films: A three-dimensional kinetic Monte Carlo simulation

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Abstract

A three-dimensional (3D) kinetic Monte Carlo simulation was performed for the growth of polycrystalline Ni films on a Ni(1 0 0) substrate via pulsed-laser deposition (PLD) on the basis of the deposition of the incident atoms that nucleate randomly and the adatoms surface diffusion combining with a growth restriction within identically oriented grains. The simulations showed that the grains grow rapidly in PLD until they reach the critical grain size that is about 7 monolayer (ML) for the substrate temperature of $T = 300$ K, and then grow slowly with the time span of the simulations. Moreover, we compared PLD with molecular beam epitaxy (MBE), and found that PLD is characteristically different from MBE at the beginning of the deposition under the condition of the same deposition rate in both cases. However, the differences became not obvious as time unfolds and growth proceeds later.

Keywords: Kinetic Monte Carlo simulations; Pulsed-laser deposition; Polycrystalline thin film growth; Nickel

1. Introduction

Researches of the epitaxial growth of thin films have been of increasing interest in recent years, due to their extensive applications in electronic devices and optical components [1–4]. Although most studies are is experimental, the theoretical simulation has come to play an important role in analyzing the experimental data and providing the mechanistic information that is inaccessible experimentally. Kinetic Monte Carlo simulations have been proven to be useful for increasing the understanding of the atomistic details of thin film growth, as demonstrated by the numerous literatures, concerning computer simulations of the thin film growth, that have been published in the last 10 years (see e.g. Refs. [5–8]). These simulations

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Violet up-converted emission in Er^{3+}:Y_2O_3 nanocrystals

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Abstract

Er^{3+} ion-doped Y_2O_3 nanocrystals have been synthesized by co-precipitation technique. Up-conversion properties of Er^{3+} in Y_2O_3 nanocrystals under 488 nm laser excitation have been investigated. It is found that the luminescence intensities of the $^2P_{3/2} \rightarrow {}^4I_{13/2}$ and $^2P_{3/2} \rightarrow {}^4I_{11/2}$ transitions which originate from $^2P_{3/2}$ level are much stronger comparing with that of other up-converted transitions. The study implies that developing Er^{3+}:Y_2O_3 nanocrystalline materials might be promising for an up-converted violet laser application.

Considerable attention has been devoted to the energy conversion in rare-earth doped materials for the development of shorter wavelength radiation due to its potential application to undersea communication, medical diagnostics, information technology, color displays and so on [1–5]. Green up-converted lasers have been developed at room temperature by pumping erbium-doped fibers with near-infrared lasers [6–9]. However, for some applications, such as information storage–retrieval, shorter wavelengths are better. Great progress in blue–green diode laser has been made in recent years [10,11]. Thus, in the future, it is possible to use the blue and green diode laser as pumping sources to realize compact solid-state violet and ultraviolet lasers with the development of diode laser technology. Up-converting the visible light to higher frequency emission through rare-earth doped materials might be a feasible approach. Nanometer-sized crystals, on the other hand, have attracted much attention more recently because strongly sized-dependent optical properties have disclosed applications including optoelectronic devices of high performance [12]. For RE doped nanocrystals, it is believed that the doped

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Investigation of an anisotropic plate model to evaluate the interface adhesion of thin film with cross-sectional nanoindentation method

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Abstract

Cross-sectional nano-indentation is a new technology especially designed for measuring interface adhesion of thin film with nano-indenter and atomic force microscopy or scanning electron microscopy. In the paper, the delamination area induced by nano-indenter pressing on the cross-section of multiple-layer thin film structure was regarded as a semi-circular interfacial crack system, and thin film delaminated from the oxide-layer/substrate composite assumed as rigid was simplified as a bending circular plate. Based on the anisotropic plate theory, in which the effect of transverse shear is considered, the analytical relationship of the critical energy release rates per unit new crack with the radii of interfacial crack area, the size of oxide-layer/substrate composite extrapolated, and the displacement of thin film extrapolated by the indenter was derived. As example, the interfacial adhesion of $BaTiO_3$, $CoFe_2O_4$, and PZT-4 thin films evaluated by the anisotropic plate and the previous tapered beams models were simulated and discussed.

Keywords: Thin film; Interfacial adhesion; Cross-sectional nano-indentation; Delamination; Plate theory

1. Introduction

Since the emergence of thin and thick films at the end of 1970s and their subsequent applications in microelectromechanical systems (MEMS), there has been continuous effort for materials development and technology innovation in this field, leading to a significant number of industrial and commercial applications [1]. Spearing pointed out the basic premise behind MEMS concept is that the high volume production and low unit cost achieved by the microelectronics industry over the past 50 years could also be accomplished in devices where mechanical and electrical components are integrated into a single silicon chip or equivalent structure [2]. They are widely used in the high technological field of information techniques, new material techniques and aviation, and appear great superiority increasingly. MEMS are usually composed of multiple-layer piezoelectric thin film structures, such as actuators, detectors, memories, and sensors [3,4]. Additionally, the application of these piezoelectric thin film materials as dielectric layers in extreme high density, new generation dynamic random access memory (DRAM) looks promising.

Interface adhesion is becoming a critical material property for improving the reliability of multiple-layer thin film structures used in MEMS. As we know, it is natural that the film may fail due to the heating loads, electric loads as well as mechanical loads in the case of the film at operating state. Therefore, it is important

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Thermal fatigue of particle reinforced metal–matrix composite induced by laser heating and mechanical load

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Abstract

The thermal fatigue of particle reinforced metal–matrix composite induced by repetition-pulsed laser heating and mechanical load was experimentally and numerically studied. It is found that the fatigue damage is initial at the intersection region of laser irradiated brim region and the perpendicular direction of tensile load. The initial damage is induced by void nucleation, growth and subsequent coalescence in the matrix material or interface separation. The fatigue cracks are constituted of void in the matrix, interface separation and particle fracture. The propagation direction of fatigue crack is the perpendicular direction of the tensile load. The fields of temperature, macroscopical stress and microscopical stress and the histories of temperature, macroscopical stress and microscopical stress induced by the repetition pulsed laser and tensile load were simulated by ANSYS-DYNA finite element code. It is found that with the times of laser-irradiated increasing, the maximum temperature within every pulsed laser is increasing. The time of the maximum temperature lagged in the time of the maximum intensity of laser. The maximum stress took place at the intersection region of laser heating brim region and the perpendicular direction of tensile load. Therefore, the damage would be initial at these regions. The results are agreement with the experiment results.

Keywords: A. Metal–matrix composites (MMCs); B. Fatigue; C. Damage mechanics; D. Scanning electron microscopy (SEM); Laser heating

1. Introduction

Particle reinforced metal–matrix composite (PMMC) can be fabricated by standard techniques, considerably reducing the manufacturing cost and providing a good balance between price and mechanical properties. They are excellent candidates for structural components in the aerospace and automotive industries due to their high specific modulus, strength, and thermal stability [1,2]. Many papers have been devoted to the preparation, microstructure, corrosion behavior, creep properties and fatigue properties of PMMC [1–6]. However, the structural components applied for the aerospace and automotive industries are often subjected to severe thermal and mechanical loads simultaneously produced by aerodynamic heating, laser irradiation, localized intense fire and other mechanical loads [7–10]. Thermal load will lead to intense thermal stress concentration in the components of PMMC because of the mismatch of thermal and mechanical properties between the metal–matrix and ceramic reinforced particle. Such a concentration of thermal stress around defects often results in catastrophic failure of components. The thermal and mechanical loads are usually cycled, i.e., cycled thermal load and constant mechanical load, cycled mechanical load and constant thermal load or cycled thermal load and cycled mechanical load.

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Electrical properties of Nd-substituted $Bi_4Ti_3O_{12}$ thin films fabricated by chemical solution deposition

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Abstract

Nd-substituted $Bi_4Ti_3O_{12}$ (BNT) ferroelectric thin films have been fabricated on $Pt/Ti/SiO_2/Si(1\,0\,0)$ substrates by chemical solution deposition (CSD). X-ray diffraction (XRD) and scanning electron microscopy (SEM) were used to identify the crystal structure, the surface and cross-section morphology of the deposited ferroelectric films. After annealing at 700 °C, the $Bi_{3.15}Nd_{0.85}Ti_3O_{12}$ and $Bi_{3.54}Nd_{0.46}Ti_3O_{12}$ films are crystallized and exhibit a polycrystalline structure, but however show different preferred orientations. The experimental results show the ferroelectric and dielectric properties of the $Bi_{3.15}Nd_{0.85}Ti_3O_{12}$ thin films are better than those of $Bi_{3.54}Nd_{0.46}Ti_3O_{12}$ thin films. $Bi_{3.15}Nd_{0.85}Ti_3O_{12}$ thin films show a large remanent polarization ($2P_r$) of 65.4 μC/cm^2 under a maximum applied field of 356 kV/cm and high dielectric constant (ε_r) of 521 at the frequency of 10 kHz. This work clearly reveals that $Bi_{3.15}Nd_{0.85}Ti_3O_{12}$ thin film has the more promising potential application in the non-volatile ferroelectric random access memories and dynamic random access memories.

PACS: 77.55.+f; 77.80.−e; 77.84.−s

Keywords: BNT thin films; Chemical solution deposition; Ferroelectric material

1. Introduction

Ferroelectric thin films have attracted considerable attention for the potential applications in non-volatile ferroelectric random access memories (NvFeRAMs) [1]. The applications of $PbZr_xTi_{1-x}O_3$ (PZT) thin films have been most widely studied because PZT films have many advantages, such as large remnant polarization ($2P_r$) and a low processing temperature. However, it has some serious drawbacks such as the lead toxicity, fatigue and leakage current for use.

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Radial spherical ZnO structures with nanorods grown on both sides of a hollow sphere-like core

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Abstract

Radial spherical ZnO structures with nanorods grown on both inside and outside of a hollow sphere-like core along the *c*-axis direction have been produced by thermal evaporation of Zn powder in the absence of catalysts. Scanning electron microscopy and X-ray diffraction investigation show that the radial spherical ZnO structures are of high purity nanocrystal with a wurtzite structure. It is found that the formation of the sphere-shaped liquid Zn droplets before adding oxygen is a key factor to control the morphology of the radial spherical ZnO structures. The radial spherical structures could possibly be used as a building block and open up new opportunities for the self-assembly of functional nanodevices.

PACS: 81.05; 81.15.G; 68.65

Keywords: A1. Nanostructures; A3. Chemical vapor deposition processes; B1. ZnO; B2. Semiconducting materials

1. Introduction

Nanostructures exhibit peculiar and fascinating properties compared with their bulk counterparts due to the minuscule structures. Since it is very important for future nanotechnology to synthesize nanostructures of different shapes, which could be the building blocks in self-assembled process, and the novel properties of nanostructures depend sensitively on their shape and size, the ability to generate new types of nanostructures and to understand the growth mechanism is essential to nanoscience and nanotechnology development. Recently one-dimensional (1-D) nanostructures,

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Low Potential Amperometric Determination of Ascorbic Acid at a Single-Wall Carbon Nanotubes-Dihexadecyl Hydrogen Phosphate Composite Film Modified Electrode

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A sensitive and selective electrochemical method was developed for the amperometric determination of ascorbic acid (AA) at a glassy carbon electrode (GCE) modified with single-wall carbon nanotubes-dihexadecyl hydrogen phosphate (SWNT-DHP) composite film. The SWNT-DHP composite film modified GCE was characterized with SEM. The SWNT-DHP composite film modified GCE exhibited excellent electrocatalytic behaviors toward the oxidation of AA. Compared with the bare GCE, the oxidation current of AA increased greatly and the oxidation peak potential of AA shifted negatively to about –0.018 V (vs. SCE) at the SWNT-DHP composite film modified GCE. The experimental parameters, which influence the oxidation current of AA, were optimized. Under the optimal conditions, the amperometric measurements were performed at a applied potential of –0.015 V and a linear response of AA was obtained in the range from 4×10^{-7} to 1×10^{-4} mol L^{-1} and with a limit of detect (LOD) of 1.5×10^{-7} mol L^{-1}. The interferences study showed that the SWNT-DHP composite film modified GCE exhibited good sensitivity and excellent selectivity in the presence of high concentration uric acid and dopamine. The proposed procedure was successfully applied to detect AA in human urine samples with satisfactory results.

Key Words : Amperometry, Ascorbic acid, Single-wall carbon nanotubes, Electrocatalysis

Introduction

It is well known that ascorbic acid (AA) exists extensively in fruit and joins in many biological reactions. Recently there has been a considerable effort in the development of the voltammetric procedures for the determination of AA selectively and sensitively in biological organization and food etc. It is generally believed that direct electrooxidation of AA at bare electrodes is irreversible and therefore requires high overpotential.[1] Moreover the direct redox reaction of uric acid (UA), dopamine (DA), and AA take place at very similar potentials and often suffer from a pronounced touling effect, which resulting in rather poor selectivity. Although various electrochemical methods, mainly based on the chemically modified electrodes, have been proposed[2-11] for determination of AA, seldom procedure could well resolve this problem by eliminating the interferes of high concentration DA and UA at the same time.

There has been much interest in the research of carbon nanotubes since their discovery.[12] Carbon nanotubes are molecular-scale wires with high electrical conductivity, high chemical stability, and extremely high mechanical strength and modulus.[13] Utilization of these properties has lead to application of carbon nanotubes as scanning probes,[14] electron field emission sources,[15] actuators,[16] nanoelectronic devices,[17] batteries,[18] nanotubes-reinforced materials,[19] potential hydrogen storage material[20] and chemical sensors.[21] The subtle electronic behaviors of carbon nanotubes reveal that they have the ability to promote electron-transfer reactions when used as an electrode material in electrochemical reactions. However, since carbon nanotubes have a large dimension and hydrophobic surface, the aqueous suspension of intact carbon nanotubes was usually unstable, which limited the applications of carbon nanotubes in electroanalytical chemistry. Carbon nanotubes consisting of cylindrical shells of graphitic sheets with nanometer diameter were found in two distinct types of structures: the single-wall carbon nanotubes (SWNT) and multi-wall carbon nanotubes (MWNT). The multi-wall carbon nanotubes (MWNT) were firstly used to fabricate carbon nanotubes electrodes by mixing them with binders such as bromoform, mineral oil or liquid paraffin, which was applied in the oxidation of DA,[22] electrocatalysis of oxygen[23] and electrochemistry of protein.[24] Then MWNT was either treated with concentrated acids[25] or heated in the air[26] to produce hydroxyl, carboxyl and ketone groups at the terminus and dispersed in concentrated sulfuric acid[25] or organic solvents.[26] The resulting suspensions were then cast on the electrode surface and dried. However, these electrodes often suffered from the lack of stability or controllable dispersion on the electrode surfaces, i.e. attaching carbon nanotubes to an electric circuit in a controlled way is still a problem. Our previous work[27-29] reported that MWNT could be easily dispersed into water in the presence of dihexadecyl hydrogen phosphate (DHP). Based on the stable suspension of MWNT in the aqueous suspension of DHP, MWNT-DHP composite film modified GCEs have been developed. These electrode exhibited catalytic activity towards several biomolecules. Compared

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FIRST-PRINCIPLES STUDY OF DOPED SINGLE WALL CARBON NANOTUBES

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We investigate boron and nitrogen substitutional doping single wall carbon nanotubes (SWCNTs) by first-principles calculations. The optimized geometres of boron and nitrogen substituted SWCNTs exhibit bamboo-like structures. Boron and nitrogen impurities form acceptor and donor states in semiconductor SWCNTs. The highest occupied molecular orbital (HOMO) indicates the trend of forming inter-tube bonds in doping SWCNTs. It may start a new way to form inter-tube bonds by doping in SWCNTs.

Keywords: Carbon nanotube; impurity; electronic structure.

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As a new quasi-one-dimensional structure, single wall carbon nanotubes (SWCNTs) have received much attention since they exhibit rich phonon and electronic properties connected closely with the geometric properties.[1–10] It is found that the variation in the structure of SWCNTs causes remarkable changes in their properties, such as semiconductor–metal–semiconductor phase transitions.[11] It means that one could modify the properties of SWCNTs by changing the geometric symmetry or atomic structures, for example, by doping in the form of substitution of carbon by impurity in SWCNTs. To our knowledge, the first nanotube simulations by Yi and Bernholc[12] developed *ab initio* molecular dynamics method to study the atomic and electronic structure of doped microtubules of graphitic carbon. It

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Numerical Analysis of Electrodeposited Nickel Coating in Multistage Drawing Processes

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The elastic-plastic finite element method of a dynamic explicit algorithm was used to simulate the deep drawing processes of nickel coating electrodeposited on a steel substrate to form an advanced battery shell. The Belytschko-Wong-Chiang shell element was used to mesh the materials, the kinematical work-hardening model was adopted for the components, and the tied-with-failure contact criterion was given to the interfacial combination. The rate-type elastic-plastic constitute law was employed to handle the large deformation, and the central difference method was utilized to solve the finite element equations. The simulations of the materials in the first and final processes illustrated that the steel substrate and the nickel coating were simultaneously deformed and yielded in the die fillet profile and the flange area. The thickness variation of the nickel coating and steel substrate was dependent on the main principal stress, and their variation rule was consistent. In the entire drawing processes, the thinnest region after forming was at the lower part of the cup near the cup bottom, the extent of the coating being thinned after drawing was acceptable, and the material was capable of forming the battery shell. The simulated results were partly compared with tests and other analysis and showed good agreement.

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Residual Stress and Stress-Strain Relationship of Electrodeposited Nickel Coatings

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Keywords: coating; mechanical properties; stress/strain relationship.

Abstract The uniform nickel coatings on substrate of low carbon steel were prepared by an electrodeposition method. The chemical composition near the interface between electrodeposited nickel coating and low carbon steel substrate was graded. The residual stress in the electrodeposited nickel coating was measured by X-ray diffraction (XRD). It was tensile when the coating was not treated. The mechanism of residual stress in nickel coating is discussed based on free energy. Laser beam thermal shock was used to modify the mechanical properties of the nickel coating. Laser beam thermal shock could redistribute the residual stress in the nickel coating. The residual stress could be converted from tensile to compressive. A tensile method to determine the stress-strain curve of the coating is proposed where the stress-strain relationship of the substrate without coating was determined for the specimen loaded by an applied tensile force.

Introduction

Electrodeposited coatings are used as wear-resistant, corrosion-resistant, decorative and functional surface layers in many fields, such as aviation, space flight and electron. Nano-electrodeposits [1,2] are attracting much interest since the potential application in nano-materials. Electroplated nickel coating is widely used in the fabrication of metallic microdevices or microsystems due to some outstanding properties, such as soft, ductile, machinable and dense[3]. The electrodeposited nickel coating can also be used as the shell of high quality and high energy-storing battery. As a good corrosive-resistant coating, electrodeposited nickel coating must have high interface strength, good thermal-mechanical match between substrate and coating, and good residual stress distribution.

Thermal Shock and Thermal Fatigue of Ferroelectric Thin Film due to Pulsed Laser Heating

Introduction

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Failure of Thermal Barrier Ceramic Coating Induced By Buckling Due to the Temperature Gradient and Creep

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Keywords: thermal barrier ceramic coatings, residual thermal stress, thermal cycle, buckling failure

Abstract. The intent of this article was to study the failure mechanism of thermal barrier coatings (TBCs) induced by buckling. The main content included the following two parts. The first part investigated the thermal/residual stresses fields in TBCs with thermal cycles, which induced by the non-linear coupled effect of a large thermal gradient, thermal fatigue and creep strain of TBCs. One found that the residual stresses in the ceramic coating were compressive and accumulated with thermal cycles, which may be high enough to induce the buckling failure of the ceramic coating. The second part studied the critical buckling failure loading of the ceramic coating in TBCs under the condition of the compressive loading by use a theoretical model. Finally, a buckling plane, i.e. $N - T_s - s_r$ plane, was obtained by combined the above parts and applied to predict the service life of the TBCs system. In this plane, it was divided into the two parts, i.e., non-buckling region and buckling region.

Introduction

During the last decades, the thermal barrier ceramic coatings (TBCs) had been recognized as showing considerable promise for various applications involving high heat flux and/or moderately high temperature environments [1,2]. The TBCs system consisting of the ceramic coating, bond coat and substrate was now employed in most turbine engines, permitting gas temperature to be raised substantially above those for uncoated systems. The optimized TBC systems could make turbine process more efficient. The ceramic coating (i.e.7-9wt% yttria stabilized zirconia) had wide application due to its low thermal conductivity and diffusivity as well as its acceptable thermal shock resistance. This protective coating provided thermal insulation and could be used to prolong the life of the turbine components.

However, there are many factors that can degrade the thermal function of the TBCs. Zhou and Evans et al. have reviewed the mainly failure mechanisms of the TBCs system [3,4,5,6]. In some cases, the interface oxidation occurs between the ceramic coating/bond coat interface at high temperature. Many kinds of oxides (mainly alumina) form and may result in the interface delamination/crack [7,8,9]. Once nucleated, the many small cracks extend and coalesce, but the TBCs may remain attached at the remnant ligaments. Failure happens when the ligaments are detached over a sufficient area that a separation becomes large enough to create either a large-scale buckle or an edge delamination that eventually spalls from the substrate under the effect of the accumulated residual stresses in TBCs [10].

In this paper, the thermal/residual stresses fields in TBCs are firstly studied and obtained the relationship of that with thermal cycles, discussed in the section 2. A theoretical model in the section 3 is also proposed to predict the critical buckling loading of the ceramic coating under the condition of the compressive loading.

Study on the Creep Properties and Rheological Viscosity of Carbon Constructional Quality Steels

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Keywords: creep test, constitutive equation, carbon constructional quality steels, rheological viscosity, rheological model.

Abstract. In this paper, creep tests under the same temperature and different stress levels have been done on carbon constructional quality steels, the integral creep constitutive equation and differential stress-strain constitutive relationship can be established according to relevant rheological model, the integral core of the creep has been achieved through the experiments. Moreover, the coefficient related with viscosity of 35 steel was obtained through creep experiments' data. The viscosity coefficients of TC11 titanium alloy and Lc4 aluminum alloy were also compared and analyzed.

Introduction

Creep of materials is usually associated with time-dependent visco-plasticity under a fixed stress at an elevated temperature. Some important internal and external factors such as temperature, time, stress and material structure, etc. have influence on the creep performance of metals. Creep is an extremely complicated phenomenon that can't be ignored, because its existence (especially under high temperature) may lead to a serious accident. Cliftom R J. from the Engineering College of Brown classified it as the first item of the schedule of the items to be researched in his article of the plasticity of metal in 1985 [1], and suggested to seek a unified method to link up the creep strain and basic mechanism by combining microstructure with simulation.

A typical creep curve can be usually divided into three stages [2]. Stage one, or primary creep, which denotes that the creep-rate decreases with increasing viscoplastic strain or time. Stage two, or steady-state creep, the strain rate increases to a value that is constant over a range of strain. Eventually, an increase in the apparent strain-rate is observed, this region is termed Stage three, or accelerating creep, and leads to fracture. As far as the rheology of model is concerned, frature or rupturing means the failure of rheological forming, so we mainly consider the creep of the first stage and the second stage.

We have studied the creep properties of TC11 titanium alloy and Lc4 aluminum alloy and draw some important conclusions. In this paper, creep tests of 35 steel under the same temperature and different stress levels were carried out. The experimental curve is shown as Fig.1.

Determination on the creep constitutive equation

The rheology models used to describe metal materials are Kelvin's model or Voigt's model, Maxwell's model, Bingham's model, Burgers' model, six elements union of Kelvin-Maxwell model and series of Kelvin-Bingham model [3-5], etc. From the curve of 35 steel's creep experiment data, we can see that it is very short at the first stage and very similar with the creep curve of the modified Burgers' model, so we adopt the model to describe its creep deformation. The modified Burgers rheology model is shown in Fig.2.

It is not difficult to determine the constitutive equation of the rheological model for modified Burgers' model, and its expression is as follows:

$$\varepsilon(t)=\frac{\sigma_0}{E_1}+\frac{\sigma_0}{E_2}\left[1-\exp\left[-\frac{E_2}{K_2}t\right]\right]+\frac{(\sigma_0-\sigma_s)}{K_3}t\ ,\ \sigma_0\geq\sigma\ . \tag{1}$$

According to the results of the creep experiments of the material 35 steel, the parameters of this model can be determined; furthermore the creep equation can be obtained. The creep equation of 35 steel under the stress of 150MPa and the temperature of 500℃ is shown as below:

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Numerical Simulation and Experimental Study on Stress Relaxation Behavior of Polymers

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Keywords: polymers, displacement control, stress relaxation, finite element.

Abstract. The stress relaxation behavior of PP is investigated at room-temperature. Displacement controlled experiment is simulated using engineering computational software ANSYS and performed on PP. Both results were compared with each other. The experiment results show a good agreement with the numerical ones. The utility of numerical simulation is also discussed.

Introduction

As the development of industry and technology, there are all kinds of new demands for materials. To satisfy the needs of technology of different fields, including aeronautic industry, electronic information, modern automobile, electronic appliance and so on, we should improve the mechanical properties, heat-resistance, endurance, and corrupt-resistance of materials. Thus, the exploitation and investigation of polymers have become an important aspect in polymer science recently. Therefore, deformation and destruction regularity or relation between structure and properties of polymers have become one of the topics which are concerned and investigated by materials' and mechanical workers [1-5].

Recently, with the rapid development of computer technology and computational method, complex engineering problems can acquire good numerical solution by computer using discrete numerical computation method. Numerical simulation technology has become one of the impetus of forming and developing of modern engineering. Simultaneously the FEM (Finite Element Method) is also the most practical and broad way in engineering. In this paper, we investigated stress relaxation behavior of PP under room-temperature. The mechanical response is studied using ANSYS for finite element analysis. In this way, we get mechanical properties of this viscoelastic material. The stress relaxation behavior of it is verified and incarnated at the same time.

Finite element analysis

The material model in ANSYS

The property of material is determined by Generalized Maxwell Model [6], we have

$$G(\xi) = \sum_{i=1}^{I} G_i e^{(-\xi/\lambda_i)} + G(\infty), \tag{1}$$

where $G(\xi)$ presents condition evaluation of material property; I is the approximate relaxation coefficient of material used in Maxwell Principle; $G_i = C_i(G(0) - G(\infty))$, where C_i are constants associated with transitory response, $G(0)$ is initiation modulus and $G(\infty)$ is final modulus; ξ is decay time; λ_i is discrete relaxation spectrum.

Determining material parameter by experiment

Stress relaxation experiment under room-temperature is performed on Electronic Universal Test Machine CCS 44020. The curve of stress relaxation of PP specimen is shown in Fig.1. The values of relaxation modulus decreases quickly at beginning, then the relaxation velocity slows and gradually approaches equilibrium at last. The relaxation curve has oddity at time $t = 0$.

Taking the logarithm to the base 10 of Williams-Landel-Ferry equation [7-8], then

$$\mathrm{A} = \log_{10} \frac{C_1(T(t') - T_{base})}{C_2 + (T(t') - T_{base})}, \tag{2}$$

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The Finite Element Method of a Kind of New Variational Principle

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Keywords: the least work consumption principle, variational principle, finite element method, elasticity, plasticity, rheology.

Abstract: The variational problem of the variational principle, which is so called in Mechanics, is very useful when building more reasonable calculating theory of the finite element. This paper focuses on how to derive the corresponding calculating formula of the finite element method according to a kind of new variational principle. And the specific instances are given, and the results are correct.This finite element method of the new variational principle is appropriate to the general situations including elasticity, plasticity and rheology, besides, it offered a new alternative way for some more complicated problems, such as the study of elastic-plastic interface in the elastic-plastic analysis.

Introduction

It is generally known that the calculating formula also can be derived by the void work principle, which has nothing to do with stress-strain relation (namely, physical equation) of materials, so the finite element method derived by void work principle attaches no limitations to stress-strain relation of materials and is appropriate to general circumstances including elastic, plastic, and rheological theory. However, in the aspect of treating boundary conditions of finite element reasonably, in the aspect of approximate solutions, which adopt the simplest interpolating function to get the result that the stresses extend between every finite element after using mixed-mode finite element, and in the aspect of eliminating the non-continuance of stress of displacement-type finite element and so on , which are relative with finite element method, variational principle has important value of application[1] ,and it is difficult to settle these problems according to finite element method derived by void work principle, so in many situations, people would rather build more reasonable calculating theory of finite element method with the aid of variational principle. But some variational principles existing always attach some restrictive conditions, which obviously bring inconvenience when solving a kind of structure analysis problem in which different areas are described with different stress-strain relations. Therefore it is necessary to search a kind of variational principle which sets no limits to physical equations, that is, appropriate to general situations including elasticity, plasticity and rheology so as to establish establish the reasonable finite element method.

Zhou Zhubao [2] proposed and proved a least work consumption principle, from which three types of new variational principles which solve problems by stress, displacement and mixed method are derived. Since this least work consumption principle adds no limitations to physical equations and whether the structure has "dissipation" under loading, the derived new variational principles are just what we want: appropriate to general situations including elasticity, plasticity and rheology.

The finite element formula for calculating is established based on this new variational principle in this paper, the calculating instances are given and the results are correct.

Calculating formula of finite element of the new variational principle

Take the new variational principle solving by displacement for example, its expression is given as follows [2]

$$\delta\left\{\iiint_V F(u_k(t))dV + \iiint_V \lambda_i(t)\left[\sigma_{ij,j}(u_k(t)) + F_i(t)\right]dV + \iint_{S_u} \lambda_i^*(t)\left[u_i(t) - \overline{u}_i\right]dS \right.$$

$$\left. + \iint_{S_p} \lambda_i^{**}(t)\left[\sigma_{ij}(u_k(t))n_j - T_i(t)\right]dS \right\} = 0 . \qquad (1)$$

where $u_k(t)$(or $u_i(t)$) is the displacement component; $F(u_k(t))$ is the external work consumption rate; $F_i(t)$ is the body force component; $\overline{u}_i$ is the given boundary displacement component; $\sigma_{ij}(u_k(t))$ is the stress component ;

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Research on Identification Technology Based on Constitutive Model Database of Geotechnical Material

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Keywords: Geo-material, Constitutive Model, Database, Model Identification

Abstract. Constitutive model back analysis is important aspect and difficult point in geo-material back analysis, in which the identification of geo-material constitutive model is precondition and foundation of constitutive model back analysis. Based on the present circumstances about the model identification methods of geo-material constitutive researching, this paper begins with the fundamental principle of identification, puts forward the researching train of thought taking the geo-material constitutive model database as a platform, combining several identification algorithms.

Introduction

Early in 1977, the investigation of identification problems about the constitutive model were at earliest put forward by L. Jurina, G. Maier and K. Podolak [1]. In 1981, the problem of how to choose rational model was mentioned by G. Gioda and S. Sakurai[2]. However, the research in this field is far from the attention paid in the parameter inversion analysis. Entering the 1990's, Chinese scholars started to set foot in the field of constitutive model identification research. In 1991, having adopted systematical identification theory, statistics information theory and decision-making principle of mode identification, Dr Yuan Yong approached the problem of rock constitutive model identification[3]. In 1997, Liu Baoguo established one general mothod for viscoelastic constitutive model identification in tunnel surrounding rock system by analytical method[4]. In 1999, Academician Sun Jun introduced the fundamental thinking about geotechnical constitutive model recognition in his monograph, and researched the identification for rock mass elastic-viscoelasticity and elastic-viscoplasticity constitutive model under complicated conditions by least square method[5]. At the same time, since 1998, Professor Feng Xiating, as the representative, led the intelligence technique (artificial nerve network, genetic algorithm and evolution algorithm) into the research on the geotechnical material constitutive model identification, so that came into existence of the intelligence identification for constitutive model[6-8].

To sum up, rich fruits have been obtained in the research on the geotechnical constitutive. However, most of the research took those as the key point, which are establishing suitable criterion function[3,4], choosing effective input-output information[6,7], or looking for efficient parameter inversion algorithm[8], while with less consideration given to the establishment and exploitation of constitutive model database. In fact, through longtime researches, a lot of data about the constitutive model has been accumulated for the geotechnical engineering circles which has set up a solid foundation for establishment of constitutive model database. Based on the above consideration, this paper poses the researching train of thought taking the database of geo-material constitutive model as one platform, combining a few identification algorithms, such as the least square method, the intelligence identification algorithm and so on.

Fundamental principle for identification of geo-material constitutive model

Early in 1962, L. A. Zadeh made the definition for identification: identification is to define one model equivalent to the system being measured in one group of given model classification on the basis of input-output data. The three essential factors for identification are evidently pointed out in the definition, namely, data, model classification and criterion. Just the same, this definition is also followed by the identification of geo-material constitutive model; the fundamental identification loop chart is seen as Fig. 1[5]. Within the exact identification, one set of data collected through actual observation are usually stress σ (input) measured on-site, and actually measured U (input), where

$$U = \{U_i(x_i, y_i, \Delta t)\} \qquad i \in [1, N],\ \Delta t \geq 0 \quad , \tag{1}$$

Where Δt is a stretch of observation. The constitutive model classification set being marked as M ,

$$M = \{M_1, M_2, \cdots, M_j, \cdots, M_l\} \quad j \in [1, l], \tag{2}$$

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Effects of Entraining Velocity of Lubricant and Sliding Velocity on Friction Behavior in Stainless Steel Sheet Rolling

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Keywords: friction, lubrication, sheet metal rolling, entraining velocity of lubricant, sliding velocity, slide/roll ratio.

Abstract. A series of experiments was carried out using a rolling-type tribometer to investigate the effects on friction behavior of the entraining velocity of the lubricant at the inlet to the contact zone ($\boldsymbol{V}$) and sliding velocity during deformation ($\boldsymbol{\Delta V}$). Experiments with stainless steel sheets of two different surface roughnesses showed that the variations in the friction coefficient with entraining velocity $\boldsymbol{V}$ and sliding velocity $\boldsymbol{\Delta V}$ are largely dependent on the initial surface texture of the workpiece. For a smooth workpiece, the friction coefficient decreases with increasing sliding velocity $\boldsymbol{\Delta V}$ but keeps almost constant with increasing entraining velocity $\boldsymbol{V}$. However, for a rough workpiece, the friction coefficient initially decreases slowly and increases largely with increasing sliding velocity $\boldsymbol{\Delta V}$ or decreasing entraining velocity $\boldsymbol{V}$. Observation of the rolled surface for a smooth workpiece shows that, with increasing entraining velocity $\boldsymbol{V}$, the slip band becomes more marked, and with increasing sliding velocity $\boldsymbol{\Delta V}$, the rubbed portions become more conspicuous. For a rough workpiece, galling occurs at high sliding velocity $\boldsymbol{\Delta V}$. The critical condition for galling outbreak is shown on the $\boldsymbol{V}$-$\boldsymbol{\Delta V}$ graph. The galling outbreak process is observed by interrupting the rolling process.

Nomenclature

F = friction force on friction roll
h = lubricant film thickness
N = normal force on traction roll
p = yield pressure of workpiece
$r = (t_0 - t_1)/t_0 \times 100\%$, reduction in workpiece thickness
R_F = friction roll radius (35 mm)
R_T = traction roll radius (55 mm)
R_y = maximum roughness height
t_0 = workpiece thickness at inlet
t_1 = workpiece thickness at outlet
$V = (V_0 + V_F)/2$, entraining velocity of lubricant
V_0 = workpiece velocity at inlet
V_1 = workpiece velocity at outlet
V_F = friction roll velocity
$V_m = (V_0 + V_1)/2$, average velocity of workpiece
V_T = traction roll velocity (rolling velocity)
α = pressure viscosity index of lubricant
$\delta = (V_m - V_F)/ (V_m + V_F)/2$, slide/roll ratio
η_0 = viscosity of lubricant at ambient pressure
$\Delta V = V_m - V_F$, relative sliding velocity between workpiece and friction roll
$\mu = F/N$, friction coefficient between workpiece and friction roll
θ = inlet angle

Introduction

It has been realized that friction in the lubricated forming process is determined by the amount of lubricant entering the work zone and its performance at the interface between the tool and workpiece [1]. The amount of lubricant carried into the contact interface has been calculated by Mizuno based on hydrodynamic theory [1]. Mizuno showed that the thickness of the lubricant film is proportional to the entraining velocity of the lubricant at the inlet to the contact zone. This was revised by Wilson [2], who considered the thermal effects due to viscous shear, and by Sutcliffe and Johnson [3], who took the influence of surface roughness into consideration. On the other side, the viscous shear stress of the lubricant film is determined by the lubricant properties at high pressure, the film thickness, and the relative sliding velocity. The relative sliding velocity especially affects the lubricant performance at the interface [4]. This suggests that the entraining velocity of the lubricant at the contact zone inlet

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Research on the Tensile Rheological Properties to Temperature, Deformation Speed Dependence of TC1 Titanium Alloy Sheet

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Keywords: TC1 Ti-alloy sheet, deformation speed, thermo-rheology, mechanics properties.

Abstract. Combining closely with the practical production of one rectifier internal hood deep-drawing thermal forming, in order to provide parameters of material properties for the numerical simulation “experiments” of it, the standard samples of TC1 Ti-alloy thin plate of 0.8mm thickness were made, the tensile tests under different temperatures and strain-rates have been done so that the effects of their material’s thermo-rheological mechanics properties have been inquired out.

Introduction

Being a novel alloy material, TC1 titanium alloy has its broad prospect in application of aerospace-aviation which has been used in one model of aeroengine rectification hood made in China, and has a sound effect. However, the fundamental research is not sufficient on the mechanics properties of this new material, especially the investigation on the mechanics property of dependence on temperate, deformation speed has not unfolded yet. But actually, this kind of investigation in other sorts of material has gone on deeply, and has gotten good results, such as , the research on the influence of deformation speed and temperature on pure titanium friction coefficient was made by P.VENUGOPAL in India[1]; the research on the influence of deformation degree and temperature on Ti-31 alloy was done by Li Baoxun in the Institute of Shipping Material of Luoyang, in China [2]; the approaching on the effect of temperature and deformation speed on the relation of stress-strain of aluminum alloy A6061 was done by Yingshe Luo, in Xiangtan University of China, and Toshihiko Mori in Japan [3]. These show that it has the same important significance for TC1 titanium alloy to spread out these researches in this field. Based on this consideration, having adopted the method of combining testing analysis with numerical calculating, the influence of temperature and speed on tensile mechanics property of TC1 titanium alloy has been researched in this paper and the relevant mechanics parameters have been achieved.

The tensile experiment for TC1 titanium alloy

The experiment condition, equipment and scheme. An identical TC1 titanium alloy sheet has been used to have been made into standard samples. The tensile test is done at 8 kinds of different temperature and 5 sorts of tensile speed. The standard samples of titanium alloy thin sheets of TC1(Ti-2Al-1.5Mn) are shown as Fig. 1; the equipments for tensile test are shown as Fig. 2.

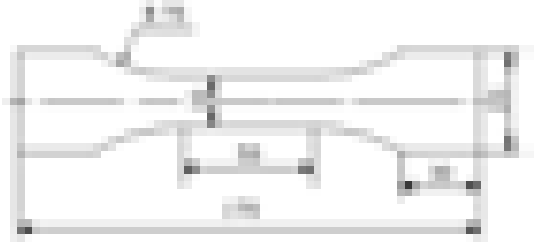
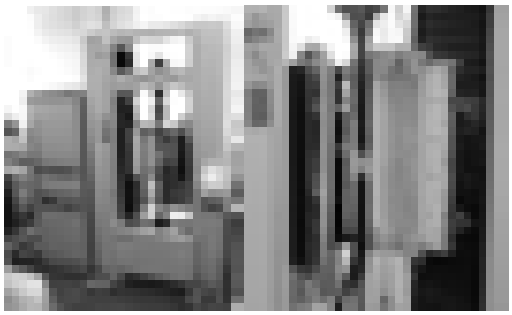


Fig. 1. The shape and size of the sample(t=0.8mm).



(a) The shape of the experiment machine (b) High-temperature hearth

Fig. 2. Experimental system of AG-1 type

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Measurement of Residual Stress in PZT Thin Films Based on Statistic Average of Micro-mechanics

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Keywords: PZT ferroelectric thin film, Residual stress, Statistic average of micro-mechanics, XRD

Abstract. Based on piezoelectric constitutive equations and statistic average of micro-mechanics, a method is proposed to measure residual stresses in ferroelectric thin films with X-ray diffraction (XRD). Considering an unit cell in the crystallite coordinate, the crystallite lattice strains are determined by the mismatches of lattice constants and thermal expansion coefficients, and its residual stresses are expressed using piezoelectric constitutive equation. Residual stresses in any oriented crystallite can be obtained via a transformation matrix, and residual stresses in thin films can be statistically averaged by orientations. Experimentally, PZT ferroelectric thin films were grown by pulsed laser deposition (PLD) method. Residual stresses in PZT thin films were evaluated by the statistic average of micro-mechanics and conventional $\sin^2\psi$ method. The measured results and the statistic average model of micro-mechanics are discussed.

Introduction

$Pb(Zr_xTi_{1-x})O_3$ (PZT) thin films have been intensively investigated for their widely use in high-value capacitors, sensors and actuators, ferroelectric field-effect transistors and nonvolatile memories. Residual stresses will be produced inevitably in thin films during the deposition [1,2], and the determination of residual stress in ferroelectric thin films is indispensable. Several techniques have been used to measure macroscopical surface residual stresses in thin films. For XRD methods, the most widely used model is conventional $\sin^2\psi$ method, in which thin films are assumed as isotropic and the piezoelectric coupling effects are neglected. However, as we know, it is inappropriate to evaluate the residual stresses in ferroelectric thin films.

In this paper, we propose a micro-mechanical model to measure residual stresses in ferroelectric thin films. Experimentally, PZT thin films were prepared by PLD method. XRD patterns of thin films were measured by X-ray diffractometer and texture goniometer. Residual stresses in PZT thin films were evaluated by the statistic average of micro-mechanics and conventional $\sin^2\psi$ method. The results were compared and discussed.

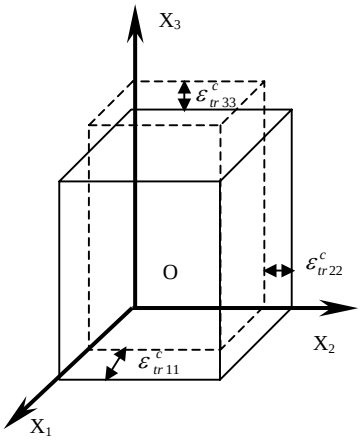

Fig. 1 An unit cell of PZT thin film and phase transition from cubic phase to tetragonal phase in the crystallite coordinate O-$X_1X_2X_3$ (solid lines: cubic structure, broken lines: tetragonal structure)

Model

An unit cell of PZT thin film in the crystallite coordinate O-$X_1X_2X_3$ is shown as Fig. 1, in which X_1-axis, X_2-axis and X_3-axis are parallel to crystallographic directions [100], [010] and [001], respectively.

Considering the piezoelectric effect and inherent anisotropy, the constitutive equations can be specifically expressed as

$$\begin{cases} \sigma_p^c = C_{pq}^E \varepsilon_q^c - e_{pn} E_n^c \\ D_m^c = e_{mq} \varepsilon_q^c + \kappa_{mn} E_n^c \end{cases} \quad (p,q = 1,\cdots,6; m,n = 1,2,3) \tag{1}$$

Where σ_p^c and ε_q^c are elastic stress and strain of the unit cell in the crystallite coordinate O-$X_1X_2X_3$. D_m^c and E_n^c are electric displacement and electric field. C_{pq}^E, e_{mq} and κ_{mn} are elastic stiffness tensor, piezoelectric tensor and dielectric tensor, respectively.

In the deposition, strains will be developed due to misfit between the film and substrate. According to the minimum energy principium, there are four stresses in thin films: intrinsic stress σ_{in}, thermal stress σ_{th}, transformation stress σ_{tr} and epitaxial stress σ_{ep} [3].

The intrinsic stress σ_{in} is generally caused by an incomplete structural order. Kweon and his group [2] considered that σ_{in} could be determined by the differences of lattice constants before and after annealing. The elements of intrinsic strain tensor of tetragonal grain ε_{inij}^c of unit cell in O-$X_1X_2X_3$ can be expressed as Eq. 2, where *a* and *c* denote a-axis and c-axis tetragonal lattice constants at room

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Evaluation of the effective elastic constants for polycrystalline PZT thin films by XRD patterns and pole figures

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Keywords: PZT thin film，Effective elastic constant，XRD pattern，Pole figure，Orientation average，Gaussian fitting.

Abstract. Polycrystalline $PbZr_{0.52}Ti_{0.48}O_3$ (PZT) thin films with different thickness were prepared by metal-organic decomposition (MOD) at different thermal decomposition temperatures. Their effective elastic constants were evaluated by x-ray diffraction (XRD) technology. XRD patterns were used to analyze the relative intensities of textures in the films, from which the effective elastic constants were evaluated by averaging over orientations. In the meantime, Gaussian distribution functions were used to describe the grains' orientation distribution, and the effective elastic constants of PZT thin films were evaluated by (001) pole figures. The results show that the effective elastic constants of PZT polycrystalline thin films evaluated by XRD patterns are in good agreement with those evaluated by pole figures. The polycrystalline thin films prepared with different experimental parameters are of different elastic properties.

Introduction

Ferroelectric thin films have attracted a great deal of attention recently due to their potential application in ferroelectric random access memories (FeRAM), microelectromechanical systems (MEMS) and photoelectronic fields. Ferroelectric $PbZr_{1-x}Ti_xO_3$ (PZT) thin films have been widely investigated for their excellent characteristics, such as high dielectric constants, large remnant polarization and fast switching [1]. In the case of polycrystalline PZT thin films, the mechanical properties are deeply dependent on their microstructures especially textures. Researchers have paid much attention on the correlation between the elastic properties and textures in traditional materials [2,3]. However, along with the wide use of MEMS, it's urgent to investigate the elastic properties of ferroelectric thin films for better understanding their mechanical behavior in these devices.

The present work reports on the evaluation of effective elastic constants for polycrystalline PZT thin films with x-ray diffraction (XRD) technology. First, PZT thin films were fabricated by metal-organic decomposition (MOD). Then, XRD techniques including XRD pattern and pole figure were used to analyze the grains' orientation distribution in PZT thin films, and the effective elastic stiffness constants were calculated. Finally, the experimental results evaluated by XRD patterns and pole figures were compared and discussed.

Experimental Procedure

Polycrystalline $PbZr_{0.52}Ti_{0.48}O_3$ thin films were deposited on $Pt/Ti/SiO_2/Si$ (100) substrates by metal-organic decomposition (MOD). The precursor compound solution [4] was 0.4 mol/L. The rotational speed of spin coating was 200 rpm for 5-7 seconds, and then it was changed into 3000 rpm for 20 seconds. Wet films were roasted on a hot plane at different thermal decomposition temperatures after each coating. After the dry films with needed thickness were obtained, the rapid treatment annealing (RTA) was adopted for 1 minute at $700\,^0$C under an O_2 gas flow. The samples were respectively labeled as A, B, C and D, and corresponding thickness and thermal decomposition temperatures were listed in Table 1.

The Philips X'Pert MRD x-ray diffractometer with monochromatic Cu-K_α radiation was used to measure XRD patterns of PZT thin films and PZT powder. The scan speed was 4°/min with a degree increment of 0.01°. (001) pole figures were measured by the X'Pert texture goniometer, in which the covered angular ranges were $0° \le \alpha \le 70°$ for the pole angles and $0° \le \beta \le 360°$ for the azimuth angles with a degree increment of 5°.

Evaluation Methods

In order to calculate the macroscopic elastic properties of a polycrystalline sample with texture, the sample fixed coordinate system O-xyz and the crystal fixed coordinate system O-XYZ are established. In the O-xyz system, x- and y-axis are two orthogonal directions in the sample's surface, and z-axis aligns along the normal direction of the surface. In the O-XYZ system, X-, Y- and Z-axis are parallel to crystallographic directions [100], [010] and [001], respectively. The orientation of the O-XYZ system with respect to the O-xyz system is determined by three Euler angles φ_1, φ_2 and ϕ (in Roe's notation [5]).

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碱性电池钢壳用镀镍钢带耐腐蚀性能研究

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摘要：利用 SEM、XRD 分析了不同厂家生产的碱性电池钢壳用镀镍钢带。比较了不同镀镍钢带的力学性能，并利用电化学方法详细讨论了不同镀镍钢带在 40%KOH 环境中的耐腐蚀行为，结果表明：湖南利德材料公司生产的电池钢壳用镀镍钢带已达到国际同类产品水平。

关键词：镀镍钢带；腐蚀性能；电池钢壳；碱性电池

Studies of Anti-corrosion Properties of Nickel-plated Steel Strips for Alkaline Battery Can

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Abstract: Nickel plated steel strips are widely used for battery can of alkaline battery. Samples of different facilities were examined by scanning electron microscopy (SEM) and X-ray diffraction (XRD). Mechanical properties of different nickel plated steel strips were compared. With electrochemical technology, corrosion behaviors in 40% KOH solution were discussed in detail. Results showed that battery can using nickel plated steel strips produced by Hunan Leed Material Company have reached the same lever with the international counterparts.

Keywords: nickel plated steel strip; corrosion properties; battery can; alkaline battery

电池钢壳是碱性电池一个重要的组成部分，为了防止正极活性材料对电池钢壳的氧化，及提高对电池液强碱环境的耐腐蚀性能，通常用镀镍的方法来保护铁基底。从现有的生产实践来看，电池钢壳有两种生产方式：一是由冷轧低碳钢带直接冲制成电池钢壳后，滚镀镍；另一种是由钢带镀镍后拉伸制壳，称为预镀钢壳。前者生产工艺简单，易操作，但钢壳内外镀镍层厚度不均，易造成电池均一性能差，容易出现漏镀的情况，且污染大。国外著名的电池生产厂家均采用预镀钢壳，因为其生产污染小、镀层厚度均一、次品率低、生产效率高，适于大规模产业化生产，所生产的电池性能均一，存放周期长。因此，从滚镀钢壳向预镀钢壳发展，研制出适于冲制、有较强耐腐蚀性能的碱性电池用高性能镀镍深冲钢带将是大势所趋[1-2]。

目前，国外只有德国和日本有能力生产这种电池钢壳用镀镍钢带。2002 年，湘潭大学研制出高性能电池钢壳用覆镍深冲钢带，并在湖南利德材料科技股份公司产业化生产电池钢壳用预镀镍深冲钢带。本文采用 SEM、XRD 及电化学方法等来对各种电池钢壳用镀镍钢带的力学性能和腐蚀行为进行比较研究。

1 实验

1.1 实验对象

实验用镀镍钢带分别为湖南利德材料科技股份有限公司生产提供的覆镍深冲钢带及德国和日本

脉冲激光沉积法制备的PZT铁电薄膜的残余应力

Residual Stress in $Pb(Zr_{0.52}Ti_{0.48})O_3$ Ferroelectric Thin Films Prepared by Pulsed Laser Deposition

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1 引 言

用纳米压痕法测量电沉积镍镀层的力学性能*

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[摘要]　随着科学技术的发展和薄膜材料的广泛应用，对于薄膜材料的性能的研究已经越来越引起人们的重视，尤其是其力学性能.因此，着重对电沉积镍涂层中的力学性能如硬度和杨氏模量等进行了研究.首先介绍了用纳米压痕的方法测量薄膜的硬度与杨氏模量的原理和方法，然后对电沉积后未经处理、经真空热处理和激光处理的样品进行了载荷–深度曲线的测试.结果表明，经过真空热处理的样品硬度明显减小，而经激光处理后的样品的硬度比未经处理的样品要高.同时，对于同一样品，加不同的载荷导致压痕深度不同，随着压痕深度的增加其测得的硬度值和杨氏模量值都会有明显的下降.

关　键　词：电沉积镍镀层；纳米压痕法；硬度；杨氏模量
中图分类号：O343.4　　文献标识码：A　　文章编号：1000－5900(2005)03－0050－08

Mechanical Properties of the Electrodeposited Nickel Coating by Nanoindentation

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【Abstract】 With the development of the science and the widely uses of the films or coatings, the research of the properties of the films attachs much interest of the researchers, especially mechanical properties. In the paper, the hardness and Young's modulus of nickel coating are investigated. The principles of nano－indenter to measure the hardness and Young's modulus of nickel coating are introduced. The relation curves of the load and displacement are obtained, including the original electrodeposited samples and the samples undergoing annealing and laser thermal shock. The results revealed that the hardness of the samples undergoing annealing is less small while that of undergoing laser thermal shock is slightly lager compared with the original electrodeposited samples. Moreover, the indentation depths change with the load, the hardness decrease with the increasing of the depth.

Key words: Nickel coating; Nano－indentation; Hardness; Young's modulus

随着科学技术的发展和薄膜材料的广泛应用，对于薄膜材料的各种性能的研究已越来越引起人们的重视[1,2]，特别是其力学性能.当然，对于薄膜与基底复合体的力学性能研究相对来说不是一件难事，但仅研究薄膜性能如硬度和弹性模量、应力－应变关系等力学性能却比较复杂.近几年由于新的实验装置出现，如纳米硬度计，使得一些方法不受试样尺寸的限制，对于纳米级的材料同样适用.

压痕法是一种很有发展前途的力学性能测量方法，它是在硬度法的基础上发展起来的. Tsui[3]、Bolshakov[4]和 Carlsson[5]等用纳米压痕技术和数值的方法研究了 8009 铝合金中的残余应力对硬度、接触面积和弹性模量的影响.结果表明，硬度不受残余应力的影响，而压痕的接触面积和深度却对残余应力的存在很敏感.基于以上特点，有许多学者对纳米压痕法测量薄膜中的残余应力产生了极大的兴趣. Suresh 和 Giannakopoulos[6]根据 Tsui[3]和 Bolshakov[4]的结果，假设材料中存在的是等双轴残余应力和残余应变场，提出了一种用尖的维氏压痕确定表面残余应力的方法，得出了有残余应力存在时的压痕面积和

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20号钢热拉伸流变特性的研究(Ⅱ)*

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[摘要] 为了进一步研究温度和应变速率对固体金属材料的粘性性质及其流变力学特性的影响,在温度为450 ℃、500 ℃、550 ℃和等应变速率(0.05/s~0.2/s)下对20号钢进行了一系列恒温恒应变速率实验,在Perzyna模型和Johnson-Cook模型的基础上建立了20号钢的高温流变应力模型,求出了与金属粘性有关的系数γ,并将模型计算结果与实验结果进行了比较,证实了该模型能更好的描述20号钢的温度效应和应变率效应.

关 键 词:20号钢;流变应力;本构模型;应变率效应
中图分类号:O341;TB301 文献标识码:A 文章编号:1000-5900(2005)01-0025-05

Study on the Rheological Properties of 20 Steel under Thermal Tension(Part Ⅱ)

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【Abstract】 In order to study the influences of temperature and strain rate upon viscosity and rheological properties of solid metal materials, a series of experiments under the same strain rates in the range of 0.05 /s~0.20 /s and at the constant temperatures in the range of 450~500 ℃ were done on the 20 steel. The rheological constitutive model of 20 steel is established on the basis of the Perzyna model and Johnson-Cook model. Furthermore, the coefficient γ related the viscosity was obtained. Comparing the results calculated from the model with the experiment results, it proves that the model can reflect the temperature effect and strain rate effect of 20 steel better.

Key words: 20 steel; rheological ptress; constitutive model; strain-rate effect

从文献[1]的实验曲线,可以看出:应变速率对碳素钢这种材料的屈服极限有明显的影响,所以可以称之为应变率敏感材料.波兰学者Perzyna P.在Hohenemser K., Prager W.和Freudenthal A.M.的基础上发展的刚粘塑性材料的本构方程,既考虑了材料的塑性特性,又包含了率型敏感的非线性性质,不失为一种较全面描述金属材料的粘塑性特性的本构模型[2~7].遗憾的是:该模型只考虑了材料的应变率和粘性效应,没有考虑金属材料的加工硬化效应和温度软化效应,而且没有将温度显式表示在方程式中.1983年,Johnson G. R.,Cook W. H.提出了一种新的经验型的粘塑性本构模型Johnson-Cook模型(简称JC模型)[8],这种模型能较好的描述金属材料的加工硬化效应、应变率效应和温度软化效应.并且由于其形式简单,使用方便,与实验结果吻合较好,使这一模型在工程中得到了广泛使用.这一模型是当前国内外较受欢迎的一种粘塑性模型,很多学者在原有形式的基础上进行了修正,以便更好地来描述特定金属的本构关系[9~11].但是JC模型也有缺陷,它没有全面考虑变形过程中材料热力学参数和微观机理,只是一个经验型公式.我们在Perzyna模型和JC模型基础上提出了一种修正模型,此模型能更好的描述优质碳素钢的流变性质[12].

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用于热障涂层氧化测量的复阻抗谱中等效电路参数的确定*

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[摘要] 建立了热障涂层在不同氧化阶段的等效电路,确立了等效电路中各元件参数与阻抗表征值之间的关系,确定了各元件的参数值,以达到对热障涂层微观结构以及TGO(其界面氧化物称为热生成氧化物(TGO))生长过程的检测.运用EQU软件模拟发现,等效电路阻抗谱与实测阻抗谱有很好的一致性,同时等效电路中参数值的计算与模拟的结果符合得很好.

关 键 词:复阻抗谱;热障涂层;等效电路;参数
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Determination of the equivalent circuit parameters for the impedance spectroscopy on the oxidation measurement in the thermal barrier coating

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【Abstract】 The simple equivalent circuits of thermal barrier coatings at different oxidation periods were proposed. The relationship between impedance spectroscopy and the parameters of the equivalent circuit of TBCs has been analyzed, meanwhile, the parameters of the equivalent circuit have been analytically obtained, so as to evaluate the degradation and the growth of TGO (The oxidation between ceramic coat and bond coat was named as thermal growth oxidation, i.e., TGO) in TBCs. It was found that the results of the impedance spectroscopy were fit to an idealized model circuit and the parameters obtained by the model were in good agreement with the simulated results by EQU program.

Key words: impedance spectroscopy; thermal barrier coatings; equivalent circuits; parameters

热障涂层是一层陶瓷涂层(Thermal Barrier Coatings,TBCs),它沉积在耐高温金属或超合金的表面,用以保护基底材料,使得用其制成的发动机涡轮叶片能在1 600 ℃的高温下运行,以提高发动机的热效率达60%以上[1].热障涂层一般由顶层(TC)陶瓷层(Ceramic Layer)、中间过渡层(Boad Coat)和基底(Sub)组成,如图1(a)所示.中间过渡层(MCrAlY)的作用是使得陶瓷层与基底层很好地粘结在一起,并提高基底的抗氧化性能;陶瓷层($ZrO_2-7-9\%Y_2O_2$)用来降低基底的工作温度,提高其热疲劳寿命;基底的作用主要是承受机械载荷.热障涂层在高温环境下工作时,中间过渡层中的金属元素会发生离化,成为金属离子;另外,陶瓷层中的氧也会离化成为氧离子,金属离子与氧离子都有向陶瓷层与过渡层的界面聚集的趋势,形成氧化物,通常称为TGO(thermal growth oxidation)[2],TGO一般是Al_2O_3,如图1(b)所示.由于TGO与中间过渡层的热不匹配性,以及TGO易于脆断,涂层中的残余应力使得界面处易于形成裂纹.随着TGO厚度的增加最终将可能导致涂层的剥落失效,显然TGO是影响热障涂层寿命的一个十分重要的因素[3].因而,无损检测TGO的生长与微观结构的变化就成了预测热障涂层寿命的重要内容.

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在制备过程中热障涂层系统内残余应力场预测©

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摘要　在热障涂层系统制备工艺冷却过程中，各层材料参数不匹配(如弹性模量、泊松比、热膨胀系数、热传导参数等)将导致其体内各层材料冷却速率不一样，同时在各层界面上热障涂层系统为了保持应变协调和位移连续，最终在冷却后热障涂层系统各层内均存在热残余应力。本文通过建立相应的理论模型得到了热障涂层系统各层热残余应力的解析解表达式。通过计算分析，我们得到了冷却方式和陶瓷喷涂厚度对各层残余应力的影响，最终希望得到一组最优化工艺参数来指导热障涂层制备工艺和生产。

关键词：热障涂层、残余应力
中图法分类号：0343

Prediction of residual stress in thermal barrier coating during the deposition process

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Abstract　The material parameters (such as Young's modulus, Poisson's ratio and thermal expansion coefficient) of each layer will result in the different cooling velocity of thermal barrier coatings (TBCs) system during the deposition process. Moreover, to satisfy the condition of strain compatibility at the free boundaries, residual stresses in TBCs occur after cooling to the ambient. In this paper, the analytical solution has been obtained by using a theoretical model. We have obtained the effect of cooling kinds and the thickness of ceramic coating on the magnitude of residual stress in TBCs. Finally, we will use a group of optimize parameters to control the deposition technology of TBCs.
Key words　thermal barrier coating, residual stress

热障涂层(Thermal Barrier Coating，**简称** TBC)**技术是表面技术的一种，早期应用在航空工业中，用于发动机高温零件的表面改性，防止热端部件受氧化和腐蚀及其危害，延长发动机的使用寿命。热障涂层是一层陶瓷涂层，它沉积在耐高温金属或超合金的表面，热障涂层是用于保护基底材料，使得用其制成的发动机涡轮叶片能在 1600°C 的高温下运行，以提高发动机的热效率达到 60%以上。图 1 就是典型的热障涂层系统横截面的微观简图。顶层是陶瓷涂层(ZrO_2-7%Y_2O_3)，其主要功能是起隔热作用，使基底处于相对比较低的工作温度；中间**

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