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# 凝结时空精华，铸就序构材料，力促大尺寸功能晶体新发展

薛冬峰[1]，苏良碧[2]，徐 军[3]

(1. 中国科学院 深圳先进技术研究院，多尺度晶体材料研究中心，深圳 518055; 2. 中国科学院 上海硅酸盐研究所，上海 201899; 3. 同济大学 物理科学与工程学院，上海 200092)

中国科学技术协会发布的 2021 年重大科学问题、工程技术难题和产业技术问题，将“如何突破大尺寸晶体材料的制备理论和技术”列为首要问题，位居十个对科学发展具有导向作用的前沿科学问题之首。这不仅对于进一步激发功能晶体材料领域研究人员的好奇心和自由探索热情，引领科技创新趋势和科研攻关方向，服务国家科技创新发展具有重要意义，而且将引导功能晶体材料领域广大科技工作者围绕问题开展原创性、引领性的科技攻关，为加快建设科技强国作出更大贡献，以优异成绩丰富中国式现代化内涵。大尺寸晶体材料在矿物学领域自然天成，常常令材料科技工作者感到震惊。例如，在所有已获认证的晶体中，最大尺寸的晶体是来自马达加斯加共和国的绿柱石，长 18 m，直径 3.5 m，体积约为 143 $m^3$，质量约为 380 t。追溯矿物的形成过程，人们不难发现形成大尺寸晶体在时空上的基本要求是时间长、空间大。因此，道法自然，生长大尺寸功能材料装备的研制与晶体生长动力学研究是两个关键自由度。由于晶体生长动力学与热力学互为函数，晶体生长的宏观行为不但在多尺度水平上受到结晶学结构对称性、组成元素间键合行为、晶体缺陷等多种物理化学因素制约，而且在多层次上受到生长装备塑造的生长环境的影响。随着数值模拟计算、SolidWorks 和 COMSOL 多物理场仿真软件，以及结晶固液界面形态可视化技术、装备自动化升级和多种原位检测技术的广泛应用，可利用电子背散射衍射和中子衍射等检测手段，从多维度、多尺度表征晶体的色心、局域配位结构、位错和晶界缺陷。开展晶体生长动力学与热力学研究可以依赖越来越丰富的精确数据。基于对“零缺陷”功能晶体的发展需求，大尺寸人工晶体总体上呈现从传统的单温区向多温区、传统的单加热体向多加热体耦合方向发展，更多深入系统的研究成果将会越来越振奋人心。

经过我国科研工作者一代代的传承和努力，中国科学院上海硅酸盐研究所的“米”级 BGO、中国科学院理化研究所和天津理工大学的 4.798 kg LBO、北京雷生强式科技有限责任公司的 8 英寸 Yb:YAG、中国科学院上海光学精密机械研究所的 $\phi$235 mm 钛宝石、天通控股股份有限公司和晶盛机电股份有限公司的 800 kg 泡生法蓝宝石、同济大学的 415 mm×810 mm×12 mm 导模法蓝宝石等成果均居于世界第一方阵水平。大尺寸光伏和电子级单晶硅、AlN、GaN、金刚石、SiC、$Ga_2O_3$、InP、$CaF_2$ 等系列重要功能晶体也得到迅猛发展，为我国光伏产业、LED 产业、集成电路产业、先进制造、医疗、大科学工程、国防等提供了材料支撑和保障。2021 年 8 月，由中国科协先进材料学会联合体主办，中国晶体学会、中国稀土学会、中国科学院深圳先进技术研究院承办了“如何突破大尺寸晶体材料的制备理论和技术”线上学术研讨会，来自多所高校及科研院所的一线科研人员参加了研讨。研讨会凝聚了晶体学学科专家学者的智力资源，着重分析了晶体学领域代表性的难点问题，对于进一步推动我国晶体学学科的发展具有重要意义。研讨会还围绕大尺寸晶体材料的基础科学、产业化、制造装备、加工装备等方面形成了政策建议报告并递呈国家相关部门。

2022 年上半年,《无机材料学报》编辑部邀请中国科学院深圳先进技术研究院薛冬峰研究员、中国科学院上海硅酸盐研究所苏良碧研究员和同济大学徐军教授共同担任特邀编辑，以“大尺寸功能晶体材料新进展”为主题组织出版专辑。本专辑收录了我国部分大尺寸功能晶体材料的最新研究成果和综述文章，体现了我国大尺寸功能晶体材料研究的前沿进展。希望本专辑能够抛砖引玉，为促进我国大尺寸功能晶体材料研究与应用发展提供有益参考。我们期待在全球学者的不懈努力和推动下，凝结时空之精华，铸就序构之新材，力促大尺寸功能晶体新发展。

# Developing Large-size Functional Crystals through Condensing Essence of Time-space and Modulating Order of Materials

XUE Dongfeng[1], SU Liangbi[2], XU Jun[3]

(1. Multiscale Crystal Materials Research Center, Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences, Shenzhen 518055, China; 2. Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai 201899, China; 3. School of Physics Science and Engineering, Tongji University, Shanghai 200092, China)

In 2001, China Association for Science and Technology released the major scientific issues, engineering technical problems and industrial technology issues. Among them, “How to break through the preparation theory and technology of large-size crystal materials” was listed as the primary issue, and the top one of 10 frontier scientific issues. This issue plays a significant role in related scientific research by stimulating curiosity and free exploration enthusiasm of the researchers in the field of functional crystal materials, guiding trend of innovation and research direction, and pushing researchers to carry out original and leading research focusing on the challenges to make greater contributions to accelerating construction of a strong scientific and technological country, and enriching the connotation of the Chinese-style modernization.

Natural formation of large-size crystalline materials in the field of mineralogy often shocked material scientists. For example, among all the certified crystals, the largest one is the beryl found in the Republic of Madagascar, which is 18 m in length, 3.5 m in diameter, 143 $m^3$ in volume, and 380 t in weight. Tracing the process of mineral formation, it is not difficult to figure out that the basic requirements of large-size crystals are long-time and large-space. So, developing the growth equipment and researching the crystal growth kinetics are two key degrees of freedom for artificial preparation of large-size functional crystals. Since crystal growth kinetics and thermodynamics are functions of each other, the macroscopic behavior of crystal growth is not only restricted by physicochemical factors (such as crystallography structure symmetry, bonding behavior between constituent elements), but also affected by growth environment shaped by growth equipment on a multi-scale level. Due to the wide application of numerical simulation calculation, SolidWorks and COMSOL multi-physical field simulation software, solid-liquid interface morphology visualization technology, equipment automation promotion, and a variety of *in-situ* detection technologies, the color centers, local coordination structures, dislocations, and grain boundary defects were researched from multi-dimension and multiscale with electron backscattering diffraction (EBSD), neutron diffraction, *etc*. More and more abundant accurate data can be used when researching the crystal growth kinetics and thermodynamics. Based on the demand of zero-defect crystals, the general development trend of the large-size artificial crystals is involved from the traditional single heating zone to the multi-heating zones, and from the traditional single heater to the coupling of multi-heaters. The results of more in-depth research in this field will become increasingly encouraging.

In recent years, through the inheritance and efforts of Chinese scientific researchers from generation to generation, many achievements have been placed in the first camp in the world, such as the meter-level BGO crystals of Shanghai Institute of Ceramics, CAS, LBO crystals with the weight of 4.798 kg of Technical Institute of Physics and Chemistry, CAS and Tianjin University of Technology, 8-inch Yb:YAG crystals of Beijing Opto-Electronics Technology Co., Ltd., Ti:sapphire crystals with the diameter of $\phi$235 mm of Shanghai Institute of Optics and Fine Mechanics, CAS, 800 kg-level sapphire crystals grown with Kyropoulos method of TDG Holding Co., Ltd. and Zhejiang Jingsheng Mechanical & Electrical Co. Ltd., and the large sapphire plates with the size of 415 mm×810 mm×12 mm grown with EFG method of Tongji University. Large-size photovoltaic and electronic grade monocrystalline silicon, AlN, GaN, diamond, SiC, $Ga_2O_3$, InP, $CaF_2$, and other functional crystals are also developing rapidly, which provide materials support and guarantee for Chinese photovoltaic industry, LED industry, integrated circuit industry, advanced manufacturing, medical industry, large science project, and national defense. In August 2021, front-line researchers from many universities and research institutes participated the online academic conference “How to break through the preparation theory and technology of large-size crystal materials”, which was sponsored by Advanced Materials Alliance of CAST Member Societies and organized by Chinese Crystallographic Society (CCrS), Chinese Society of Rare Earths (CSRE) and Shenzhen Institute of Advanced Technology, CAS. The conference, gathered the intellectual resources of experts and scholars in the field of crystallography, and analyzed the typical difficult problems of the field, which was of great significance for further developing crystallography. Through the conference, policy proposals focused on the basic science, industrialization, preparation equipment, processing equipment, and other aspects of large-size crystal materials were formed and submitted to the relevant national departments.

In the first half of 2022, the editor board of the *Journal of Inorganic Materials* invited Professor XUE Dongfeng from Shenzhen Institute of Advanced Technology, CAS, Professor SU Liangbi from Shanghai

Institute of Ceramics, CAS and Professor XU Jun from Tongji University as co-editors to organize a special issue with the theme of "New Progress in Large-size Functional Crystal Materials". This issue includes the latest research results and review articles of some large-size functional crystals in China, and reflects the frontier progress of the above crystal materials. It is hoped that this issue can provide useful reference for promoting the research and application of large-scale functional crystal materials in China. With the unremitting efforts and promotion of global scholars, we can condense the essence of time and space, modulate order of materials, and promote the development of large-scale functional crystals.

薛冬峰，教授、博士生导师，享受国务院政府特殊津贴，现任中国科学院深圳先进技术研究院多尺度晶体材料研究中心主任、深圳理工大学材料学院科研讲席教授，致力于新型晶体材料与储能技术研究。2003 年起历任大连理工大学化工学院材料化工系主任、中国科学院长春应用化学研究所稀土资源利用国家重点实验室主任和副所长、山东大学晶体材料国家重点实验主任和晶体所所长。西澳大利亚大学 Gledden 高级访问学者，国家杰出青年科学基金、中国科学院百人计划择优支持者，教育部新世纪优秀人才支持计划入选者，国家万人计划科技创新领军人才，国家新材料产业发展专家咨询委员会委员，中国建筑材料联合会专家委员会新材料学部委员，英国皇家化学会会士。在 *Journal of the American Chemical Society, Advanced Materials, Physical Review Letters* 等期刊上发表论文 600 余篇。学术成果获得湖南省自然科学一等奖、山东省科技进步一等奖、中国颗粒学会自然科学一等奖、中国化工学会基础研究二等奖等奖项。担任中国稀土学会稀土晶体专委会主任，兼任 *CrystEngComm* 副主编，任 *SCIENCE CHINA Technological Sciences*, *Journal of Rare Earths*,《无机化学学报》,《结构化学》,《人工晶体学报》等期刊编委。

E-mail: df.xue@siat.ac.cn

苏良碧，研究员、博士生导师，现任中国科学院上海硅酸盐研究所副所长。长期从事激光与光学晶体材料的研究，在国际上首次提出激活离子“局域格位结构设计和调控”的学术思想，成功地发展了一类具有优异光谱和激光性能的掺钕氟化钙/锶激光晶体；发展了热交换坩埚下降法(HEB)，成功研制出大尺寸、高透过率、高光学均匀性的深紫外级氟化钙晶体，并实现成果转移转化，保障国产光刻机关键光学元件的自主可控。在国内外 SCI 刊物上发表学术论文 200 多篇，获得授权发明专利 30 余项，合作出版学术专著 6 本。2014 年获得国家优秀青年科学基金资助，2017 年获得第十二届中国硅酸盐学会青年科技奖，2019 年获得国家杰出青年科学基金资助。应邀担任《人工晶体学报》副主编，美国 *Applied Optics* 期刊专题编辑，《无机材料学报》、《硅酸盐学报》、《激光与光电子学进展》等期刊编委，中国激光杂志社青年编委。

E-mail: suliangbi@mail.sic.ac.cn

徐军，同济大学物理科学与工程学院长聘教授、博士生导师，上海蓝宝石单晶工程技术研究中心主任、上海物理气相沉积(PVD)超硬涂层及装备工程技术研究中心技术委员会主任、上海光探测材料与器件工程技术研究中心技术委员会副主任、中国有色金属学会半导体材料学术委员会副主任。《人工晶体学报》副主编，《无机材料学报》顾问编委，中国硅酸盐学会晶体生长和材料专业委员会理事。主要研究方向为激光与光学晶体、晶体生长技术。首次提出并成功生长出大尺寸掺锶偏硼酸钡紫外双折射晶体并实用化；提出 $Cr^{4+}$和 Yb 共掺 YAG 自调制激光晶体并实用化；提出“激活离子局域配位调控”概念，发现 Yb,Na:$CaF_2$、Nd,Lu:$CaF_2$ 等系列氟化物晶体，Yb,Na:$CaF_2$ 晶体率先实现太瓦级(TW)激光输出；大尺寸钛宝石晶体实现百太瓦级激光输出；研制成功大尺寸倍半氧化物($Sc_2O_3$)晶体和氧化镓晶体；研制成功大尺寸蓝宝石衬底片、蓝宝石整流罩、蓝宝石氢原子钟谐振腔、400 kg 泡生法晶体、同步 22 片导模法蓝宝石片、导模法蓝宝石透明装甲板材等。发表 SCI 论文 500 余篇，授权发明专利 100 余项，出版著作 6 部。国家杰出青年科学基金、中国科学院百人计划择优支持者和百千万人才工程国家级人选获得者。先后获得国家科技进步二等奖(1/9)、上海市科技进步一等奖(1/9)和上海市自然科学一等奖(1/5)、中国科学院科技进步二等奖、中国科学院青年科学家奖、上海市自然科学牡丹奖、上海市十大杰出青年等奖励。已培养博士生 40 余名。

E-mail: 15503@tongji.edu.cn