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Volume 2 (2022)



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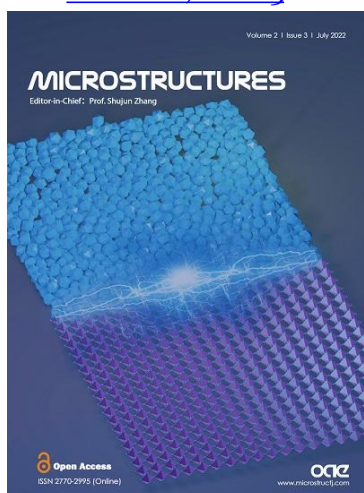
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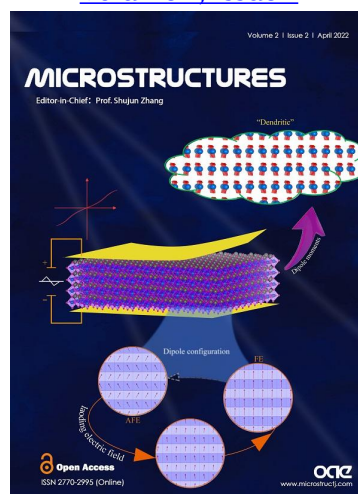
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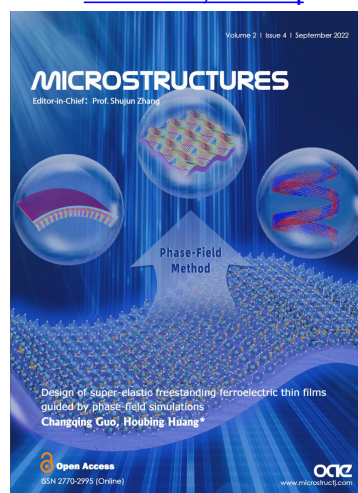
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Cover Picture

1. Hollow microstructural regulation of single-atom catalysts for optimized electrocatalytic performance

A-Wu Zhou, Ding-Sheng Wang*, Ya-Dong Li

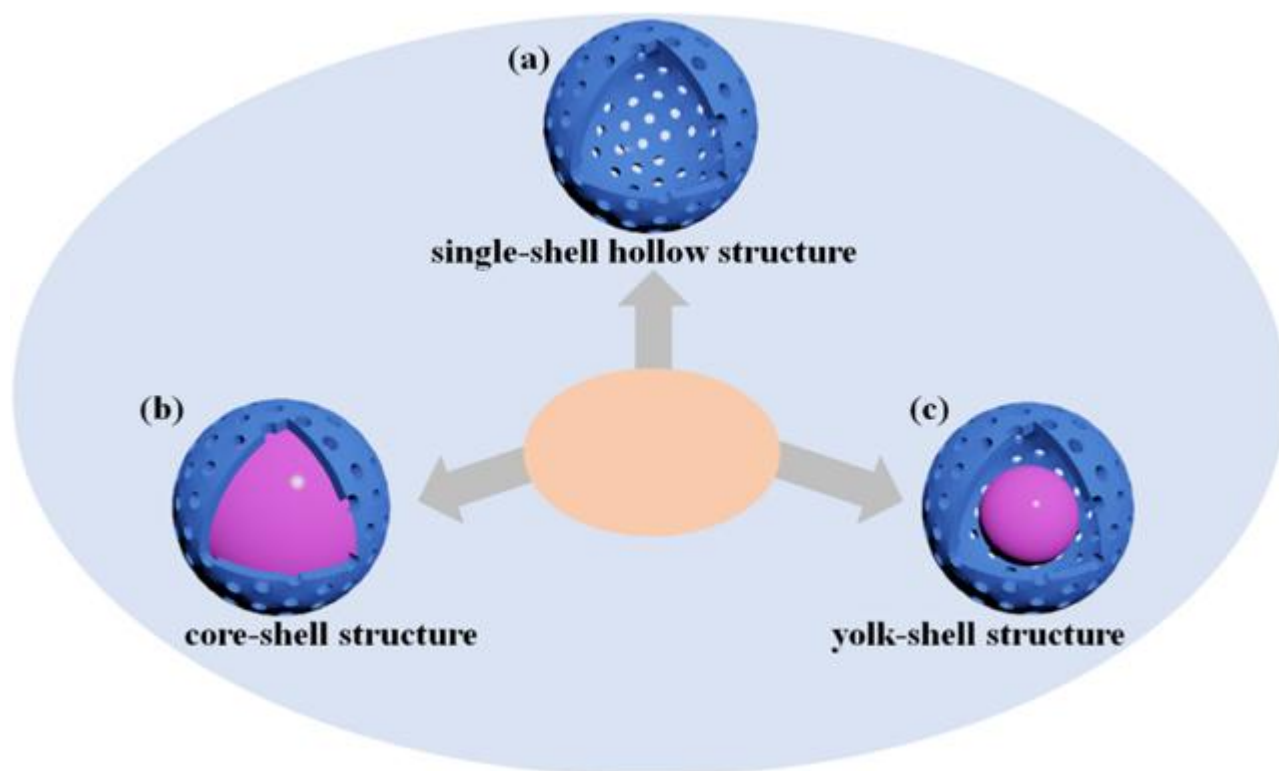
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Graphical Abstract



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Zhou AW, Wang DS, Li YD. Hollow microstructural regulation of single-atom catalysts for optimized electrocatalytic performance. *Microstructures* 2022;2:2022005.

<http://dx.doi.org/10.20517/microstructures.2021.08>

2. An intriguing canting dipole configuration and its evolution under an electric field in

La-doped $\text{Pb}(\text{Zr},\text{Sn},\text{Ti})\text{O}_3$ perovskites

Botao Gao, Hui Liu, Zhengyang Zhou, Ke Xu, He Qi, Shiqing Deng, Yang Ren, Junliang Sun, Houbing Huang, Jun Chen*

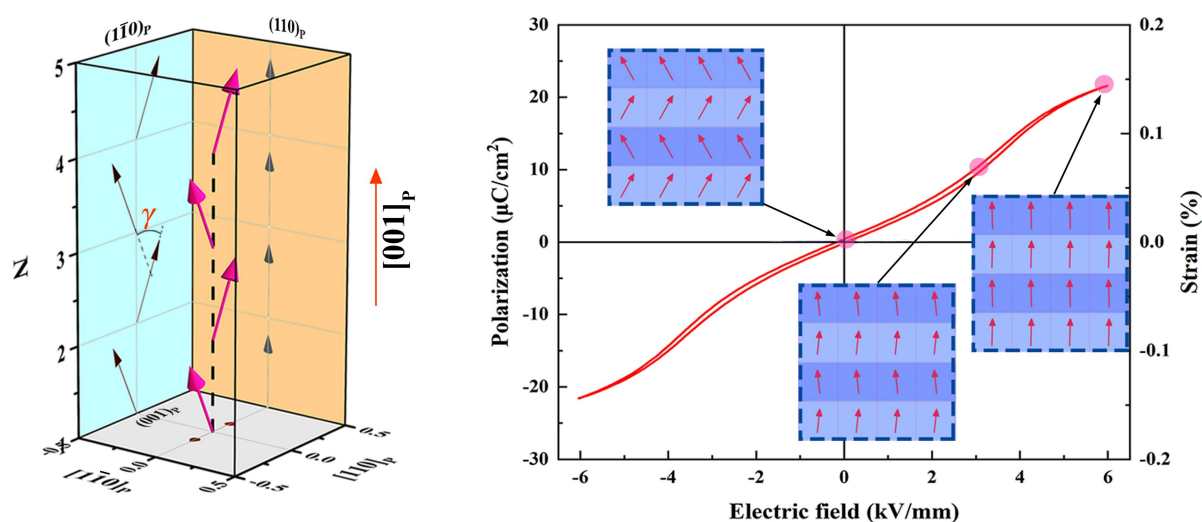
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Graphical Abstract



Cite this article

Gao B, Liu H, Zhou Z, Xu K, Qi H, Deng S, Ren Y, Sun J, Huang H, Chen J. An intriguing canting dipole configuration and its evolution under an electric field in La-doped $\text{Pb}(\text{Zr},\text{Sn},\text{Ti})\text{O}_3$ perovskites.

Microstructures 2022;2:2022010. <http://dx.doi.org/10.20517/microstructures.2022.03>

3. Metal-organic framework-tailored perovskite solar cells

Peng Chen¹, Jingwei Hou, Lianzhou Wang*

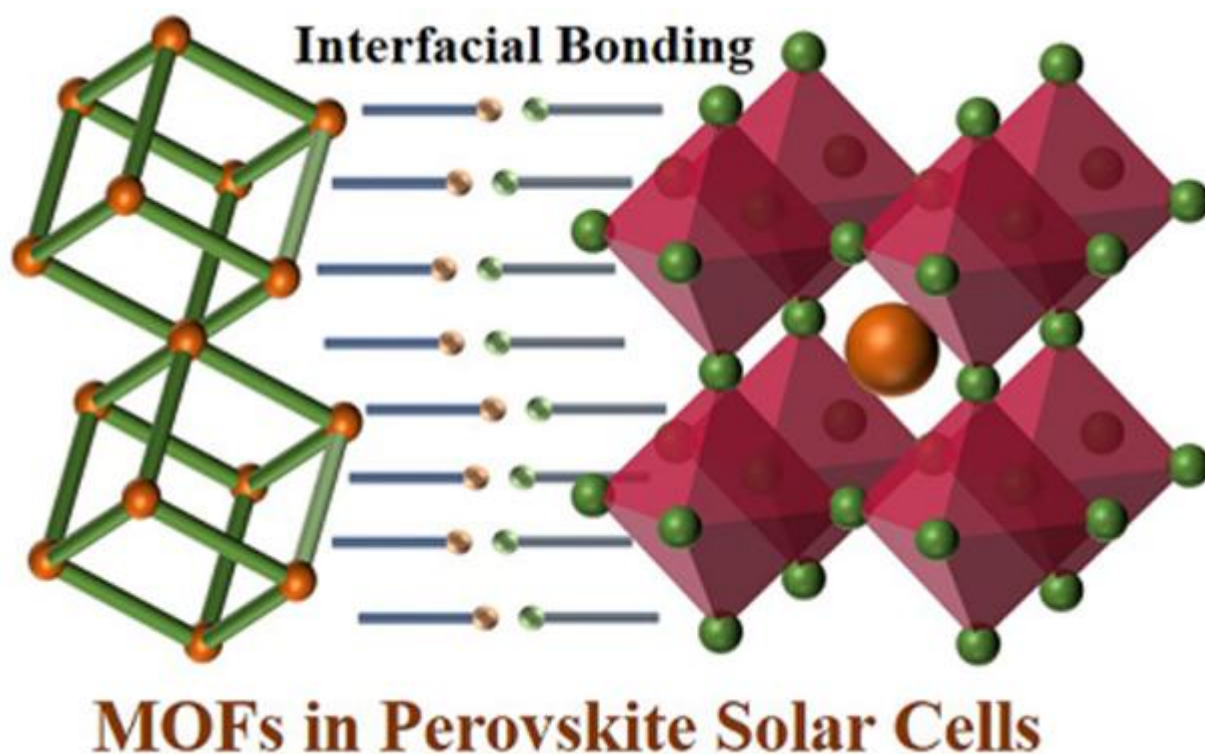
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Graphical Abstract



Cite this article

Chen P, Hou J, Wang L. Metal-organic framework-tailored perovskite solar cells. *Microstructures* 2022;2:2022014. <http://dx.doi.org/10.20517/microstructures.2022.05>

4. Design of super-elastic freestanding ferroelectric thin films guided by phase-field simulations

Changqing Guo, Houbing Huang*

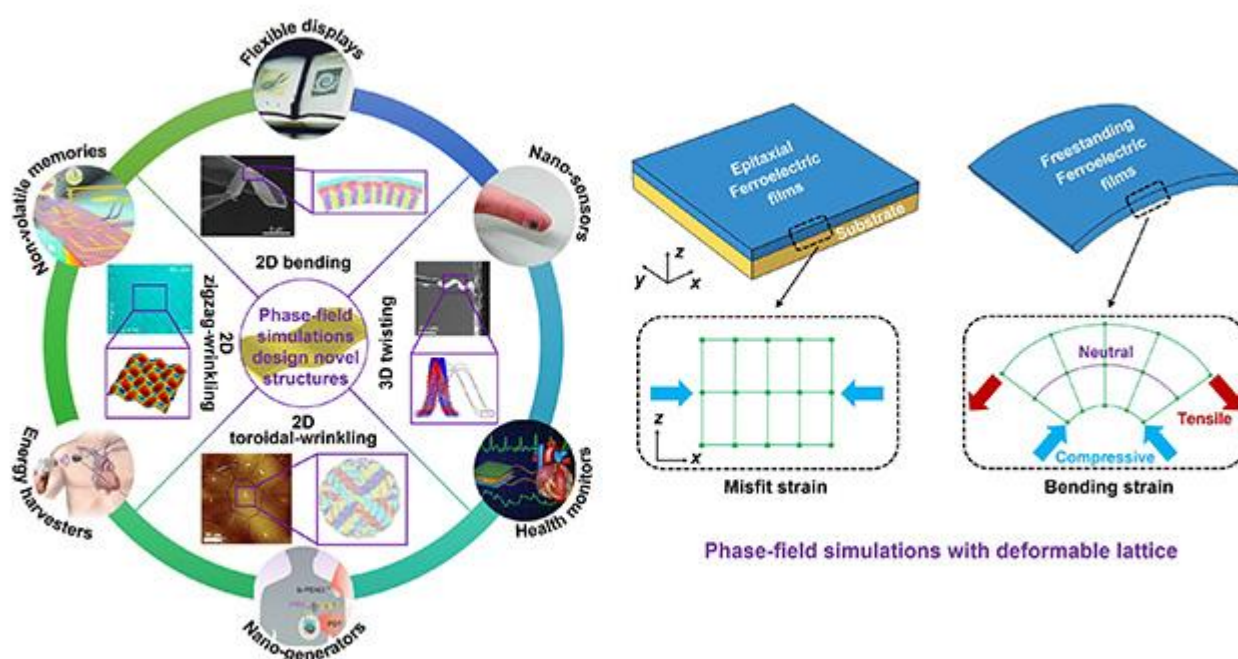
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Graphical Abstract



Cite this article

Guo C, Huang H. Design of super-elastic freestanding ferroelectric thin films guided by phase-field simulations. *Microstructures* 2022;2:2022021. <http://dx.doi.org/10.20517/microstructures.2022.20>

Review

1. Hollow microstructural regulation of single-atom catalysts for optimized electrocatalytic performance

A-Wu Zhou, Ding-Sheng Wang*, Ya-Dong Li

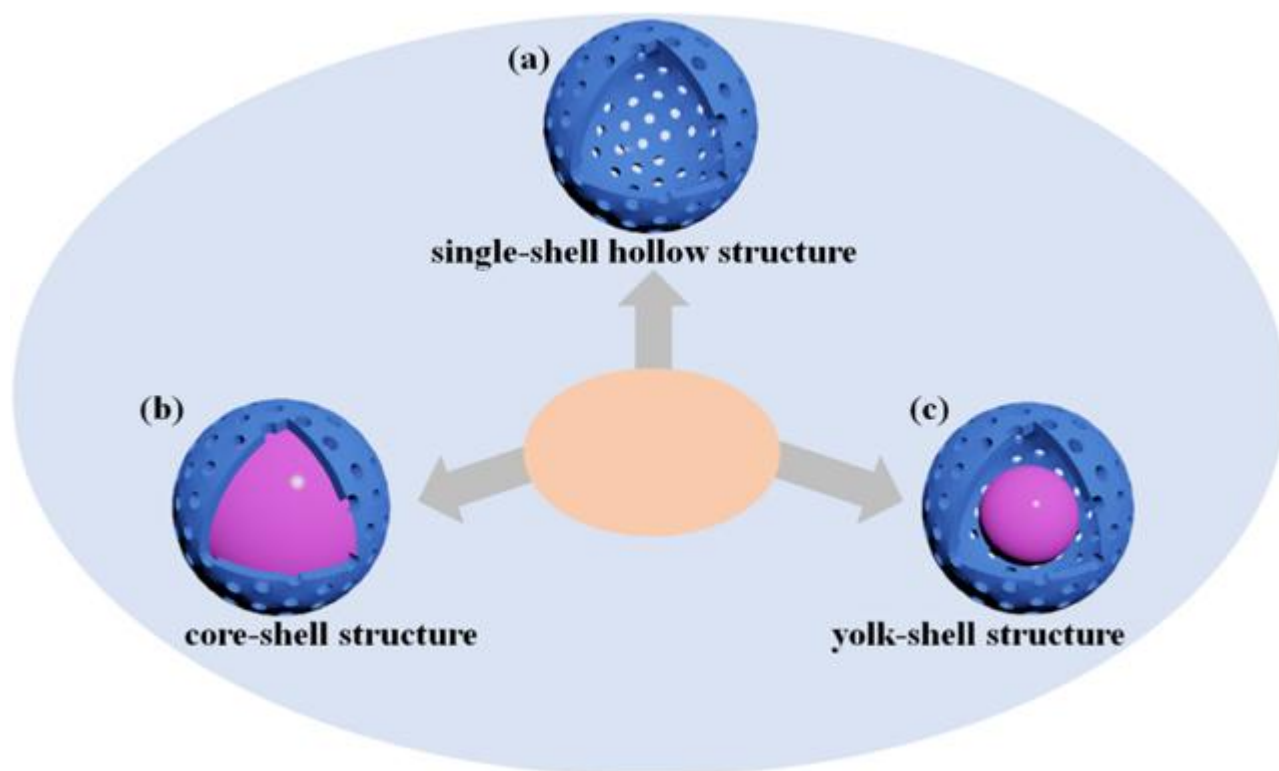
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Graphical Abstract



Abstract

Single-atom catalysts (SACs) and hollow microstructured materials have recently undergone significant advancements in the field of catalysis. The combination of SACs and hollow microstructured materials can further endow them with extraordinary characteristics, such as high loadings, uniform active sites and unique metal-support interactions and electronic structures. In this review, we focus on the design and construction of SACs supported on hollow microstructured materials for enhancing electrocatalytic reactions. Due to these unique hollow microstructures, most of the active sites can be fully exposed in catalysis. Therefore, the atomic utilization rate is greatly improved. Furthermore, the synergistic effect of SACs and hollow microstructured supports can bring about unpredictable characteristics. The hollow microstructures not only adjust the geometry and electronic structure of the SACs to improve their activity but the SACs can also serve as an auxiliary stimulus to the intrinsic activity of the support to achieve better performance. Compared with the reported traditional dual atomic catalysts, hollow microstructures are conducive for the isolation of atomically dispersed binary atom active sites on both sides of the particle shell. Combined with the current development status, we summarize the challenges and prospects in this area. This review is conducive to the reasonable design and manufacture of advanced SACs supported on hollow materials and the promotion of their future industrial usage in energy applications.

Keywords

Microstructures, single-atom catalysts, hollow structures, electrocatalytic activity, energy conversion

Cite this article

Zhou AW, Wang DS, Li YD. Hollow microstructural regulation of single-atom catalysts for optimized electrocatalytic performance. *Microstructures* 2022;2:2022005.

<http://dx.doi.org/10.20517/microstructures.2021.08>

2. A critical review of the mechanical properties of CoCrNi-based medium-entropy alloys

Dingfeng Xu, Mingliang Wang, Tianxin Li, Xiangsai Wei, Yiping Lu

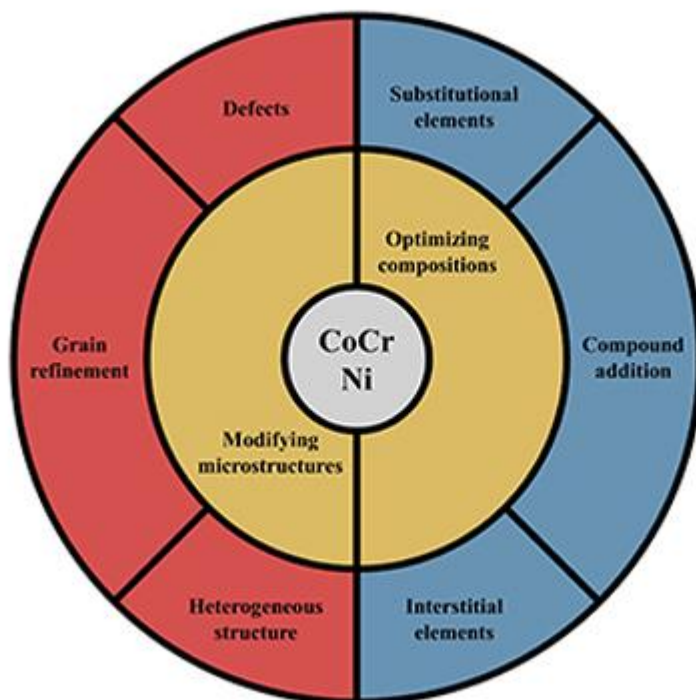
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Graphical Abstract



Abstract

The CoCrFeMnNi alloy is one of the most notable first-generation high-entropy alloys and is also

known as a Cantor alloy. This alloy was first proposed in 2004 and shows promising performance at cryogenic temperatures (CTs). Subsequent research has indicated that the equiatomic ternary CoCrNi medium-entropy alloy (MEA), as a subset of the Cantor alloy family, has better mechanical properties than the CoCrFeMnNi alloy. Interestingly, both the strength and ductility of the CoCrNi MEA are higher at CTs than at room temperature. CoCrNi-based alloys have attracted considerable attention in the metallic materials community and it is therefore important to generalize and summarize the latest progress in CoCrNi-based MEA research. The present review initially briefly introduces the discovery of the CoCrNi MEA. Subsequently, its tensile response and deformation mechanisms are summarized. In particular, the effects of parameters, such as critical resolved shear stress, stacking fault energy and short-range ordering, on the deformation behavior are discussed in detail. The methods for strengthening the CoCrNi MEA are then reviewed and divided into two categories, namely, modifying microstructures and adjusting chemical compositions. In addition, the mechanical performance of CoCrNi-based MEAs, including their dynamic shear properties, creep behavior and fracture toughness, is also deliberated. Finally, the development prospects of CoCrNi-based MEAs are proposed.

Keywords

Medium-entropy alloys, mechanical properties, deformation mechanism, strengthening mechanism

Cite this article

Xu D, Wang M, Li T, Wei X, Lu Y. A critical review of the mechanical properties of CoCrNi-based medium-entropy alloys. *Microstructures* 2022;2:2022001.

<http://dx.doi.org/10.20517/microstructures.2021.10>

3. Applications of *in situ* electron microscopy in oxygen electrocatalysis

Zhi-Peng Wu, Hui Zhang, Cailing Chen, Guanxing Li, Yu Han*

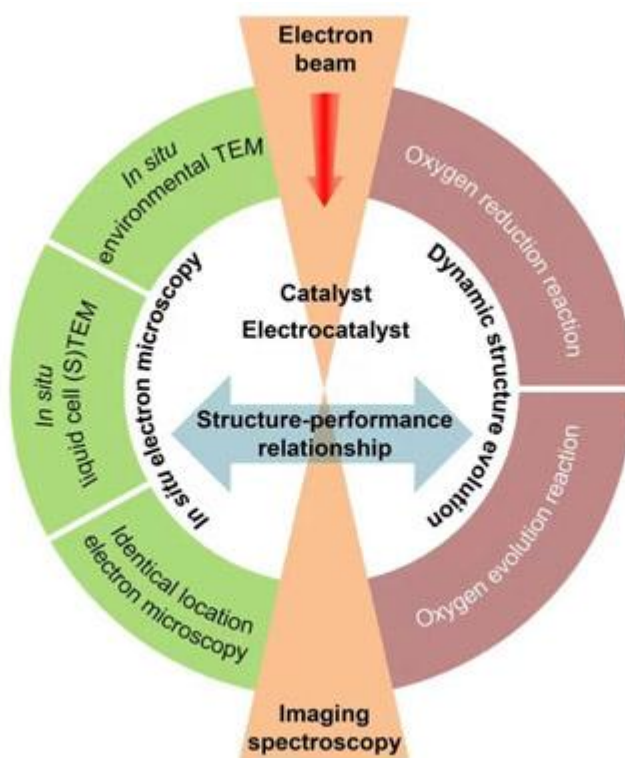
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Graphical Abstract



Abstract

Oxygen electrocatalysis involving the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) plays a vital role in cutting-edge energy conversion and storage technologies. In situ studies of the evolution of catalysts during oxygen electrocatalysis can provide important insights into their structure - activity relationships and stabilities under working conditions. Among the various in situ characterization tools available, in situ electron microscopy has the unique ability to perform structural and compositional analyzes with high spatial resolution. In this review, we present the latest developments in in situ and quasi-in situ electron microscopic techniques, including identical location electron microscopy, in situ liquid cell (scanning) transmission electron microscopy and in situ environmental transmission electron microscopy, and elaborate their applications in the ORR and OER. Our discussion centers on the degradation mechanism, structural evolution and structure - performance correlations of electrocatalysts. Finally, we summarize the earlier discussions and share our perspectives on the current challenges and future research directions of using in situ electron microscopy to explore oxygen electrocatalysis and related processes.

Keywords

In situ electron microscopy, oxygen electrocatalysis, OER, ORR, liquid cell (scanning) transmission electron microscopy, identical location electron microscopy

Cite this article

Wu ZP, Zhang H, Chen C, Li G, Han Y. Applications of in situ electron microscopy in oxygen electrocatalysis. *Microstructures* 2022;2:2022002. <http://dx.doi.org/10.20517/microstructures.2021.12>

4. Recent advances in two-dimensional van der Waals magnets

Hang Xu, Shengjie Xu, Xun Xu, Jincheng Zhuang, Weichang Hao*, Yi Du*

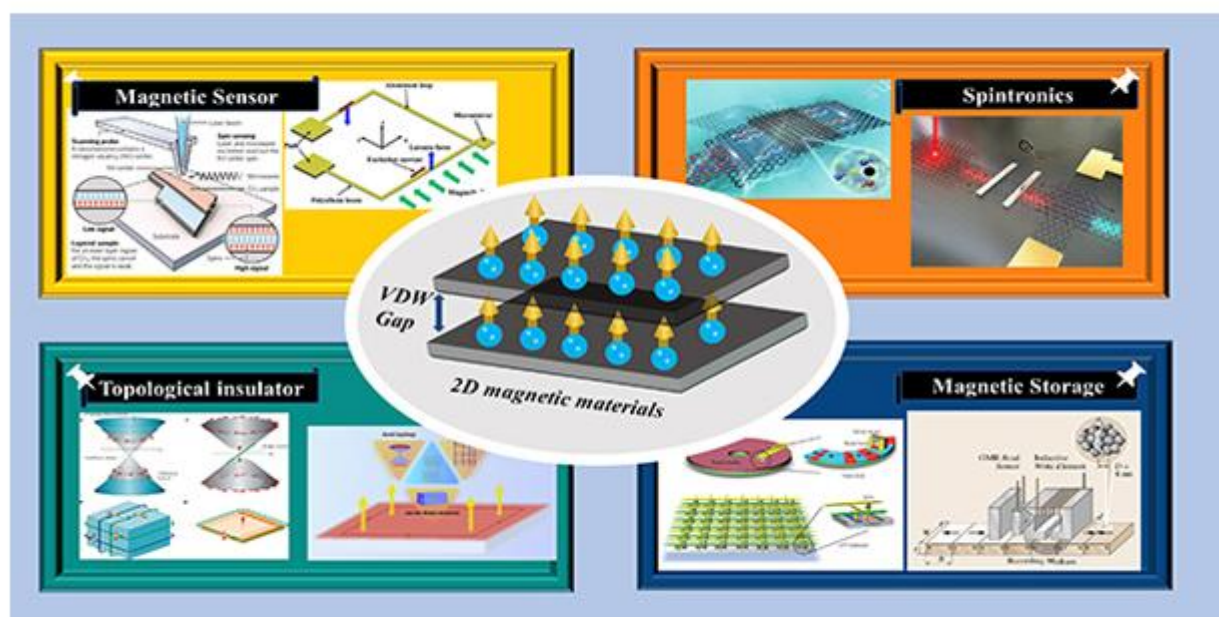
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Graphical Abstract



Abstract

Two-dimensional (2D) magnets have evoked tremendous interest within the research community due to their fascinating features and novel mechanisms, as well as their potential applications in magnetic nanodevices. In this review, state-of-the-art research into the exploration of 2D magnets from the perspective of their magnetic interaction and order mechanisms is discussed. The properties of these magnets can be effectively modulated by varying the external parameters, such as the charge carrier

doping, thickness effect, pressure and strain. The potential applications of heterostructures of these 2D magnets in terms of the interlayer coupling strength are reviewed, and the challenges and outlook for this field are proposed.

Keywords

Two-dimensional (2D) ferromagnetism, van der Waals (vdW) crystal, magnetic interaction, physical properties

Cite this article

Xu H, Xu S, Xu X, Zhuang J, Hao W, Du Y. Recent advances in two-dimensional van der Waals magnets.

Microstructures 2022;2:2022011. <http://dx.doi.org/10.20517/microstructures.2022.02>

5. Polarization boosted catalysis: progress and outlook

Lin Ju, Xiao Tang, Liangzhi Kou*

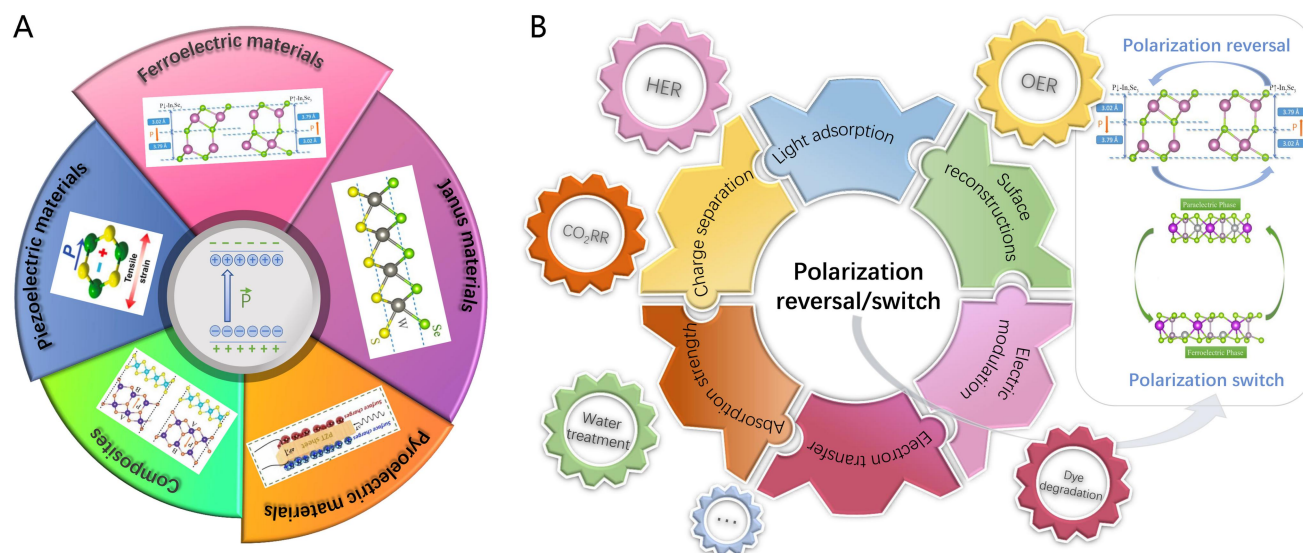
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Graphical Abstract



Abstract

Polarization has a significant impact on chemical reactions, as demonstrated by recent research of photo-/electrocatalytic water splitting, electrocatalytic CO₂ reduction, water treatment, dye

degradation and so on. This review summarizes the fundamental influence of polarization on the physical/chemical properties of catalysts and discusses polarization-dependent catalytic processes. Based on the research progress of polarization-modulated chemical reactions, we draw the conclusion that the control of polarization can be used to adjust the reactivity and selectivity of various catalytic reactions by tuning the miscellaneous fundamental properties of polarized catalysts. At the end of the review, the future research challenges are also discussed, including the ultrafast reversal of polarization, the magnetic-field control of chemical reactions through the magnetoelectric effect and in-plane polarization.

Keywords

Polarization reversal, electrocatalysis, water splitting, photocatalysis

Cite this article

Ju L, Tang X, Kou L. Polarization boosted catalysis: progress and outlook. *Microstructures* 2022;2:2022008. <http://dx.doi.org/10.20517/microstructures.2021.14>

6. Microstructural evolution and ferroelectricity in HfO₂ films

Dou Zhao, Zibin Chen*, Xiaozhou Liao*

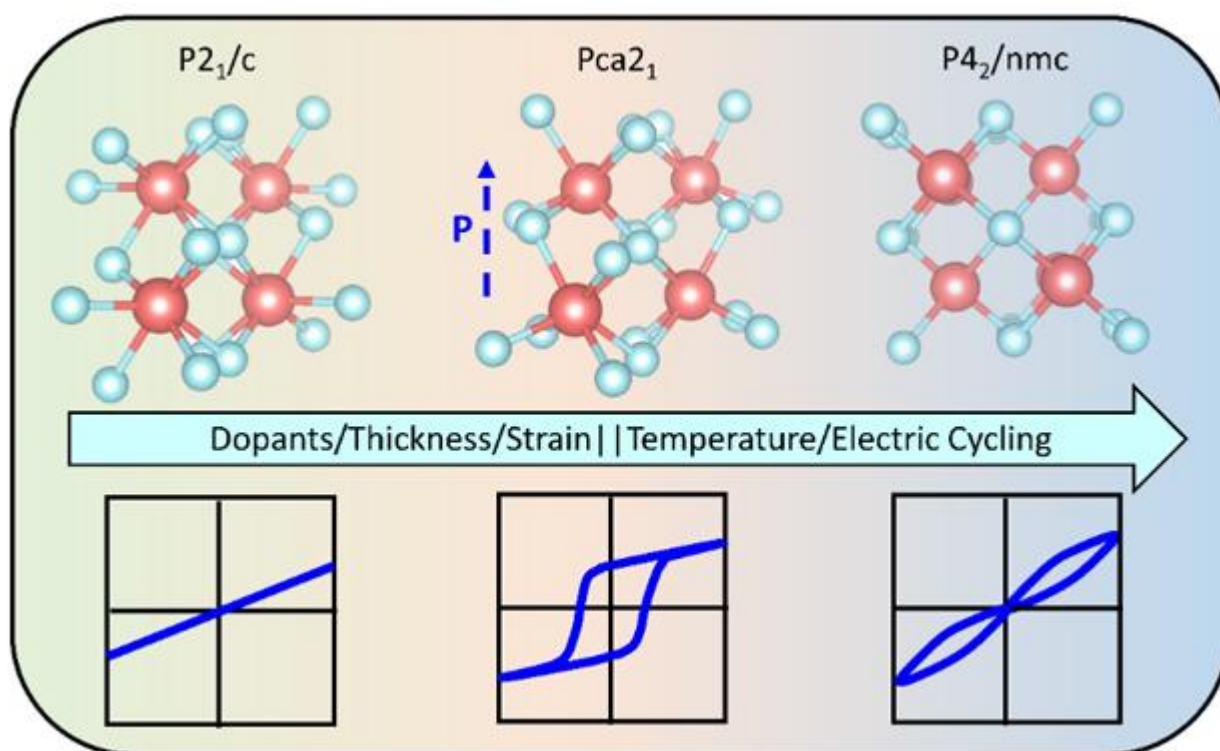
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Graphical Abstract



Abstract

Ferroelectric (FE) materials, which typically adopt the perovskite structure with non-centrosymmetry and exhibit spontaneous polarization, are promising for applications in memory, electromechanical and energy storage devices. However, these advanced applications suffer from the intrinsic limitations of perovskite FEs, including poor complementary metal oxide semiconductor (CMOS) compatibility and environmental issues associated with lead. Hafnium oxide (HfO_2), with stable bulk centrosymmetric phases, possesses robust ferroelectricity in nanoscale thin films due to the formation of non-centrosymmetric phases. Owing to its high CMOS compatibility and high scalability, HfO_2 has attracted significant attention. In the last decade, significant efforts have been made to explore the origin of the ferroelectricity and factors that influence the FE properties in HfO_2 films, particularly regarding the role of microstructure, which is vital in clarifying these issues. Although several comprehensive reviews of HfO_2 films have been published, there is currently no review focused on the relationship between microstructure and FE properties. This review focuses on the microstructure-property relationships in FE polycrystalline and epitaxial HfO_2 films. The crystallographic structures and characterization methods for HfO_2 polymorphs are first discussed. For polycrystalline HfO_2 films, the microstructure-FE properties relationships, driving force and kinetic pathway of phase transformations under growth parameters or external stimuli are reviewed. For

epitaxial films, the lattice matching relations between HfO₂ films and substrates and the corresponding impact on the FE properties are discussed. The FE properties between polycrystalline and epitaxial HfO₂ films are compared based on their different microstructural characteristics. Finally, a future perspective is given for further investigating FE HfO₂ films.

Keywords

HfO₂ films, ferroelectricity, phase transformations, oxygen vacancies, transmission electron microscopy

Cite this article

Zhao D, Chen Z, Liao X. Microstructural evolution and ferroelectricity in HfO₂ films. *Microstructures* 2022;2:2022007. <http://dx.doi.org/10.20517/microstructures.2021.11>

7. Design and manufacture of high-performance microbatteries: lithium and beyond

Feiyang Chen, Zheng-Long Xu*

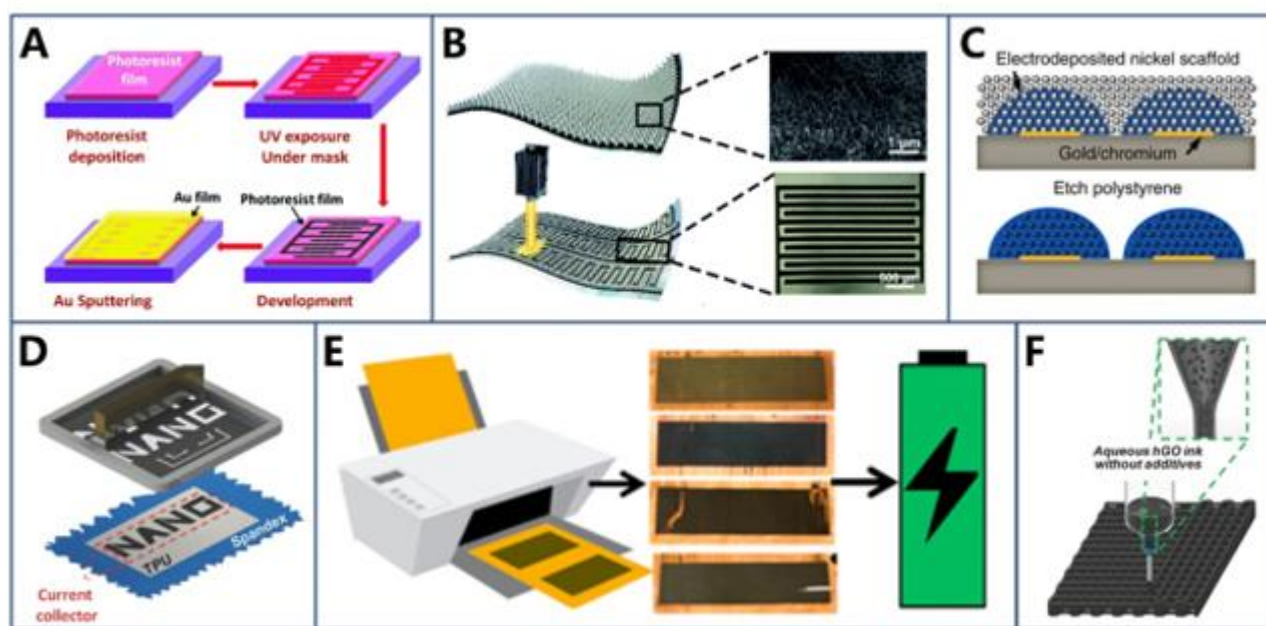
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Abstract

The accelerated development of miniaturized and customized electronics has stimulated the demand for high-energy microbatteries (MBs) as on-chip power sources for autonomous state operations. However, commercial MBs with thin-film configurations exhibit insufficient energy and power density due to their limited active materials and sluggish ion diffusion kinetics. In order to simultaneously enhance electrochemical performance and maintain low-cost production, efforts have been devoted to constructing three-dimensional battery architectures. This review summarizes the state-of-the-art progress in designing and fabricating microelectrodes for microbattery assembly, including the top-down etching and bottom-up printing techniques, with a particular focus on elucidating the correlations between electrode structures, battery performance, and cost-effectiveness. More importantly, advancements in post-lithium batteries based on sodium, zinc and aluminum are also surveyed to offer alternative options with potentially higher energy densities and/or lower battery manufacturing costs. The applications of advanced MBs in on-chip microsystems and wearable electronics are also highlighted. Finally, conclusions and perspectives for the future development of MBs are proposed.

Keywords

Microbatteries, lithium-ion batteries, post-lithium batteries, etching and printing techniques,

microelectronics

Cite this article

Chen F, Xu ZL. Design and manufacture of high-performance microbatteries: lithium and beyond.

Microstructures 2022;2:2022012. <http://dx.doi.org/10.20517/microstructures.2022.10>

8. Design of super-elastic freestanding ferroelectric thin films guided by phase-field simulations

Changqing Guo, Houbing Huang*

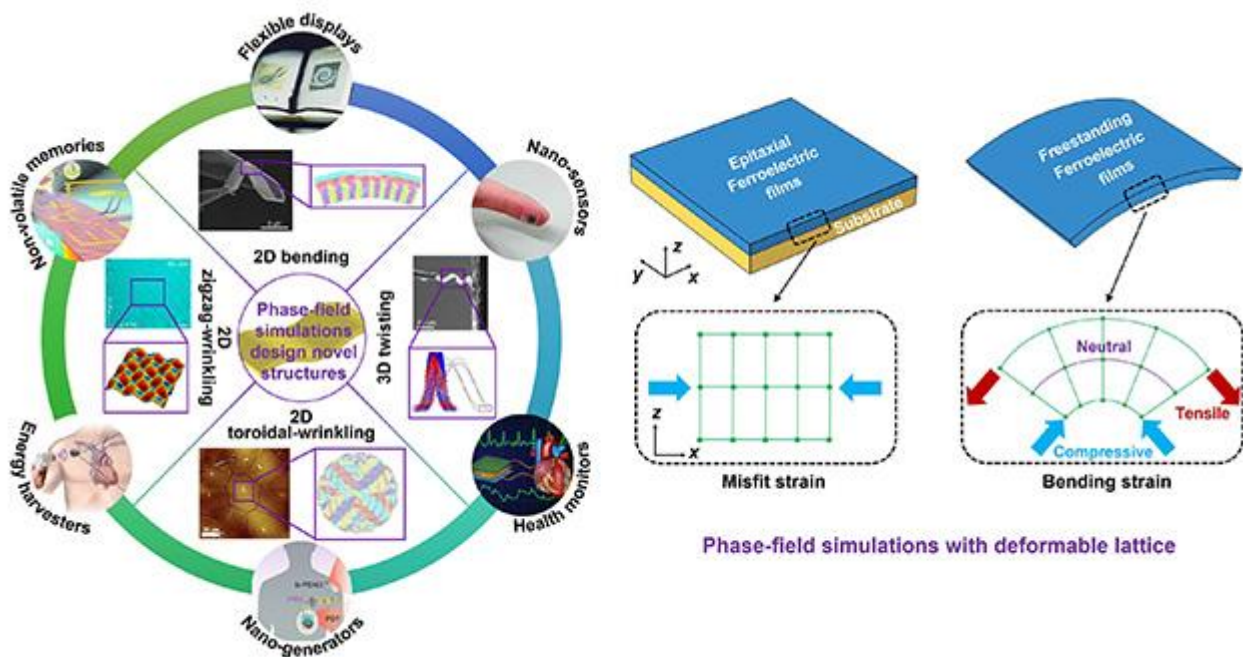
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Graphical Abstract



Abstract

Understanding the dynamic behavior of domain structures is critical to the design and application of super-elastic freestanding ferroelectric thin films. Phase-field simulations represent a powerful tool for observing, exploring and revealing the domain-switching

behavior and phase transitions in ferroelectric materials at the mesoscopic scale. This review summarizes the recent theoretical progress regarding phase-field methods in freestanding ferroelectric thin films and novel buckling-induced wrinkled and helical structures. Furthermore, the strong coupling relationship between strain and ferroelectric polarization in super-elastic ferroelectric nanostructures is confirmed and discussed, resulting in new design strategies for the strain engineering of freestanding ferroelectric thin film systems. Finally, to further promote the innovative development and application of freestanding ferroelectric thin film systems, this review provides a summary and outlook on the theoretical modeling of freestanding ferroelectric thin films.

Keywords

Freestanding ferroelectric thin films, super-elastic, mechanical structure, topological domain structure, phase-field simulations

Cite this article

Guo C, Huang H. Design of super-elastic freestanding ferroelectric thin films guided by phase-field simulations. *Microstructures* 2022;2:2022021. <http://dx.doi.org/10.20517/microstructures.2022.20>

Perspective

1. Metal-organic framework-tailored perovskite solar cells

Peng Chen¹, Jingwei Hou, Lianzhou Wang*

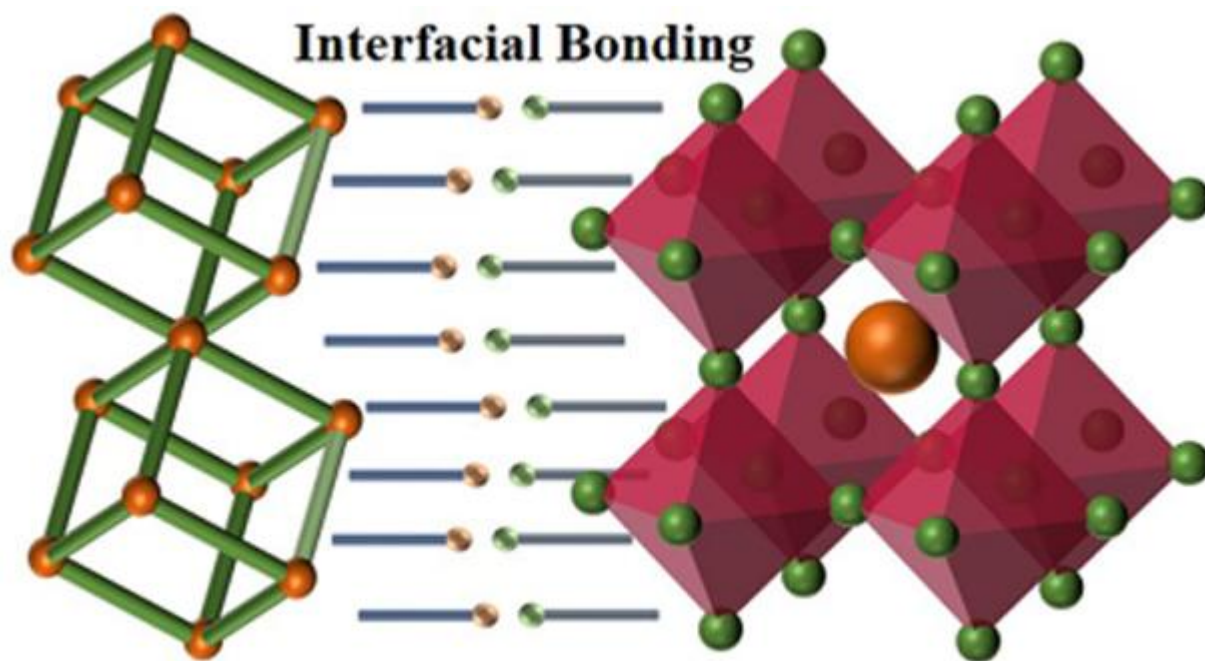
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MOFs in Perovskite Solar Cells

Abstract

Metal-organic frameworks (MOFs) with tailorable structures and building blocks have demonstrated their advantages in improving the long-term stability of perovskite solar cells (PSCs). However, the inferior conductivity of MOFs and their lack of strong chemical interaction with perovskites cause undesirable interfacial charge carrier recombination and then deteriorate the photovoltaic (PV) performance of PSCs. This perspective offers an insightful overview of the versatile functionalities and key merits of MOFs for stabilizing PSCs under various external stimuli in terms of MOF interlayers and MOF-perovskite heterostructures. To tackle the charge transport problem of MOFs, promising strategies are outlined to improve the intrinsic conductivity and chemical coordination of MOFs, with the aim of achieving long-term stable PSCs without compromising their PV performance. The current challenging issues and potential solutions are also discussed to provide a roadmap for MOF-tailored PSCs towards practical applications.

Keywords

Perovskite solar cells, metal-organic frameworks, charge carrier mobility, interfacial bonds, intrinsic conductivity

Cite this article

Chen P, Hou J, Wang L. Metal-organic framework-tailored perovskite solar cells. *Microstructures* 2022;2:2022014. <http://dx.doi.org/10.20517/microstructures.2022.05>

Research Article

1. Low neutron cross-section FeCrVTiNi based high-entropy alloys: design, additive manufacturing and characterization

Bosheng Dong, Zhiyang Wang*, Hanliang Zhu, Ondrej Muránsky, Zhijun Qiu, Chen Shen, Zengxi Pan, Huijun Li

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Abstract

The development of high-entropy alloys (HEAs) based on the novel alloying concept of multi-principal components presents opportunities for achieving new materials with desired properties for increasingly demanding applications. In this study, a low neutron cross-section FeCrVTiNi-based HEA was developed for potential nuclear applications. A face-centred cubic (FCC) HEA with the nominal composition of $\text{FeCr}_{0.4}\text{V}_{0.3}\text{Ti}_{0.2}\text{Ni}_{1.3}$ is proposed based on the empirical thermodynamic models and the CALculation of PHase diagrams (CALPHAD) calculation. Verifications of the predictions were performed, including the additive manufacturing of the proposal material and a range of microstructural characterizations and mechanical property tests. Consistent with the prediction, the as-fabricated HEA consists of a dominant FCC phase and minor Ni_3Ti precipitates. Moreover, significant chemical segregation in the alloy, as predicted by the CALPHAD modelling, was observed experimentally in the produced dendritic microstructure showing the enrichment of Ni and Ti elements in the interdendritic regions and the segregation of Cr and V elements in the dendritic cores. Heterogenous mechanical properties, including microhardness and tensile strengths, were observed along the building direction of the additively manufactured HEA. The various solid solution

strengthening effects, due to the chemical segregation (in particular Cr and V elements) during solidification, are identified as significant contributing factors to the observed mechanical heterogeneity. Our study provides useful knowledge for the design and additive manufacturing of compositionally complex HEAs and their composition-microstructure-mechanical property correlation.

Keywords

High-entropy alloys, materials design, additive manufacturing, microstructures, materials characterization

Cite this article

Dong B, Wang Z, Zhu H, Muránsky O, Qiu Z, Shen C, Pan Z, Li H. Low neutron cross-section FeCrVTiNi based high-entropy alloys: design, additive manufacturing and characterization.

Microstructures 2022;2:2022003. <http://dx.doi.org/10.20517/microstructures.2021.09>

2. $K_6Sn_4F_{12}I_2 \cdot 0.5H_2O$: a zero-dimensional alkali metal tin mixed halide compound exhibiting color change due to crystal water loss

Pifu Gong, Siyang Luo, Zheshuai Lin*

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Abstract

A new zero-dimensional alkali-metal tin mixed halide, $K_6Sn_4F_{12}I_2 \cdot 0.5H_2O$, is synthesized by a hydrothermal method. It crystallizes in the cubic centrosymmetric space group of $Fd-3m$ (No. 227) and its structure consists of crystal water molecules and ordered arranged $[Sn_4F_{12}I_4]$ fundamental structural blocks trapped in $[K_{18}]$ cages. Interestingly, $K_6Sn_4F_{12}I_2 \cdot 0.5H_2O$ exhibits a color change from colorless to orange when exposed to air. Experimental measurements combined with theoretical calculations reveal that the color change in $K_6Sn_4F_{12}I_2 \cdot 0.5H_2O$ is attributed to the loss of crystal water.

Keywords

Metal halide, color change, new material exploration

Cite this article

Gong P, Luo S, Lin Z. $\text{K}_6\text{Sn}_4\text{F}_{12}\text{I}_2 \cdot 0.5\text{H}_2\text{O}$: a zero-dimensional alkali metal tin mixed halide compound exhibiting color change due to crystal water loss. *Microstructures* 2022;2:2022004.

<http://dx.doi.org/10.20517/microstructures.2021.07>

3. An intriguing canting dipole configuration and its evolution under an electric field in La-doped $\text{Pb}(\text{Zr},\text{Sn},\text{Ti})\text{O}_3$ perovskites

Botao Gao, Hui Liu, Zhengyang Zhou, Ke Xu, He Qi, Shiqing Deng, Yang Ren, Junliang Sun, Houbing Huang, Jun Chen*

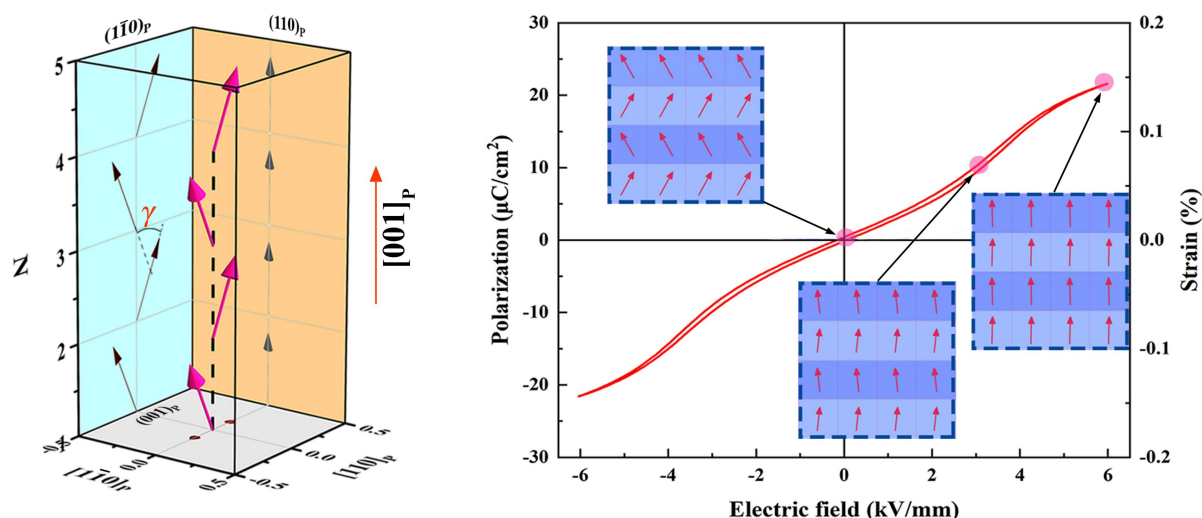
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Graphical Abstract



Abstract

Despite the fact that electric dipole ordering plays a key role in the unique physical properties of dielectric materials, electric dipole configurations mostly appear simply as either parallel or antiparallel. Here, we report a canting electric dipole configuration in La-doped $\text{Pb}(\text{Zr},\text{Sn},\text{Ti})\text{O}_3$ perovskites based on advanced neutron, synchrotron X-ray and three-dimensional electron diffraction techniques. It is revealed that, arising from the coupling between the atomic displacement and oxygen octahedral

tilting, this unique electric dipole configuration displays a canting arrangement aligned in the (110)_p plane that possesses an antiparallel component along the [110]_P direction and a parallel component along the [001]_P direction. Remarkably, under an in-situ electric field, the electric dipoles continuously rotate with a gradually reduced canting angle, as confirmed by phase-field simulations, and ultimately evolve into a ferroelectric ordering. Such an evolution gives rises to a small hysteresis and an equivalent lattice strain to the macroscopic strain. These findings enrich the current understanding of the types of electric dipole configurations in dielectric materials and are expected to aid the design of new dielectric materials with emergent properties.

Keywords

Antiferroelectric, electric dipole configurations, canting, perovskite

Cite this article

Gao B, Liu H, Zhou Z, Xu K, Qi H, Deng S, Ren Y, Sun J, Huang H, Chen J. An intriguing canting dipole configuration and its evolution under an electric field in La-doped Pb(Zr,Sn,Ti)O₃ perovskites.

Microstructures 2022;2:2022010. <http://dx.doi.org/10.20517/microstructures.2022.03>

4. Influence of softening annealing on microstructural heredity and mechanical properties of medium-Mn steel

Fanglin Ding, Qinyi Guo, Bin Hu, Haiwen Luo*

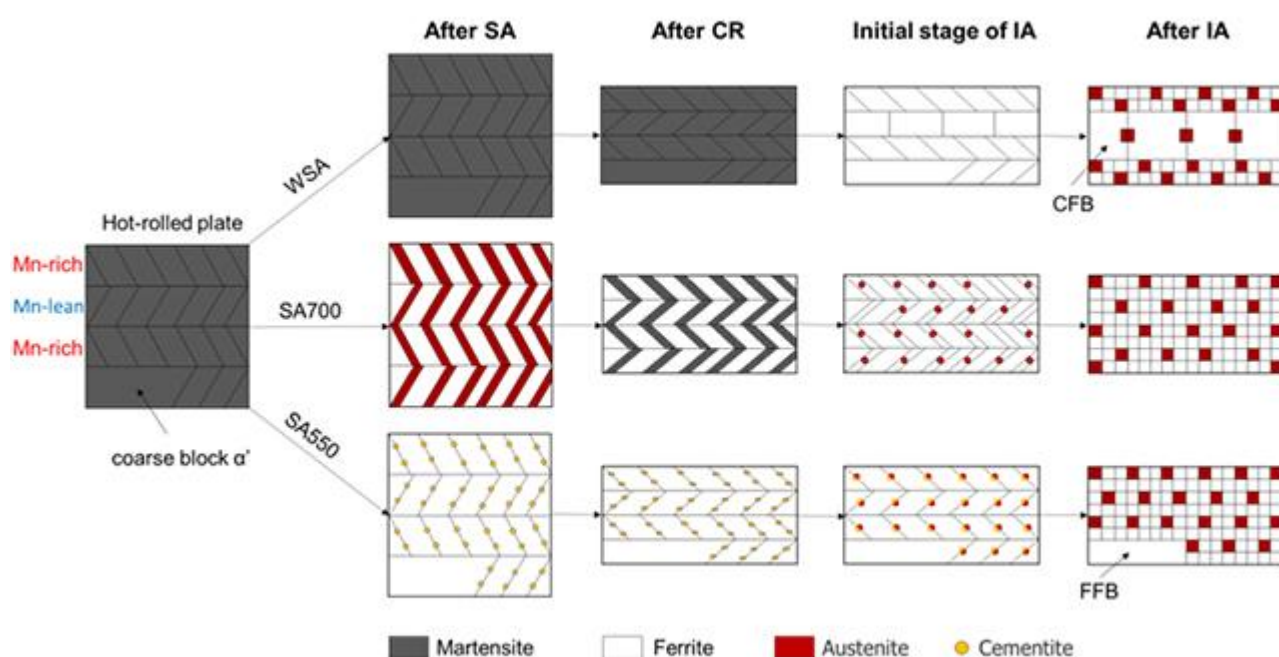
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Graphical Abstract



Abstract

Softening annealing (SA) is often required for producing medium-Mn steels (MMS) as it lowers hardness so that they can be cold rolled to reduce thickness. The influences of different SA processes on the microstructural heredity during the processing route and the final tensile properties were studied. It was found that the SA process could either intensify or weaken the influence of the Mn segregation resulting from solidification on the subsequent microstructural evolution during the process, i.e., microstructural heredity. In the case when no SA was employed, both recrystallization and rapid growth of ferrite grains preceded the reverse austenitic transformation during the intercritical annealing (IA) in the Mn-lean regions, where very coarse ferrite grains were formed. This deteriorated ductility due to the propagation of cracking along the boundary of the coarse-grained and fine-grained regions. In contrast, SA at a sufficiently high temperature could dissolve cementite, producing uniformly distributed austenite grains. They transformed to martensite during cold rolling but were reborn during IA. As a result, ultrafine austenite and ferrite grains were uniformly distributed, which improved ductility significantly. This study hints at a new approach to altering the microstructural heredity resulting from the heterogeneous Mn distribution in MMS.

Keywords

Medium-Mn steels, intercritical annealing, Mn segregation, recrystallization, mechanical properties

Cite this article

Ding F, Guo Q, Hu B, Luo H. Influence of softening annealing on microstructural heredity and mechanical properties of medium-Mn steel. *Microstructures* 2022;2:2022009.

<http://dx.doi.org/10.20517/microstructures.2022.01>

5. Topochemical synthesis and structural characteristics of orientation-controlled (Bio.5Nao.5)0.94Bao.06TiO₃ perovskite microplatelets

Yaqing Ma, Hang Xie, Yuan Sun, Qiangwei Kou, Linjing Liu, Bin Yang, Wenwu Ca, Yunfei Chang*, Fei Li

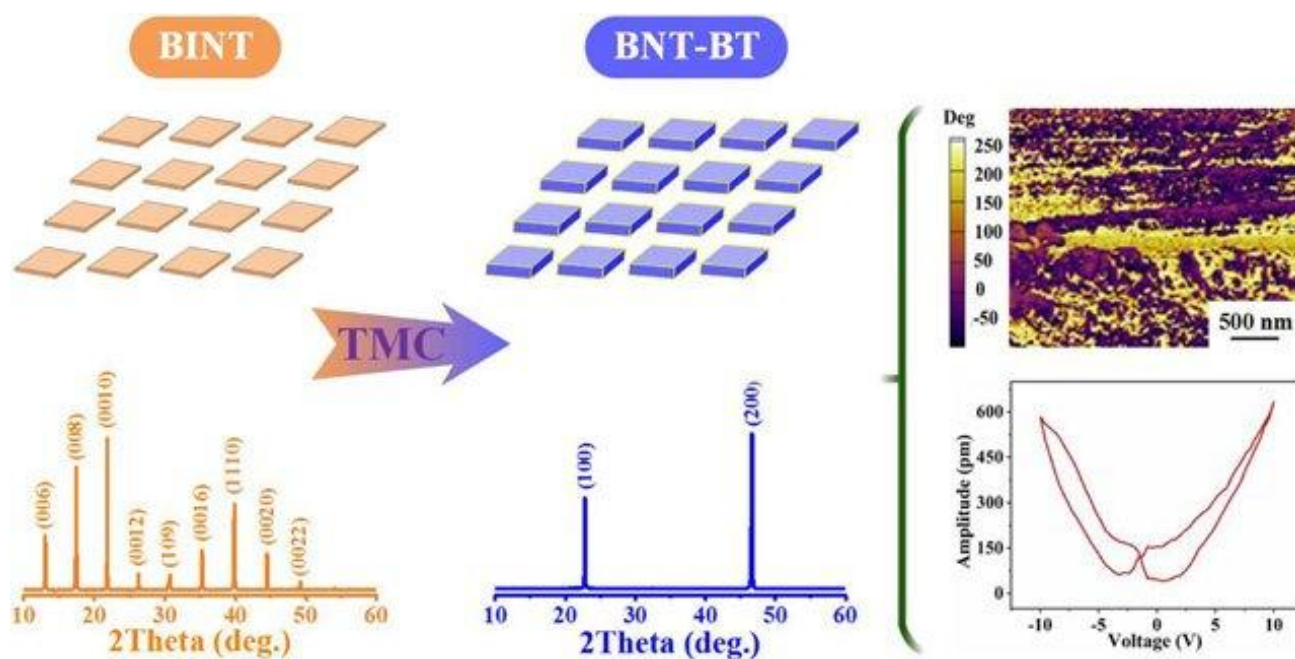
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Graphical Abstract



Abstract

Two-dimensional perovskite microcrystals have important applications in various electronic and energy devices. In this work, 0.94(Bio.5Nao.5)TiO₃-0.06BaTiO₃ (0.94BNT-0.06BT) microplatelets with a pure perovskite structure, (hoo) orientation, good crystallinity and remarkable electromechanical strain are fabricated through topochemical microcrystal conversion from Aurivillius-structured

Bi_{4.5}Na_{0.5}Ti₄O₁₅ precursors. The formation process of the Bi_{4.5}Na_{0.5}Ti₄O₁₅ precursors and the topochemical conversion mechanism of the 0.94BNT-0.06BT target are systematically studied. Intermediate phases, such as Bi₄Ti₃O₁₂ and Bi_{8.5}Na_{0.5}Ti₇O₂₇, appear before the formation of pure Bi_{4.5}Na_{0.5}Ti₄O₁₅ at 950 °C in a NaCl molten salt. For the topochemical microcrystal conversion process, although the Aurivillius to perovskite structural transformation is completed at 900 °C, the original single-crystal precursor platelets are replaced by polycrystalline aggregates because of extensive exfoliation and disintegration events. Such microstructural damage is healed by recrystallization via Ostwald ripening through further heating to produce single-crystal 0.94BNT-0.06BT microplatelets with flat surfaces, regular shapes and homogenous distributions of Bi, Na, Ba, Ti and O at 1150 °C. Both labyrinth and stripe-like domains can be detected from these microplatelets, suggesting the coexistence of both rhombohedral and tetragonal phases, in agreement with the X-ray diffraction analysis. Furthermore, local electromechanical strain with an amplitude of ~600 pm (at 10 V) is observed from the platelets along the <001>c direction.

Keywords

Topochemical conversion, (Bi_{0.5}Na_{0.5})TiO₃-BaTiO₃, microstructure, piezoelectricity

Cite this article

Ma Y, Xie H, Sun Y, Kou Q, Liu L, Yang B, Cao W, Chang Y, Li F. Topochemical synthesis and structural characteristics of orientation-controlled (Bi_{0.5}Na_{0.5})_{0.94}Ba_{0.06}TiO₃ perovskite microplatelets.

Microstructures 2022;2:2022006. <http://dx.doi.org/10.20517/microstructures.2021.13>

6. Ultrasonication-assisted fabrication of porous ZnO@C nanoplates for lithium-ion batteries

Xueting Wang, Yunchuang Wang, Meichao Wu, Ruopian Fang, Xi Yang, Da-Wei Wang*

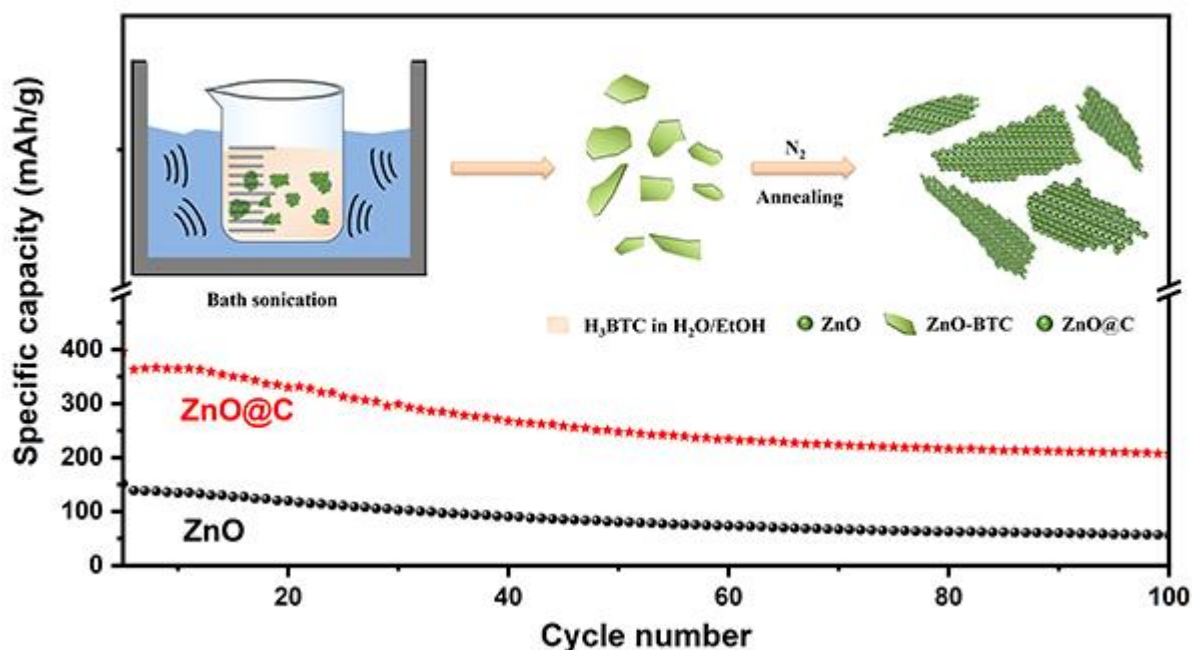
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Graphical Abstract



Abstract

Lithium-ion batteries have made significant commercial and academic progress in recent decades. Zinc oxide (ZnO) has been widely studied as a lithium-ion battery anode due to its high theoretical capacity of 987 mAh g⁻¹, natural abundance, low cost, and environmental friendliness. However, ZnO suffers from poor electronic conductivity and large volume variation during the battery discharge/charge process, leading to capacity deterioration during long-term cycling. Herein, porous ZnO@C nanoplates are developed to offer short ion diffusion pathways and good conduction networks for both Li ions and electrons. The porous nanoplates provide abundant active sites for electrochemical reactions with minimized charge transfer impedance. As a result, the porous ZnO@C nanoplates deliver higher performance for lithium-ion storage compared with a bare ZnO anode. Furthermore, with the introduction of reduced graphene oxide (rGO), the ZnO@C@rGO composite anode achieves a capacity of 229.3 mAh g⁻¹ at a high current density of 2 A g⁻¹.

Keywords

Zinc oxide, porous materials, lithium-ion batteries, anodes

Cite this article

Wang X, Wang Y, Wu M, Fang R, Yang X, Wang DW. Ultrasonication-assisted fabrication of porous ZnO@C nanoplates for lithium-ion batteries. *Microstructures* 2022;2:2022016.

<http://dx.doi.org/10.20517/microstructures.2022.11>

7. High strength and ductility in partially recrystallized Fe₄₀Mn₂₀Cr₂₀Ni₂₀ high-entropy alloys at cryogenic temperature

Qi-Xin Ma, Hui-Jun Yang, Zhong Wang, Xiao-Hui Shi, Peter K. Liaw, Jun-Wei Qiao*

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Abstract

The effects of cold rolling and subsequent annealing on the microstructures and mechanical properties of Fe₄₀Mn₂₀Cr₂₀Ni₂₀ high-entropy alloys (HEAs) are investigated. The Cr-rich secondary phases with a tetragonal structure (σ phases) in the Fe₄₀Mn₂₀Cr₂₀Ni₂₀ HEAs are precipitated upon annealing at 600 °C-900 °C for 2 h. The prepared Fe₄₀Mn₂₀Cr₂₀Ni₂₀ HEA annealed at 800 °C for 2 h after cold rolling has a good combination of strength and elongation, with a high yield strength of 438 MPa, a high ultimate tensile strength of 676 MPa, and an excellent elongation to fracture of 32%. The mechanical properties at cryogenic temperature are better than those at room temperature. Typically, for the incompletely recrystallized alloy annealed at 700 °C, the yield strength, tensile strength, and elongation after fracture are increased by 26%, 22%, and 100%, respectively. This trend mainly depends on dislocation and twinning strengthening. The σ phases also improve the cryogenic tensile properties. Furthermore, the recrystallization kinetics of the Fe₄₀Mn₂₀Cr₂₀Ni₂₀ HEAs are explored to correlate with the deformation behavior.

Keywords

High-entropy alloys, mechanical properties, plastic deformation, recrystallization kinetics, cryogenic temperature

Cite this article

Ma QX, Yang HJ, Wang Z, Shi XH, Liaw PK, Qiao JW. High strength and ductility in partially recrystallized Fe₄₀Mn₂₀Cr₂₀Ni₂₀ high-entropy alloys at cryogenic temperature. *Microstructures* 2022;2:2022015. <http://dx.doi.org/10.20517/microstructures.2022.12>

8. Near-room-temperature reversible switching of quadratic optical nonlinearities in a one-dimensional perovskite-like hybrid

Qingshun Fan, Yu Ma, Haojie Xu, Yipeng Song, Yi Liu, Junhua Luo, Zhihua Sun*

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Abstract

The switching of quadratic nonlinear optical (NLO) effects between two or more NLO states of solid-state materials represents an intriguing new branch in the field of photoelectrics and optics. While structural phase transitions have shown potential in this field, near-room-temperature reversible NLO switches have rarely been reported. To exploit new NLO switching materials within the structurally flexible class of hybrid perovskites, here, we synthesize a one-dimensional perovskite-like hybrid, (MP)PbBr₃ (where MP⁺ is a 1-methylpyrrolidinium cation), through a facile solution method, which exhibits strong second harmonic generation (SHG) activities with an intensity of ~1.6 times as large as potassium dihydrogen phosphate. Intriguingly, (MP)PbBr₃ enables the near-room-temperature reversible switching of SHG properties, showing a large NLO switching contrast of up to ~40 between its SHG-active and SHG-inactive phases, beyond most of its liquid counterparts. Further microscopic structural analyses reveal that the dynamic ordering of the organic MP⁺ cation and inorganic chain-like skeleton triggers its centrosymmetric (P6₃/mmc) to acentric (P2₁2₁2₁) phase transition at 316 K upon cooling, resulting in a crucial contribution to its NLO switching properties. This work illustrates the potential of this material as a candidate for solid-state NLO switches and will promote the development of NLO materials within the family of low-dimensional hybrid perovskites.

Keywords

Phase transition, nonlinear optical properties, NLO switching, hybrid perovskites

Cite this article

Fan Q, Ma Y, Xu H, Song Y, Liu Y, Luo J, Sun Z. Near-room-temperature reversible switching of quadratic optical nonlinearities in a one-dimensional perovskite-like hybrid. *Microstructures* 2022;2:2022013. <http://dx.doi.org/10.20517/microstructures.2022.09>

9. Chemical unit co-substitution enabling broadband and tunable near-infrared emission in garnet-type $\text{Lu}_3\text{Sc}_2\text{Ga}_3\text{O}_{12}:\text{Cr}^{3+}$ phosphors

Taoze Wang, Gaochao Liu, Zhiguo Xia*

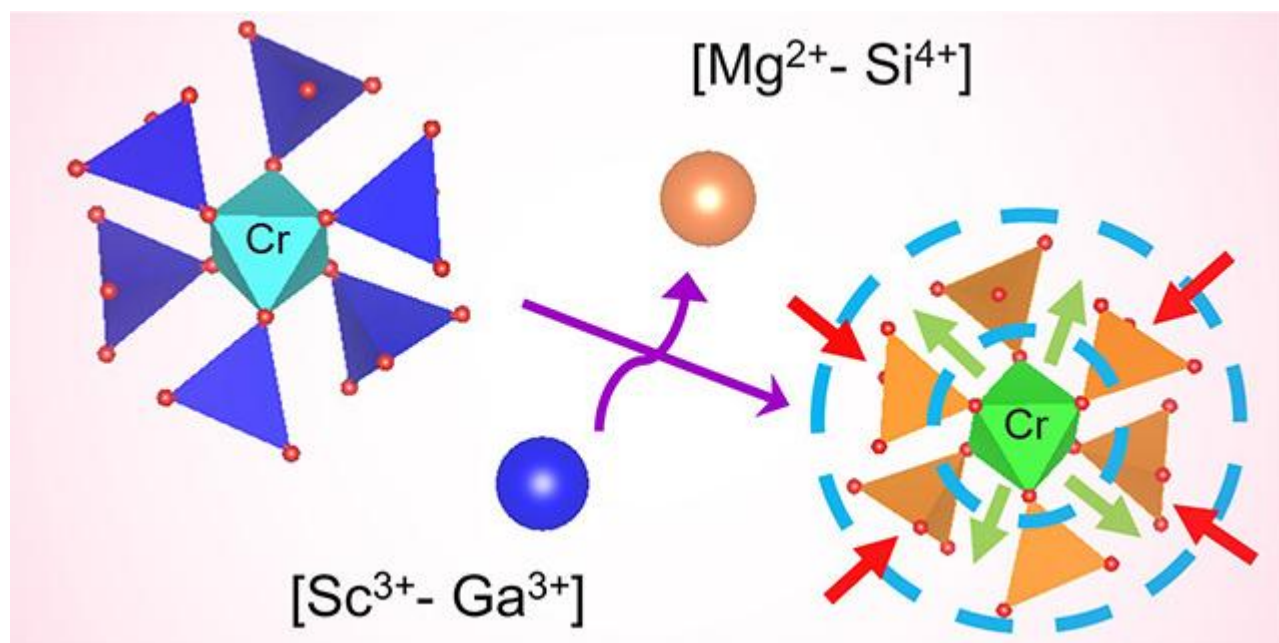
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Graphical Abstract



Abstract

Although near-infrared phosphor-converted light-emitting diodes (NIR pc-LEDs) are desired for non-visible light source applications, the design of broadband NIR phosphors remains a challenge. Inspired by the chemical unit co-substitution strategy for the modification of composition and local structure, we realize a tunable redshift emission from 706 to 765 nm in garnet-type $\text{Lu}_3\text{Sc}_2\text{Ga}_3\text{O}_{12}:\text{Cr}^{3+}$ with a broadened full width at half maximum and enhanced photoluminescence intensity by introducing a $[\text{Mg}^{2+}-\text{Si}^{4+}]$ unit into the $[\text{Sc}^{3+}-\text{Ga}^{3+}]$ couple. Structural and spectral analyzes demonstrate that the co-substitution reduces the local symmetry and crystal field strength of the $[\text{CrO}_6]$ octahedra, thus leading to inhomogeneous widening of the $4T_2 \rightarrow 4A_2$ emission and enhanced blue absorption. Furthermore, the $4T_2 \rightarrow 4A_2$ emission exhibits a phonon-assisted character at low temperatures due to the thermal coupling effect with the $2E$ level. The fabricated NIR pc-LED based on

the optimized NIR phosphor exhibits excellent potential in night vision and imaging applications.

Keywords

Near-infrared (NIR), garnet structure, Cr³⁺-doped phosphor, co-substitution

Cite this article

Wang T, Liu G, Xia Z. Chemical unit co-substitution enabling broadband and tunable near-infrared emission in garnet-type Lu₃Sc₂Ga₃O₁₂:Cr³⁺ phosphors. *Microstructures* 2022;2:2022020.

<http://dx.doi.org/10.20517/microstructures.2022.19>

10. Effects of processing parameters on a β -solidifying TiAl alloy fabricated by laser-based additive manufacturing

Danni Huang, Yangping Dong, Hancong Chen, Yinghao Zhou, Ming-Xing Zhang*, Ming Yan*

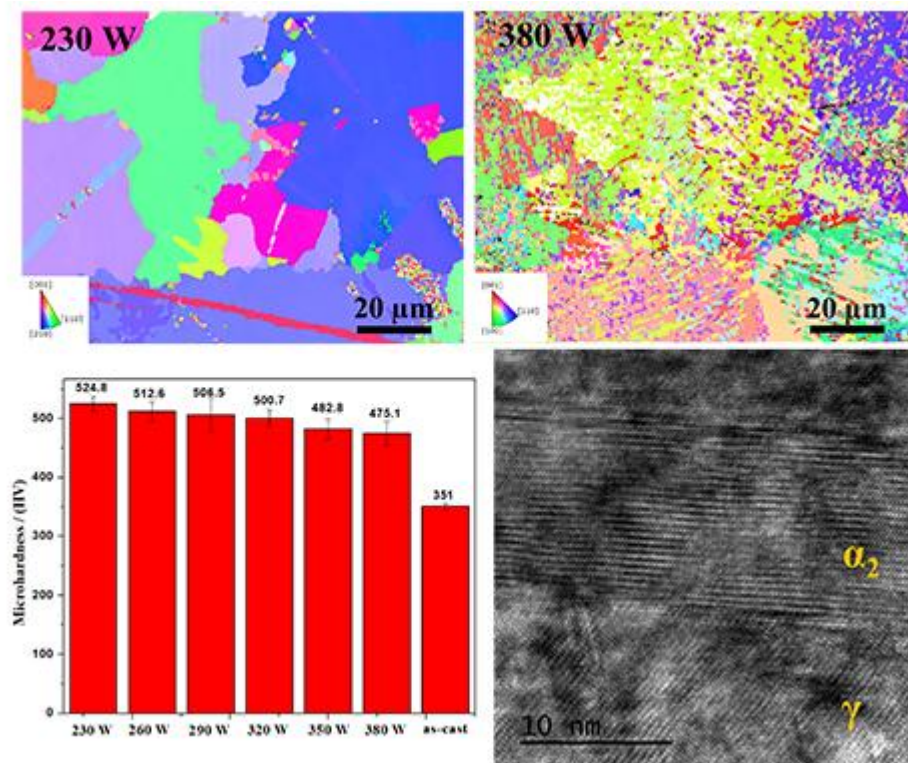
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Graphical Abstract



Abstract

β -solidifying TiAl alloys are considered as promising candidate materials for high-temperature

structural applications. Laser-based additive manufacturing (LAM) enables the fabrication of components with geometrical complexity in near-net shape, leading to time and feedstock savings. In this study, a gas-atomized Ti-44Al-4Nb-1Mo-1Cr powder is used as a feedstock material for LAM. However, the LAM of TiAl alloys remains a challenge due to serious cracking during the printing process. To minimize the cracking, the optimization of the LAM processing parameters is essential. Hence, the effects of the LAM processing parameters on the cracking susceptibility and microstructure are studied here. Our experimental results show that the cracking susceptibility can be mitigated by increasing the laser power. Accordingly, the microstructure transforms from the dominating α_2 grains to a near-lamellar microstructure with an increment in laser power, leading to a reduction in microhardness, even though it is still higher than that of its as-cast counterparts. It is concluded that changes in the laser power can directly tailor the microstructure, phase composition and microhardness of LAM-fabricated TiAl alloys.

Keywords

β -solidifying TiAl alloy, laser-based additive manufacturing, phase, microstructural evolution, microhardness

Cite this article

Huang D, Dong Y, Chen H, Zhou Y, Zhang MX, Yan M. Effects of processing parameters on a β -solidifying TiAl alloy fabricated by laser-based additive manufacturing. *Microstructures* 2022;2:2022019. <http://dx.doi.org/10.20517/microstructures.2022.17>

11. Tunable negative thermal expansion in La(Fe, Si)₁₃/resin composites with high mechanical property and long-term cycle stability

He Zhou, Yuwei Liu, Rongjin Huang, Bo Chen*, Min Xia, Ziyuan Yu, Haodong Chen, Kaiming Qiao, Junzhuang Cong, Sergey V. Taskaev, Ke Chu, Hu Zhang*

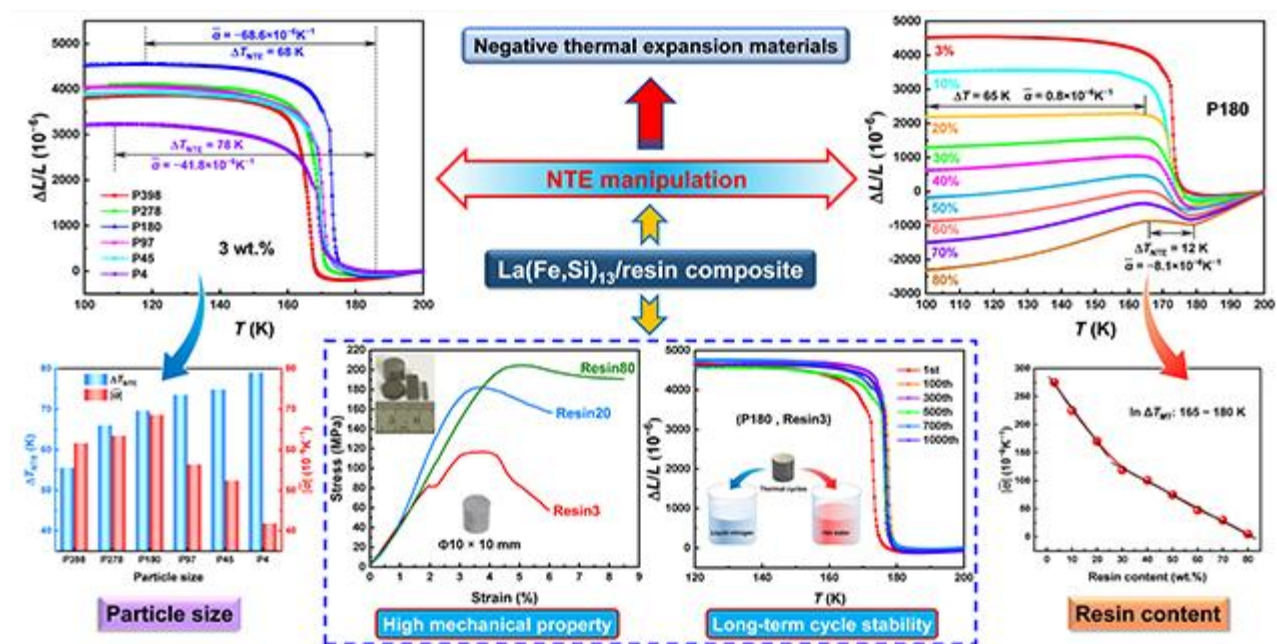
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Graphical Abstract



Abstract

Materials with tunable negative thermal expansion (NTE) are highly demanded in various functional devices. $\text{La}(\text{Fe}, \text{Si})_{13}$ -based compounds are promising NTE materials due to their outstanding NTE properties. However, their poor mechanical properties and related short service life restrict their practical applications. In this work, epoxy resin with positive thermal expansion is used to synthesize La-Fe-Si/resin composites. The NTE of La-Fe-Si/resin composites can be manipulated by optimizing the La-Fe-Si particle size and resin content, and tailoring resin content could tune the NTE more effectively. The average linear coefficient of thermal expansion of the composites decreases from $-275.0 \times 10^{-6} \text{ K}^{-1}$ to $-4.9 \times 10^{-6} \text{ K}^{-1}$ over the magnetic transition temperature range as the resin content increases from 3 wt.% to 80 wt.%. In addition, zero thermal expansion is achieved in the La-Fe-Si/resin composite with 20 wt.% resin. The resin would reinforce the binding force by filling the pores between the particles. The La-Fe-Si/resin composite with 80 wt.% resin exhibits highly improved mechanical properties; for example, its compressive strength of 205 MPa is 75% higher than that of the La-Fe-Si/resin composite with 3 wt.% resin. The prepared La-Fe-Si/resin composites can be machined into different shapes for practical applications, such as thin plates, strips, and rods. Furthermore, the La-Fe-Si/resin composites can undergo 1000 thermal cycles without NTE performance degradation and mechanical integrity loss, indicating durable cycle stability. Hence, significantly tunable NTE with high mechanical properties and long-term cycle stability makes La-Fe-Si/resin composites present great application potential as NTE materials.

Keywords

Negative thermal expansion (NTE), La-Fe-Si compounds, mechanical properties

Cite this article

Zhou H, Liu Y, Huang R, Chen B, Xia M, Yu Z, Chen H, Qiao K, Cong J, Taskaev SV, Chu K, Zhang H. Tunable negative thermal expansion in La(Fe, Si)₁₃/resin composites with high mechanical property and long-term cycle stability . *Microstructures* 2022;2:2022018.

<http://dx.doi.org/10.20517/microstructures.2022.13>

12. Detwinning/twin growth-induced phase transformation in a metastable compositionally complex alloy

Wenjun Lu*, Fengchao An, Christian H. Liebscher*

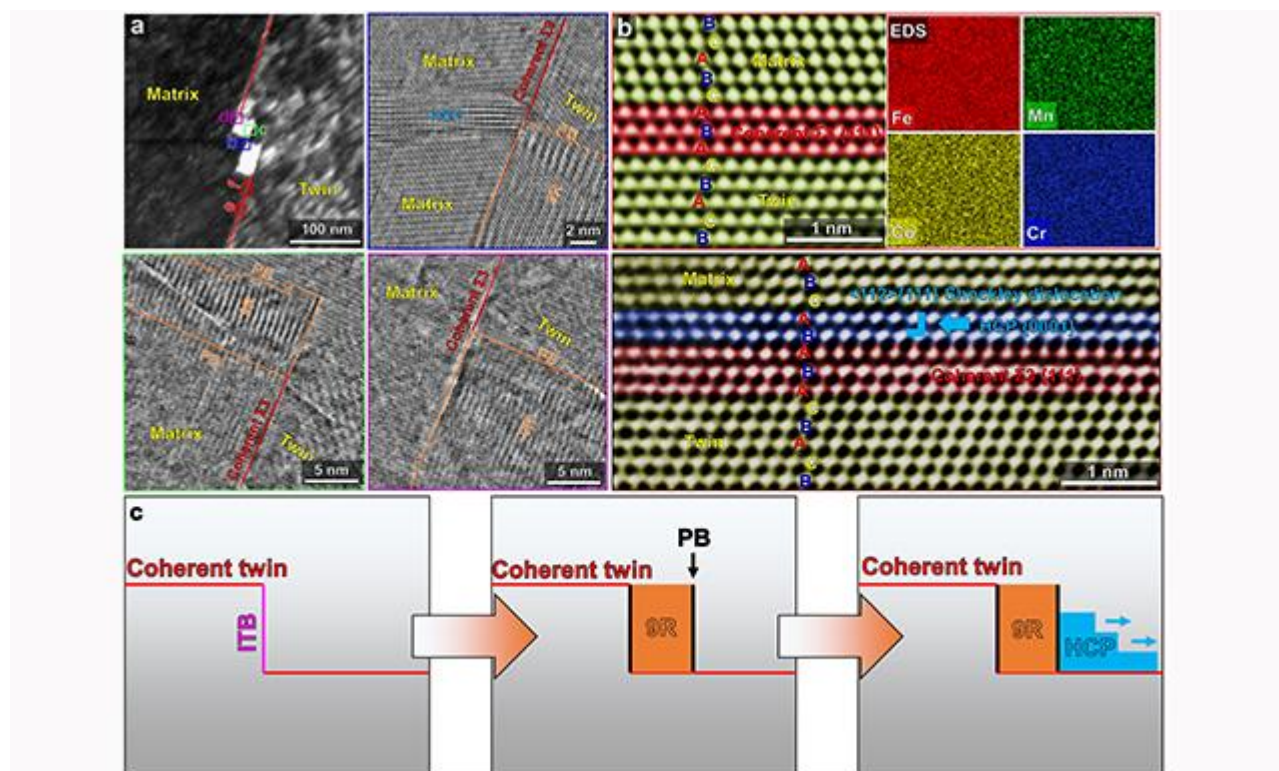
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Graphical Abstract



Abstract

Extensive experiments have shown that the transformation from the face-centered cubic to hexagonal close-packed ϵ phase usually occurs around coherent Σ_3 boundaries. However, in this letter, we reveal a different transformation mechanism in a metastable dual-phase compositionally complex alloy via a systematic high-resolution scanning transmission electron microscopy analysis. The face-centered cubic γ matrix can be transformed to the hexagonal close-packed ϵ phase (as small as one unit) around an incoherent Σ_3 boundary (~ 30 nm), i.e., the facet of the coherent Σ_3 boundary. This transformation is assisted by the detwinning/twin growth of a coherent Σ_3 boundary during annealing treatment (900 °C for 60 min).

Keywords

Detwinning/twin growth, incoherent Σ_3 boundary, 9R structure, displacive transformation, compositionally complex alloy

Cite this article

Lu W, An F, Liebscher CH. Detwinning/twin growth-induced phase transformation in a metastable compositionally complex alloy. *Microstructures* 2022;2:2022017.

<http://dx.doi.org/10.20517/microstructures.2022.14>