Forum J Intelligence Materials

qpei@seas.ucla.edu

Flexile optoelectronics are currently being investigated for applications in large-areas flat-panel displays, solid state lighting and other consumer electronics. As the important parts, flexible touch sensor, OLEDs with thin film transistors (TFT) offer potentially lower production cost and greater mechanical flexibility including elastomeric stretchability. However, for the flexible OLEDs, the experimentally determined external quantum efficiency has been limited to less than 30% without other out-coupling component. The 70% of the produced photons is lost due to trapping inside OLEDs in the form of waveguide modes in organic/ITO transparent anode layers, surface plasmon–polariton modes at the metallic electrode/organic interface, and glass substrate modes from total internal reflection at the glass substrate/air interface. The use of ITO and glass also affect the flexibility and fabrication cost of the OLEDs, touch sensor and TFT.

Firstly I will introduce a flexible touch senor based on flexible substrate and silver nanowires. The silver nanowire solution is synthesized in the lab and could realize the mass production and different application based on the different size of silver nanowire and the solid content. The flexible conductive film is fabricated by large scale roll-to-roll coating system and 1 minutes for 5 meters. We could use laser etching to pattern this conductive film and the resolution could reach to 25 um. Also we could use photolithograph to pattern this conductive film and compatible the universal product line. The transmittance of this touch sensor could reach to 92% and 50 Ohm/sq. The final products cell phone with 4 inch touch panel and flat panel with 7 inch touch panel are realized.

Secondly I will introduce a solution processed flexible polymer nanocomposite conductor to replace ITO/glass for the fabrication of high-efficiency PLEDs. The nanocomposite comprises a layer of single-walled carbon nanotubes (SWNT) and a layer of silver nanowires (AgNWs) embedded in the surface of a barium strontium titanate (BST) nanoparticle-polymer nanocomposite. The SWNT layer on the outer layer of the nanocomposite interfaces with the polymer semiconductor layer(s) to smoothen the surface roughness and to increase the conductive surface coverage, while the AgNW layer underneath the SWNT provides long range electrical conductivity. The BST nanoparticles embedded in the polymer substrate disrupt the substrate mode of trapped light. Finite-difference time-domain (FDTD) simulation indicates that the enhancement factor of the nanocomposite electrode as compared ITO/glass could be as high as 361%. The experimentally obtained enhancement factors are 246% and 224% for green and white PLEDs, respectively, comparing the nanocomposite substrate to ITO/glass substrate. The maximum external quantum efficiency of solution-processed green and white PLEDs are 38.9%

and 30.5%, respectively. Furthermore, these PLEDs are highly flexible and can be bent to 3 mm radius.

Keywords: Stretchable, Flexible, Self-healable, Transparent Conductive Electrode, Silver nanowires-polymer composite

J09

Applications of Smart Humidity-controlling Materials on Preserve in Refrigerator

Wentao Liu*, Hao Liu, Suqin He, Chengshen Zhu

School of Materials Science and Engineering, Zhengzhou University, 450001, Zhengzhou, China

Stable humidity range in high humidity environment is critical to preservation of fruits and vegetables, high humidity environment of materials has wide application prospect. A series of polyacrylamide/sepiolite and sodium polyacrylate/sepiolite humidity-controlling composite materials were prepared by aqueous intercalation solution polymerization with activated inorganic mineral sepiolite and acrylamide or sodium acrylic acid monomer, the impact of the ratio of raw materials, preparation conditions and the drying method on humidity-controlling performance of the composite were studied. The optimal parameters of polyacrylamide/sepiolite and sodium polyacrylate/sepiolite humidity-controlling composite materials have been obtained, which showed high moisture capacity and moisture absorption rate. In addition, SEM and FTIR were used to study the surface morphology and structure. At last, the application of polyacrylamide/sepiolite humidity-controlling composite materials in refrigeratorfruits and vegetablelesboxes was studied. Preliminary study on the application of polyacrylamide/sepiolite composites in refrigerator fruits and vegetablelesboxes were carried out, and compared with commercially available moisture absorption material. The results showed that polyacrylamide/sepiolite composites have certain ability in fruits and vegetableles fresh-keeping.

J10

Tunable Magnetocaloric Effect in Melt-extracted Ni-Mn-Ga Microwires

M.F. Qian¹, X.X. Zhang^{1*}, L.S. Wei¹, Y.F. Liu¹, L. Geng¹, H.X. Peng^{2*}

¹ School of Materials Science and Engineering, Harbin Institute of Technology, Harbin 150001, PR

² Institute for Composites Science Innovation (InCSI), School of Materials Science and Engineering, Zhejiang University, Hangzhou, 310027, PR China.

* Corresponding author. Tel: 86-451-86415894, 86-571-87952660, Fax: 86-451-86413921, E-mail address: <u>xxzhang@hit.edu.cn</u>; <u>hxpengwork@zju.edu.cn</u>

Magnetocaloric effect (MCE) in melt-extracted Ni-Mn-Ga microiwires were studied by tuning the temperature distance between the first-order (martensitic) and the second-order (ferromagnetic to paramagnetic) transitions. We presented that giant MCE can be achieved in annealed Ni_{50.4±0.2}Mn_{29.4±0.1}Ga_{20.2±0.2} microwires (W1) by merging the two transitions where a strong magneto-structural coupling was existed. An absolute maximum value of the isothermal magnetic entropy change of 24.9 J/kgK was achieved at the magnetic field change of 50000 Oe, being comparable to or even superior to that of polycrystalline bulk alloys. While a real magnetic refrigerator requires not only a large MCE but also a wide temperature span of the MCE. For this purpose, partial magneto-structural coupling was required. Microwires with a first and second-order transformation temperature difference of ~30K was designed and an intentional stepwise Mn-vaporizing annealing was applied for widening the transformation range. It yielded a full width at half maximum (FWHM) of ~60K from 330 to 390K and a refrigeration capacity (RC) as large as 240 J/kg at 50000 Oe in Ni_{50.6±0.2}Mn_{28.1±0.6}Ga_{21.3±0.5} (W2) microwires, which significantly improved the practicability of Ni-Mn-Ga alloys.

J11 (Invited)

Structure and Dielectric Properties of Perovskite 0.7CaTiO₃-0.3NdAlO₃ Based Microwave Ceramic with Ti Deviation from Stoichiometry

Shaojun Liu, Lijin Cheng

Powder Metallurgy Research Institute, Central South University, Changsha, China

It is well known that the densification processing and dielectric properties of perovskite ABO₃ microwave ceramics can be effectively tuned by controlling the B-site non-stoichiometry. In the present study, $0.7CaTiO_3$ - $0.3NdAlO_3$ (CTNA) based microwave ceramic with high relative density is fabricated, which is ascribed to induced point defects by B-site non-stoichiometry. The microstructure (domain) and crystal structure is tuned successfully as well. Special attention is paid on the influence of Ti deficiency on the crystal distortion and the titling of Ti-O₆ octahedral. Several findings are summarized as follows. 1) The oxygen vacancies induced by Ti deficiency effectively promote the grain boundary diffusion and volume diffusion. Single phase CTNA

ceramics are of dense microstructure and homogeneous morphology. 2) The decreased crystal volume and crystal distortion of CTNA ceramics occurs due to Ti deficiency. It is found that the crystal distortion results in enhanced dielectric loss. In contrast, the decreased crystal volume can decrease the dielectric loss by reducing the damping coefficient of crystal vibration. 3) As a substructure, the domains in CTNA ceramics are perpendicular to each other (002) crystal plane. Slight Ti deviation from sotiochiometry does not change the tilting type of anti-phase domains of CTNA ceramic. The orientation relationship between the domains is not influenced either. In contrast, oxygen vacancies induced by Ti deficiency significantly promote the growth of domain. 4) Optimized microwave properties are found for CTNA ceramics with 0.5mol% Ti deviation. The dielectric constant (ε_r), quality factor (*Q.f*), and temperature coefficient of resonant frequency (τ_r) of 0.7CaTi_{0.995}O₃-0.3NdAlO₃ ceramics with high relative density (99.25%) and large size domain (~520nm) are 46, 44000 GHz, and +2.88ppm/°C, respectively.

Note: This work is supported by National Natural Science Foundation of China through Grant Nos. 51172053

J12 (Invited) Material Preparation and Characterization of novel Magnetorheological Elastomers

Miao Yu¹, Dong Chen¹, Song Qi¹, Jie Fu¹, Mi Zhu¹,

¹Laboratory for Optoelectronic Technology and Systems of Ministry of Education, College of Optoelectronic Engineering, Chongqing University, Chongqing, China 400044; Corresponding Author: *Email: yumiao@cqu.edu.cn

Magnetorheological elastomers (MREs) are well-known smart particle reinforced elastomer, which consisting of micronized magnetic particles suspended in an elastic matrix. MRE has excellent magnetic-control mechanical properties, and it brought broad prospects of application in the fields of noise reduction, vibration attenuation and smart sensing. This paper mainly introduced the material researches of MRE which focus on the improvement of matrix, interface and magnetic-particle. In the study of the matrix, we prepared a MRE based on polyurethane /epoxy interpenetrating network structure matrix, and the damping and mechanical properties of this MRE were improved. In interface research, Fe nano-flakes coated carbonyl iron particles were prepared to improve the damping property and magnetorheological effect. For the magnetic-particle, we replaced the soft magnetism particles by NdFeB particles. The novel MRE was showed a bi-directional magnetic-control modulus. The MRE with high damping, high

strength and bi-directional magnetic-control modulus would offer promising advantages in seismologic application.

J13

Phase and Size Controlled Synthesis of ZnS Nanoparticles at Low Temperatures

Feng Huo¹, Yushu Wang², Feng Yang^{3*}, Jin-Fang Xi³, Long-Sheng Zou³, Si-Si Xie³, Yuan Pu^{4*}
¹School of Chemistry and Chemical Engineering, Analytical Testing Center, Neijiang Normal University, Neijiang, 641100, PR China

²School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA30318, USA

³Superconductivity and New Energy R&D Center, Key Laboratory of Advanced Technology of Materials (Ministry of Education of China), Mail Stop 165#, Southwest Jiaotong University, Chengdu, 610031, People's Republic of China

⁴State Key Laboratory of Organic-Inorganic Composites, Beijing University of Chemical Technology, Beijing 100029, PR China

E-mail:yf@home.swjtu.edu.cn, puyuan@mail.buct.edu.cn

We report a simple solution for the synthesis of phase and size controlled ZnS nanoparticles at low temperatures. ZnS nanoparticles of cubic form (c-ZnS), as well as hexagonal form (h-ZnS), were obtained by heating an aqueous solution of $Zn(NO_3)_2 \cdot 6H_2O$ and $Na_2S_2O_3 \cdot 5H_2O$ at different temperatures. When the system was heated at 65 °C for 24 h, crystal phase of ZnS nanoparticles obtained was assigned to the hexagonal form, according to X-ray diffraction (XRD) and selected-area electron diffraction (SEAD). c-ZnS nanoparticles were obtained when the reaction temperatures were at 100 °C under hydrothermal conditions. Results show that the size of ZnS obtained by hydrolytic method was 200-350 nm.Under hydrothermal conditions (100°C), ZnS exhibits monodispersed nanoparticles of about 4 nm. Proper rate of releasing S of $Na_2S_2O_3 \cdot 5H_2O$, tuned by the variation of temperature, is believed to be critical to stabilize the ZnS nanoparticles of hexagonal form. Compared with large size h-ZnS microspheres,c-ZnS 4 nmnanoparticles show significant quantum size effect and higher photocatalytic properites.

J14

Fuzzy Control for a Magnetorheological Elastomer Vibration Isolation

System

Jie Fu

Chongqing University

This paper addresses the problem of micro-vibration control of a precision vibration isolation system with a magnetorheological elastomer (MRE) isolator and fuzzy control strategy. Firstly, a polyurethane matrix MRE isolator working in the shear-compression mixed mode is introduced. The dynamic characteristic is experimentally tested, and the range of the frequency shift and the model parameters of the MRE isolator are obtained from experimental results. Secondly, a new semi-active control law is proposed, which uses isolation structure displacement and relative displacement between the isolation structure and base as the inputs. Considering the nonlinearity of the MRE isolator and the excitation uncertainty of an isolation system, the designed semi-active fuzzy logic controller (FLC) is independent of the model of system and is robust. Finally, the numerical simulations and experiments are conducted to evaluate the performance of the FLC with single-frequency and multiple-frequency excitation, respectively, and the experimental results show that the acceleration transmissibility is reduced by 54.04% at most, which verifies the effectiveness of the designed semi-active FLC. Moreover, the advantages of the approach are demonstrated in comparison to the passive control and ON-OFF control.

J15 (Invited)

Morphotropic Phase Boundaries and Their Corresponding Magnetic Properties in Ferromagnetic Rare Earth-transition Metal Alloys with Lavas Structure

Sen Yang

School of Science, MOE Key Laboratory for Nonequilibrium Synthesis and Modulation of Condensed Matter, Xi'an Jiaotong University, China 710049

Ferromagnetic morphotropic phase boundary (FMPB) has attracted much attention in recent years since its discovery in $Tb_{1-x}Dy_xCo_2$ (PRL 104, 197201 (2010)). Here we report our study on $Tb_{1-x}Gd_xFe_2$, $Tb_{1-x}Nd_xFe_2$ and $Tb_{1-x}Nd_xCo_2$ systems which all possess FMPB and shows interesting magnetic and magnetostrictive properties around this boundary. Systematic investigations on the crystal symmetry, magnetization, magnetic coercive field H_c , magnetostriction, magnetic anisotropy and magnetocaloric effect were performed. The results indicate the wide existence of FMPB in ferromagnetic materials especially the RE (rare

earth)-Fe₂/Co₂ alloys with Laves structure, and also suggest new routes to design new magnetic functional materials.

J16 Electrorheological Performance of Elastomers Filled with Modified TiO₂ Particles

Xufeng Dong, Chenguang Niu, Min Qi

School of Materials Science and Engineering, Dalian University of Technology, Dalian 116024,

China

As a composite, the particle/matrix interface may poly an important role on electrorheological (ER) performance of ER elastomers, which have been overlooked in previous studies. In this study, TiO_2 particles and silicon rubber was used to prepare ER elastomers. To improve the interfacial bond strength, two coupling agents, 3-(trimethoxysilyI)propyl methacrylate (A174) and triethoxyvinyIsilane (VTEO), were used to modify the surface of the TiO_2 particles. Particles characterization results illustrate that the coupling agents modified TiO_2 particles present little change in morphology but an increase in size with respect to the bare TiO_2 particles. Compared with the bare TiO_2 particles filled sample, the modified TiO_2 particles filled elastomers present bridging structures between the particles and the matrix, enhanced mechanical properties, and higher dielectric constant, indicating enhanced interfacial bond strength. The viscoelastic properties of the bare and the modified TiO_2 particles filled elastomers were tested and compared. The results indicated the ER performance, including the field-induced storage modulus and the storage modulus sensitivity, can be promoted by improving the bond strength between the TiO_2 particles and the silicon rubber.

J17

Glass-ferroic Composite: the Third Class of Ferroic Materials

Yuanchao Ji¹, Minxia Fang^{1,2}, Xiangdong Ding¹, Dong Wang¹, Kazuhiro Otsuka², Xiaobing Ren^{1,2}

¹ Frontier Institute of Science and Technology, and State Key Laboratory for Mechanical Behaviour of Materials, Xi'an Jiaotong University, Xi'an 710049, China

²Ferroic Physics Group, National Institute for Materials Science, Tsukuba, 305-0047, Ibaraki,

Email: jyc.xjtu@xjtu.edu.cn

We report a glass-ferroic composite (in short "glass-ferroic") in ferroic materials, an analogue of the composite of glassy and crystalline phases (glass-crystal composite, e.g., semicrystalline polymer). The formation of glass-ferroic (i.e. the existence of residual ferroic glass) stems from a time-dependent crystallization of the ferroic glass. Moreover, glass-ferroics show two types of transition characteristics depending on the thermal hysteresis of crystallization transition, as exemplified in Ti_{48.7}Ni_{51.3} and Pb_{0.87}La_{0.13}Zr_{0.4}Ti_{0.6}O₃. Based on experimental results, a generic phase diagram is established to include all ferroic states, i.e., ferroic crystal, ferroic glass and glass-ferroic. Being the third class of ferroic materials, glass-ferroics may open a new avenue for achieving novel properties and designing ferroic phase-change memory devices. Such one example has been given in the BaTiO₃-based material, which has simultaneously achieved large electrostrain and low hysteresis over a broad temperature range.

J18 (Invited) Nanoscaled Martensitic Transition and Its Abnormal Properties in Shape Memory Alloys

Dong Wang, Yunzhi Wang

Xi'an Jiaotong University

By impurity doping in shape memory alloys (SMAs), we show a mechanism that leads to nanoscaled martensitic transformation accompanying with superelasticity with slim hysteresis across a wide temperature range. Computer simulations using the Landau theory of phase transformations and Khachaturyan's microelasticity theory predict the formation of randomly distributed nanosized, singlevariant martensitic domains and a generic "phase diagram" including all the strain states in Fe-doped NiTi SMAs, which agrees well with experimental measurements. These nanoscale martensitic domains are frustrated and cannot evolve into long-range-ordered, internally twinned structures (i.e. long-range strain ordering). Such a structural state is found to evolve gradually upon loading and unloading or heating and cooling across a wide temperature range with narrow hysteresis. This continuous transition process shows lots of unique properties.

J19 (Invited)

Research on Application of Piezoelectric Materials in Smart Structures

Hongli Ji, Jinhao Qiu

Aeronautic Science Key Laboratory for Smart Materials and Structures, College of Aerospace Engineering

Nanjing University of Aeronautics and Astronautics, Nanjing 210016, China

Piezoelectric materials have become the most attractive functional materials for sensors and actuators in smart structures because they can directly convert mechanical energy to electrical energy and vise versa. They have excellent electromechanical coupling characteristics and excellent frequency response. In this article, some research activities on the applications of piezoelectric materials in smart structures, including semi-active vibration control based on synchronized switch damping using negative capacitance, energy harvesting using new electronic interfaces, structural health monitoring based on a new type of piezoelectric fibers with metal core, and active hysteresis control based on new modified Prandtl-Ishlinskii model at the Aeronautical Science Key Laboratory for Smart Materials and Structures, Nanjing University of Aeronautics and Astronautics are introduced.

Keywords: Piezoelectric materials, vibration control, energy harvesting, structural health monitoring, piezoelectric hysteresis

J20

Study on Optical Properties of Complex Perovskite Ceramics

Jie Shen

State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, School of Materials Science and Engineering, Wuhan University of Technology, Wuhan, 430070, P.R. China *Corresponding author Tel:+86-27-8776-0153 Fax: +86-27-8776-0129 E-mail address: shenjie@whut.edu.cn

Compared to the glass and single crystal, transparent ceramics not only have high transparency and corrosion resistance, but also can work in extreme condition. High permittivity and low dielectric loss of the complex perovskite ceramics provide the application potential of a high refractive index material with good intrinsic transmittance. Furthermore, with outstanding structure tolerant, transparent complex perovskite ceramics can be a good matrix candidate for Re doped luminescent material to improve the quenching concentration. In this study, Sn⁴⁺ doped Ba(Mg_{1/3}Nb_{2/3})O₃ (BMN) transparent ceramics were synthesized by a solid state reaction and

investigated with using of first-principle method calculation. Additionally, Sm³⁺ doped BMN luminescent ceramic was also synthesized and investigated.

Sn⁴⁺ doped BMN transparent ceramics were fabricated via the solid state reaction with using active powders and isostatic cool pressing. The transmittance of the Sn⁴⁺ doped BMN transparent ceramic is 30–53% in the visible region, and its refractive index is 2.09–2.22 in the wavelength range of 400 to 1000 nm. The cut-on wavelength shifts with doping to the edge of the visible region (410 nm), leading to effective ultraviolet absorption.

The phase structure of Sn⁴⁺: BMN was determined by Rietveld refinement. Based on the structural analysis, the electronic structure and optical properties of the material were calculated, analyzed and predicted. The theoretical analysis results show that the band gap of Sn⁴⁺: BMN is gradually widening with the increasing of additive amount of Sn⁴⁺, the absorption edge being blue-shift, and the transparent area expanding, which are consistent with experimental results.

Sm³⁺ doped BMN luminescent ceramic were synthesized by the same method as Sn⁴⁺: BMN. Structural analysis shows that Sm³⁺ enters the A-sites of BMN crystal structure. Sm³⁺:BMN ceramic shows obvious absorption peaks at 407 nm, 465 nm and 478 nm. The emission spectrum excited by 407 nm shows characteristic emission peaks from f-f orbital transitions of Sm³⁺ at 564 nm, 600 nm, 647 nm, 708 nm. Because of the structure tolerant of BMN matrix, quenching concentration of the materials were improved to 2% mol, which were nearly 25% higher than most materials of literatures.

All the above results show that doped BMN is an excellent candidate for the functional optical application.

Keywords: Complex perovskite ceramics; Transparent ceramics; Luminescent ceramic; Quenching concentration

J21

Actuation Performance of Piezoelectric Fiber Composites

Xiujuan Lin, Shifeng Huang

School of Material Science and Engineering, University of Jinan, Jinan, PR China

Piezoelectric fiber composites (PFCs) with interdigitated electrodes (IDEs) have attracted widespread attention owning to their unique structures, improved strength, excellent flexibility and higher actuation energy compared with conventional monolithic piezoceramic wafers. Though IDEs enabled PFCs to exploit the d₃₃ piezoelectric effect and enhance the actuation capability, inhomogeneous distribution of the electrical field existed in

piezofibers due to IDEs, which weakened the PFCs' actuation capability to some extent. Both electrode finger spacing and substrate thickness determined the distribution and strength of the electric field in piezofibers, and then influenced the PFCs' performance.

PFCs with different electrode finger spacing and substrate thicknesses were fabricated by viscous plastic processing (VPP). The researches focused on the influences of electrode finger spacing and substrate thicknesses on the actuation capability through the finite element modeling and experimental studies. The modeling results showed that smaller electrode finger spacing and substrate thicknesses both improved the actuation capability, which were validated by experiment results. The variation of actuation performance of PFCs as a function of applied voltages was investigated. The results showed the free strain performance was enhanced sharply from 162 microstrain to 1900 microstrain when the voltages of 500 V and 2000 V were applied, respectively. The free strain performance at 1000 V voltage amplitude decreased markedly around 27.8%, i.e. from 690 to 540 microstrain, with the increase of dc bias voltages from 0 to 500 V, respectively. The PFCs showed better free strain performance, a total increase of 26.0%, under the quasi-static condition than 50 Hz dynamic condition.

J22

The Effect of Dopamine Modified BaTiO₃ Nanoparticles on the Actuation Performance of Piezoelectric Fiber Composites

Mingliang Wu , Hang Luo, Xi Yuan, Weiwei Liu, Chao Chen, Kechao Zhou, Dou Zhang^{a)} State Key Laboratory of Powder Metallurgy, Central South University, Changsha, Hunan 410083, China

Piezoelectric fiber composites (PFCs) have attracted much interest in a variety of commercial, industrial and aerospace markets owing to their unique structures, far superior flexibility and toughness compared with conventional monolithic piezoceramic wafers. The free strain values, effective piezoelectric constant d₃₃ of PFCs and actuation property were strongly dependent on the active electric field applied to Pb(Zr_{1-x}Ti_x)O₃ (PZT) piezoceramic fibers. Reducing the dielectric mismatch between PZT fiber and the assembling epoxy would greatly increase the active electric field in PZT fiber. Therefore BaTiO₃ (BT) nanoparticles were introduced into the epoxy matrix in order to enhance the dielectric constant. Homogeneous dispersion of BT nanoparticles and tight adhesion with the epoxy were achieved owing to the surface modification by dopamine. The maximum dielectric constant of dopamine modified BT/epoxy (Dop@BT/epoxy) nanocomposites was 10.38 with 12wt% Dop@BT content at 1kHz. The maximum free strain and effective d₃₃

reached 1820 ppm and 455 pm/V, respectively, with 6 wt% Dop@BT content, while PFCs assembled by pure epoxy only showed 790 ppm and 198 pm/V at the same condition. The maximum tip displacement of cantilever beam actuated by PFCs was 19mm at the resonance frequency with 6 wt% Dop@BT content in epoxy, which improved 90% comparing to PFCs with pure epoxy.

Keywords: piezoelectric fiber composites, active electric field, free strain, actuation property

J23

Thermal and Kinetics Performance of Na-, Li-, Ca-, Ag-LSX Zeolites in the N₂-O₂ Adsorption

Hamida Panezai, Jihong Sun*

Beijing Key Laboratory for Green Catalysis and Separation, Department of Chemistry and Chemical Engineering, Beijing University of Technology, Beijing 100124, P. R. China *Corresponding author: jhsun@bjut.edu.cn

The effect of small amounts of water on the adsorption of N₂-O₂ gases on various cationic forms (Na-, Li-, Ca-, Ag-,) of LSX zeolite was investigated using thermogravimetric and derivative thermogravimetry (TG-DTG) techniques at different heating rates, which have proved to be very effective way for studying the influence of strongly adsorbed water on adsorption of less-strongly adsorbed N₂-O₂ molecules. The morphological, structural, and thermal properties of Na-, Li-, Ca-, and Ag-LSX were investigated using physicochemical characterizations such as ICP-AES, XRD, XPS, SEM, TG-DTG and N₂ adsorption-desorption isotherms. Three kinetic methods including Kissinger, Flynn-Wall-Ozawa and Coats-Redfern were employed to estimate the kinetic triplets (activation energy E, pre-exponential factor A and most probable mechanism/model) relating to the thermal desorption of water molecules exist in the skeleton of Cation-LSX zeolites. The E values calculated from these two equations were in close agreement, and thereafter corresponding thermal dehydration mechanisms and models corresponding to thermal dehydration were proposed on the basis of Coats-Redfern method. Moreover, the results demonstrated that the exponential declination of N₂ adsorption with the loading of different kinds of water is because of the significant influence of the adsorption capacity of cationic zeolites by water through reducing heterogeneity and strength of the electric field. Other than water, nature of cation also plays an important role in the association between the water and cations mainly depends on their electric charge density, showing that Li⁺ can hold the higher amounts and stronger force of water molecules than Na⁺, Ca²⁺, and Ag⁺. Their strong influence and distributions in the skeleton of LSX on the N_2 - O_2 adsorption performance in connection with the crystal water (traces) have remarkable impact on the N_2 adsorption capacity. Therefore the removal of water is essential for industrial applications particularly in air separation.

Keywords: Low silica zeolite type X, dehydration mechanism, N_2 - O_2 adsorption, Kissinger, Flynn-Wall-Ozawa, Coats-Redfern.

J24

Large Electric-field-induced Strain and Piezoelectricity in NBT-0.06BT Ceramic Prepared from Hydrothermally Synthesized Nanoparticles

Xuefan Zhou, Chao Jiang, Hang Luo, Chao Chen, Dou Zhang^{a)}

State Key Laboratory of Powder Metallurgy, Central South University, Changsha, Hunan 410083, China

In this study, 0.94Na_{0.5}Bi_{0.5}TiO₃-0.06BaTiO₃ (NBT-0.06BT) nanoparticles were synthesized by the hydrothermal method and subsequently were used to prepare NBT-0.06BT ceramic. The effects of polarization on crystalline phase, microstructures, dielectric properties and domain structures of the ceramics were investigated in detail to reveal the origin of enhanced piezoresponse and large electric field induced strain in as-prepared NBT-0.06BT ceramic.

The crystalline phases of NBT-0.06BT nanoparticles and ceramic were tested by X-ray diffraction (XRD). High-resolution transmission electron microscopy (HRTEM) images of the ceramic were taken with a JEM-2100F transmission electron microscope. A precision impedance analyzer (4294A, Agilent, PaloAlto, CA) was used to obtain the variation of dielectric constant and loss tangent as a function of frequency and temperature. The ferroelectric hysteresis loops and field-induced strain curves were obtained by using a typical Sawyer-Tower configuration and an inductive nanopositioner linear variable differential transformer (LVDT) sensor. Polarization was performed in silicone oil at 80 °C for 15 min under a electric field of 3.5 kV/mm. The piezoelectric charge coefficient, d₃₃, was measured 24 h after polarization using a Berlincourt d₃₃ meter (APC). Planar electromechanical coupling coefficient (κp) was calculated by resonance and anti-resonance technique using impedance analyzer. The ceramic was polished for investigating domain structures by the piezoresponse force microscopy (PFM) mode of an atomic force microscope (NanoManTM VS) with a conductive Pt/Ir-coated Si cantilever (SCM-PIT). The domain structures were obtained by keeping the Pt-coated tip fixed on the surface and appling an ac voltage with amplitude Vac= 10 V and frequency f= 41 kHz.

The XRD results of unpoled and poled NBT-0.06BT ceramics suggested the rhombohedraltetragonal morphotropic phase boundary (MPB) existed in as-prepared ceramics and tetragonal phase in the ceramics was enhanced after polarization. After poling at an electric field 3.5 kV/mm, the piezoelectric coefficient (d₃₃) and electromechanical coupling factor (κ_p) reached 171 pC/N and 0.31, respectively. The NBT-0.06BT ceramic exhibited a large remanent polarization of 46.10 μ C/cm² and electric field induced strain of 0.491% at 8 kV/mm with normalized strain d₃₃*=614 pC/N (Smax/Emax). It can be observed that the polar nanoregions (PNRs) were transformed into lamellar domains after polarization. The dielectric response of NBT-0.06BT ceramic also exhibited an electric-field-induced relaxor-to-ferroelectric phase transformation.

In summary, NBT-0.06BT nanoparticles were synthesized by hydrothermal method. The corresponding NBT-0.06BT ceramic possessed enhanced piezoelectric response and large electric-field-induced strain. The origin of large piezoresponse and strain of NBT-0.06BT ceramic was attributed to the coexistence of ferroelectric phase and relaxor phase under unpoled state along with domain switching and field-induced relaxor-to-ferroelectric phase transition when applying a electric field.

Keyword: NBT-0.06BT, piezoelectricity, strain, hydrothermal synthesis

J25

Study on the Properties of NBT-BT-KBT Lead-free Piezoelectric Ceramics

Kaihua liu, Gang liu

Faculty of material and energy, Southwest University, Chongqing 400715, PR China

The pure perovskite $(1-x)(0.935NBT-0.065BT-0.02KBT)-xK_2AINbO_5$ (x=0,0.001,0.003,0.005,0.007,0.009) lead-free piezoelectric ceramics was prepared by the conventional method. X- ray diffraction (XRD) and scanning electron microscopy (SEM) were utilized to analyze the phases and microstructures. With increasing the x, the proportion of tetragonal phase gradually increased, and K₂AINbO₅ could significantly promote the growth of grain within the range of this study. The addition of K₂AINbO₅ could improve the electrical properties, but more addition would deteriorate the dielectric properties of this system, and lead to strong dielectric frequency dispersion. Meanwhile, the piezoelectric properties also decreased sharply when increasing K₂AINbO₅ content. From the curves of dielectric constant versus temperatures, K₂AINbO₅ doped NBT-BT-KBT ceramics had better temperature characteristics, but it can be seen clearly that there were diffuse phase transition in this system. Moreover, the little temperature coefficient in the scope from 200°C to 350°C also made it potential to be developed as lead-free high temperature capacitors.

Keywords: NBT, lead-free piezoelectric ceramics, Al-Nb co-doped, dielectric properties