O. Electronic and Spin Electron Materials: I

Symposium Organizers :

Hongda Chen, Institute of Semiconductors, Chinese Academy of Sciences, China; Feng Pan, Tsinghua University, China; Rie Y. Umetsu(Ms.), Tohoku University, Japan; Joonyeon Chang, Korea Institute of Science and Technology (KIST), Korea; Lianzhou Wang, University of Queensland, Australia

Monday PM
August 19, 2019

Room: 312 (3rd Floor)
Symposium: O

Chairs:
Hongda Chen, Institute of Semiconductors, Chinese Academy of Sciences, China
Feng Pan, Tsinghua University, China
Rie Y. Umetsu, Tohoku University, Japan
Joonyeon Chang, Korea Institute of Science and Technology, Korea
Lianzhou Wang, The University of Queensland, Austraila

13:30-14:00 Keynote (1324853)

Imaging Topological Electron-Spin Textures by Using Atomic-Resolution Lorentz TEM

Xiuzhen Yu, RIKEN, Japan

The nanometer-scale vortex-like spin textures, such as vortex-anrivortex pairs in ferromagnetic (FM) domain walls, votices in superconductors, skyrmion (lattice) and antiskyrmions in magnets with inversion symmetry, have recently attracted enormous attention owing to their emergent phenomena. To confirm such minute complex spin textures and their dynamics with external stimuli, ultrafast real-space high-resolution imaging technique, such as time-resoved X-ray microscopy or Lorentz transmission electron microscopy (TEM) is useful.
In this talk, I will present several vortex-like spin textures realized by Lorentz TEM with atomic resolution in several systems, such as chiral magnets, ferromagnets with uniaxial anisotropy and the fluctrated magnets with Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction. In addition to the hexagonal skyrmion lattice (hex-SkL), a square lattice of merons and antimerons (sq-ML)—topologically distinguish with skyrmions—have been observed. By finely varying the external magnetic fields, the transformation between the sq-ML and a hex-SkL have been induced. We found that the skyrmions were very robust, lasting even as we lowered the temperature of the thin plate, but the merons and antimerons were much more sensitive, and relaxed into spin helices as the temperature fell.
Futhermore, the transition between skyrmions (topological "particals") and antiskyrmions ("antiparticles") via non-topological magnetic bubbles have been also demonstrated by means of the in-situ Lorentz TEM observations in a chiral system with D2d-symmetry. The control of topological nature among various magnetic vortices with external stimuli will be shown.
These works have been done in collaboration with Profs. Yoshinori Tokura, Naoto Nagaosa, Taka-hisa Arima, Yusuke Tokunaga, Shinichiro Seki and Fumitaka Kagawa, and with Drs. Wataru Koshibae, Yasujiro Taguchi, Khanh Nguyen, Daisuke Morikawa, Naoya Kanazawa, Tomoyuki Yokouchi, Kiyou Shibata, Licong Peng and Yoshio Kaneko.

14:00-14:30 Keynote (1342725)

Spin-Orbit Technologies: From Magnetic Memory to Terahertz Generation

Hyunsoo Yang, National University of Singapore, Singapore

Spintronic devices utilize an electric current to alter the state of a magnetic material and thus find great applications in magnetic memory. Over the last decade, spintronic research has focused largely on techniques based on spin-orbit coupling, such as spin-orbit torques (SOTs), to alter the magnetic state. The phenomenon of spin-orbit coupling in magnetic heterostructures was also recently used to generate terahertz emission and thus bridge the gap between spintronics and optoelectronics research.
I will introduce the basic concepts of SOTs, such as their physical origin, the effect of SOTs on a magnetic material, and how to quantitatively measure this effect. Next, I will discuss the latest trends in SOT research, such as the exploration of novel material systems like topological insulators and two-dimensional materials to improve the operation efficiency. Following this, some of the technical challenges in SOT-based magnetic memory will be highlighted. Moving forward, I will introduce the process of terahertz generation in magnetic heterostructures, where the spin-orbit coupling phenomenon plays a dominant role. I will discuss the details of how this terahertz emission process can be extended to novel material systems such as ferrimagnets and topological materials. The final section will focus on how the terahertz generation process can be used to measure SOTs in magnetic heterostructures, thus highlighting the interrelation between terahertz generation and the SOTs, which are linked by the underlying spin-orbit coupling.

14:30-14:55 Invited (1375315)

Magnetic Skyrmions-and-Bobbers-Based Racetrack Memory

Haifeng Du, High Magnetic Field Laboratory of the Chinese Academy of Sciences, China; Jing Tang,

High Magnetic Field Laboratory of the Chinese Academy of Sciences, China

Magnetic skyrmions and bobbers are two kinds of different nanoscale vortex-like spin configurations that can coexist in chiral magnets. They both possess high stability and particle-like properties and are then proposed to be utilized as binary bits to build the racetrack memory device, where the data bits are encoded by a chain of magnetic domains moving electrically along a given racetrack. The ability to controllably manipulate the two magnetic objects in confined geometries is the prerequisite to realize the device. In this talk, we show by numerical simulations that an isolated skyrmion and bobber can be interconverted by using spin-polarized current in a stepped magnetic nanostructure. They both can be driven collectively by current-induced spin torques. But, they show different dynamical behavior. In addition, we further demonstrate the feasibility of encoding data bits by a series of skyrmions and bobbers. Our results not only propose an accessible and controllable method to create the magnetic bobber by electric, but also provide a guide for future magnetic racetrack memory design based on binary magnetic topological structures.

14:55-15:20 Invited (1233171)

Spintronics in Quantum Materials

Wei Han, Peking University, China

Quantum materials have recently exhibited many unique spin-dependent properties, which could be promising material candidates for spintronics. On the other hand, pure spin current, flow of spin angular momentum without the company of any charge current, can be a useful probe for interesting quantum materials/states.
In this talk, I will present our recent experimental results on spintronics in quantum materials. I will first talk about the using topological insulators for spintronics, such as spin and charge conversion, and modificatoin of the magnetic properties in the YIG/(BixSb1-x)2Te3 heterostructures, which are due to the spin-momentum locked properties of the topological surface states. Then I will discuss the pure spin current transport in canted antiferromagnet Cr_2O_3, suggesting the existence of spin superfluid ground state at low temperatures. A large enhancement of the nonlocal spin signal is observed below ~ 20K, and it saturates from ~ 5K down to 2K. We show that the spins can propagate over very long distances (~ 20μm) in such spin superfluid ground state and the nonlocal spin signal decreases very slowly as the spacing increases with an inverse relationship, which is consistent with theoretical prediction. The experimental demonstration of the spin superfluid ground state in canted antiferromagnet will be extremely important for the fundamental physics on the BEC of spin-1 bosons and paves the way for future spin supercurrent devices, such as spin-Josephson junctions.

15:30-16:10 Tea Break

16:10-16:40 Keynote (1324017)

Magnon Valve and Magnon Junction Effects

Xiufeng Han, Institute of Physics, Chinese Academy of Sciences, China

Compared with the electron based spintronic devices, the magnon based spintronic devices have many attractive features, including minimization of Joule heating, much longer magnon coherence length and additional phase degree of freedom. It has been expected that a device, used a core structure of Magnetic insulator [MI1]/Space [S]/Magnetic insulator [MI2], can also operate by method of magnon current similar to a classical spin valve (SV) and a magnetic tunnel junction (MTJ). Here, we first demonstrated a magnon valve (MI1/S/MI2, YIG/Au/YIG) which consists of two magnetic insulators (MI=YIG) and a nonmagnetic spacer (S=Au). Instead of regulating transport of spin-polarized electrons, the magnon valve regulates flow of magnons. We used the temperature gradient to excite the magnon current in YIG, and inverse spin Hall effect (ISHE) to detect the magnon current across the magnon valve by the electrical method. Our results show that the magnon current transmission between two magnetic insulating layers (YIG) mediated by a nonmagnetic metal (Au) has high efficiency, and the transmission of the magnon current in a magnon valve becomes high (low) as magnetizations of the two magnetic insulators are parallelly (anti-parallelly) configured. We interpret the Magnon Valve Effect (MVE) by the angular momentum conversion and propagation between magnons in two YIG layers and conduction electrons in the Au layer. The temperature dependence of Magnon Valve Ratio (MVR=11% at room temperature) shows approximately a power law, supporting the above magnon-electron spin conversion mechanism. This work conceptually proves the possibility of using magnon valve structures to manipulate the magnon current in magnetic insulators, which has potential applications in magnon based devices.
Then, we designed and manufactured an all-insulating magnon junction with sandwich structure MI1/S/MI2 (S=AFI, antiferromagnetic insulator, such as YIG/NiO/YIG), in order to achieve pure magnon transport. The devices were made on magnetron sputtering system which is a technique used for industrial large-scale production. Necessarily, the transport and manipulating properties of magnon were investigated. When the temperature gradient was applied, the magnon current would flow from one MI to the other MI through the AFI. So the magnon current in any MI are easily influence by the other MI layer. Then setting a heavy metal Pt

on the top MI layer for detecting magnon, one could find an effect that the signal of ISHE is related to the magnetization structure of both MI layers, similar to the TMR effect in an MTJ. Furthermore, the magnon valve ratio in such magnon junctions can be increase to 100%. Hence, the electric-insulating magnon junctions can be used for developing magnon-based circuits, including non-Boolean logic, memory, diode, transistors, magnon waveguide and switches with sizable on-off ratio.

16:40-17:05 Invited (1390558)

A Novel Electric-Field-Assisted-Switching STT-MRAM Design for Sub-Nanosecond Low Energy Writing

Tai Min, Xi'an Jiaotong University, China

Magnetic Random Access Memory (STT-MRAM) is one of the next generation of new nonvolatile memory, which has the most industrial prospects and followed lots of new ideas. Recently, we found that under a small electric bias voltage induced by Ionic liquid gating, the synthetic anti-ferromagnetic multilayer system (FeCoB/Ru/FeCoB and $(Pt/Co)_2/Ru/(Co/Pt)_2$) can be changed from an antiferromagnetic coupling state to a ferromagnetic coupling state. Based on this phenomenon, we propose a new type of STT-MRAM with SAF free layer in which the critical write current can be reduced significantly. Micro magnetic simulation has been used to investigate the switching behavior and the magnetic dynamics of this SAF free layer design under the impact of the electric field, and found that the switching current density at sub-ns region can be reduced by three – six times of this design, making it a potential candidate to replace L1/2-SRAM at sub-10nm technology node. And to understand the physical origin of the abnormal phenomenon, a toy model has been proposed, in which, the external E-field controlled sign change of the RKKY interaction in SAF gives an extra contribution to rise up the total energy to help the spins climb over the barrier and breaking the processional switching mechanism.

17:05-17:30 Invited (1401197)

Microscopic Studies of Spin Dynamics with Combined Effect of Multidimensional Magnetic Field and Electric Current

Weisheng Zhao, Beihang University, China; Xueying Zhang, Beihang University, China; Anni Cao, Huaiwen Yang, Xiaoxuan Zhao, Vernier Nicolas, University Paris-Saclay, France

Spintronics devices play an important role in the era of information and intelligence by providing various solutions for data storage and computing. Studies on spin dynamics are interesting for the development of novel spintronic devices, for the characterization of properties of spintronic materials and for the understanding of underlying physics. In this talk, we present several recent research results on the spin dynamics under the combined effect of various stimulation conditions via a multifunctional Kerr microscope. First, using the coordinated work of fast magnetic field pulses and a permeant magnetic field, we have nucleated micron-size domain bubbles and directly observed the their spontaneous deflation induced by the effect of domain wall (DW) surface tension; Second, using the combined effect of in-plane and the perpendicular magnetic field, we are able to quantify the strength of Dzyaloshinskii-Moriya interactions in Pt/Co/MgO film by observing the asymmetrical expansion of magnetic bubble and find an effective method to tune the strength of DMI; Third, using the combined effect of perpendicular magnetic field and electrical current, we have observed the linear dependence of DW motion velocity on the current density in the Ta/CoFeB/MgO stripes; the effective spin-polarization of CoFeB is found to be as low as 0.26, which can explain the difficulty of DW motion induced by pure spin-transfer torque in this materials; Last, using the combined effect of in-planed magnetic field and electric current, we are able to observe the ultra-efficient spin-orbit toque induced magnetic switching in a W/CoFeB/MgO Hall bar structure, which is very beneficial for the development of novel SOT-based spintronic device.
We believe the above several research shows the importance of spin dynamics study with multiple test conditions. The research results are interesting for the development of novel spintronics devices based on the combined effect of various stimulations.

M: Renewable Energy Materials and Nuclear Materials: II

Symposium Organizers :

Min Zhu, South China University of Technology, China; Yuan Deng, Beihang University, China; Guanghong Lu, Beihang University, China; Tetsuya Uda, Kyoto University, Japan; Taek-Soo Kim, Korea Institute of Industrial Technology (KITECH), Korea; Dmitri Golberg, Queensland University of Technology, Australia; Assel Aitkaliyeva, University of Florida, USA

Tuesday AM
August 20, 2019

Room: 311(3rd Floor)
Symposium: M

Chairs:
Chenyang Lu, Xi'an Jiaotong University, China
Yuan Deng, Beihang University, China
Ying Chen, Deakin University, Australia
Shaojun Guo, Peking University, China

8:30-9:00 Keynote (1235346)

Solving Major Challenges in Lithium-Sulfur Batteries

Ying Chen, Deakin University, Australia

Lithium–sulphur (Li-S) batteries have a much higher energy density than Li ion batteries and thus are considered as next generation batteries. However, the problem of rapid capacity fading due to the shuttling of soluble polysulfides between electrodes remains main obstacle for practical applications. We use different approaches to decrease the charge transfer resistance and mitigate the shuttling problem. (ⅰ)The Li-S cells use a porous-CNT/S cathode coupled with a sulfur–nitrogen dual-doped graphene (SNGE) interlayer to benefit from excellent electric conductivity of SNGE and efficiently trapping LiPS ions. These cathodes exhibit ultrahigh cyclability when cycling at 8C for 1000 cycles, and a low capacity degradation rate of 0.01% per cycle. (ⅱ) A composite interlayer is built simply by coating the cathode surface with a functionalized boron nitride nanosheets (FBN). Using this thin and ultralight composite interlayer, the specific capacity and cycling stability of Li-S batteries are improved significantly with a life of over 1000 cycles, an initial specific capacity of 1100mAh·g^{-1} at 3C and a cycle decay as low as 0.0037% per cycle. (ⅲ) New separators are constructed by incorporation of FBN nanosheets with negative charged groups onto a commercial Celgard separator. The FBN separator is capable to prevent PSs migration through the separator effectively due to strong ion-repelling of negatively charged PSs by the negatively-charged FBN nanosheets. The Li-S cell with a FBN separator exhibits an excellent long-term cycling stability up to 2000 cycles and a high capacity of 585mAh·g^{-1} at a very high current of 10C (1.68A·g^{-1}). (ⅳ) For Li metal anodes, composite anodes are fabricated via melt infusion of lithium into graphene foams decorated by metal oxide nanoflake arrays, which successfully controls the formation and growth of Li dendrites, and alleviate volume change during cycling. A resulting Li-Mn/Graphene composite anode demonstrates a super long and stable lifetime for repeated Li plating/stripping of 800 cycles at 1mA cm^{-2} without voltage fluctuation, which is 8-fold longer the normal lifespan of a bare Li foil under the same conditions. (ⅴ) These huge improvements in the life time of the Li-S cells enable Li-S batteries to be used in electric vehicles and other large-scale electrochemical energy storage systems in near future.

9:00-9:25 Invited (1223818)

Stain-Controlled Energy Electrocatalysis on Multimetallic Nanomaterials

Shaojun Guo, Peking University, China

Proton exchange membrane fuel cells (PEMFCs) are generally expected to be the ideal alternative to traditional internal combustion engine as energy-supplying devices for transportation, which consumes nearly 25% of the global energy. However, to guarantee the wide-adoption of PEMFCs, it still requires an efficient electrocatalyst, with higher activity/stability and lower Pt usage than the state-of-the-art carbon supported platinum nanoparticles (Pt/C), towards the cathodic oxygen reduction reaction. But, the absence of low-platinum, high-activity and satisfied-durability electrocatalysts for oxygen reduction reaction has bottlenecked the wide-adoption of PEMFCs for decades. To address this challenge, an efficient strategy is to modify the electronic structure of Pt by alloying with other cheap transition metals (M), normally called ligand or electronic effect. Tuning or controlling the surface strain in multimetallic nanomaterials is a robust method to boost electrocatalytic performance, and tremendous progress has been made in this area in the past decade. In this talk, I will show recent important advances in how to tune the compressive and tensile strain in multimetallic nanocrystals to achieve more efficient energy conversion by electrocatalysis. I will start with the introduction of stain and the basic information on how to tune the strain for the electronic structure tuning. Then, I will give several examples on designing metal-based materials with interesting strain effects for boosting oxygen reduction and hydrogen evolution reaction catalysis. In particular, I will highlight our recent important results on making PtPb/Pt core/shell nanoplates with biaxial strain for boosting oxygen reduction catalysis, which exhibit much higher activity and stability for oxygen reduction catalysis. Furthermore, I will show that our strain tuning concept will be extended to other Pd-based and transition metal-based materials system for greatly enhancing oxygen reduction and hydrogen evolution catalysis. Finally, I will give the conclusion and perspective on the strain-tuned energy catalysis of different metal-based material system.

9:25-9:50 Invited (1296649)

High-Performance Thermoelectric Materials: Progress and Applications

Zhigang Chen, University of Southern Queensland, Australia

Thermoelectrics, enabling the interconversion between heat and electricity, become a typical component in the drive for eco-friendly energy technology. The mass-market application demands a high energy conversion efficiency, evaluated by the figure-of-merit (zT), which is proportional to power factor and reciprocal of lattice thermal conductivity. Besides, thermoelectric materials are supposed to be environmentally benign. GeTe is the competent choice to replace the highly toxic Pb-based alloys that are commonly used as mid-temperature thermoelectric materials. Recently, super-high zT over 2.0 for GeTe-based materials has been reported by several research groups. Particularly, our innovative contributions have significantly promoted the advance of high-performance GeTe (Adv. Mater. 2018, 30, 1705942 and Adv. Energy Mater. 2018, 8, 1702333).

Herein, we review the most recent research outcomes in GeTe-based thermoelectric materials. First, we summarize the features of GeTe (i.e., crystal structures, phase transition, multiple sub valence bands, and phonon dispersions), which endow diverse degrees of freedom to manipulate the thermoelectric properties for GeTe. Accordingly, the strategies for enhancing power factor are settled, including alignment of multiple valence bands, resonant distortion of density-of-states, and an increase of band degeneracy induced by slight symmetry reduction. To decrease thermal conductivity, we highlight the methods of strengthening intrinsic phonon-phonon interactions and introducing various lattice imperfections as scattering centers. Then, we overview the current GeTe-based thermoelectric devices, including the technical challenges and the solutions. In the end, we propose possible future directions for developing GeTe. The significance of this review can be summarized as: (i)The delivered information will bridge the communications among physicists, chemists, and engineers to further enhance the performance of GeTe and to facilitate the establishment of large-scale thermoelectric devices with high conversion efficiency. (ii)The achieved high thermoelectric performance in GeTe-based thermoelectric materials with the rationally developed strategies could serve as references for broader materials to pursue high performance.

9:50-10:10 (1222207)

Effect of Yttrium Contents on the Microstructure and Texture of a Hot Rolled Ferrite/Martensite12Cr-ODS Steel

Changhao Wang, Institute of Material, China Academy of Engineering Physics & School of Material Science and Engineering, Chongqing University of Technology, China; Qingzhi Yan, School of Material Science and Engineering, University of Sciences and Technology Beijing, China; Jinru Luo, Guomin Le, Institute of Material, China Academy of Engineering Physics, China; Jian Tu, Hong Ye, Zhonglin Yan, School of Material Science and Engineering, Chongqing University of Technology, China

Oxide dispersion strengthened (ODS) steel is one of the most important candidate structural material for the fuel cladding and fusion reactor cladding of the fourth generation nuclear reactor fission fast reactor for its excellent high temperature creep performance and radiation resistance, thus attract the attentions of many researchers and become a hot research topic nowadays. As a cladding tube material, hot deformation is the necessary manufactural process for the ODS steel. And the mechanical performance can be improved through hot deformation such as rolling or extrusion by means of microstructural optimization. Therefore, the understanding on the deformation and recrystallization mechanisms and the subsequent microstructural evolution of the material during hot deformation become very important for mechanical performance design and optimization. In the present study, a 12Cr-ODS ferrous alloy containing 0.3wt.% Y_2O_3 has been hot rolling to various strain levels at different temperature. The microstructure and texture of rolled samples has been characterized by optical microscope (OM), X-ray diffractometer (XRD) and a scanning electron microscope (SEM) equipped with electron back-scattered diffraction (EBSD) detector. The shape, size and distribution of the second phase particles were mainly examined by electron microscopes. The microstructural and textural evolutions of the ODS steel rolled to various strain at different temperature have been discussed with considering the effect of thermal activation and deformation energy on the dynamic recrystallization and phase transition of the matrix and the coarsening of the second phase particles. Microhardness has also been applied to estimate the mechanical performance of the deformed samples. The relationships between the microstructure the mechanical properties of the rolled samples have also been discussed in the present study by telling the effects of work hardening and grain refinement of the matrix grains and the density and particle size of the ODS phase.

10:30-10:45 Tea Break

10:45-11:10 Invited (1230121)

Enhancing Irradiation Tolerance in Single-Phase Concentrated Solid Solution Alloys by Tuning Chemical Complexity

Chenyang Lu, Xi'an Jiaotong University & University of Michigan, China; Fei Gao, Lumin Wang, University of Michigan, China.

Single-phase concentrated solid solution alloys (SP-CSAs), including high entropy alloys (HEAs) are a novel family of materials for studying defect dynamics without preexisting defect sinks. In contrast to conventional alloys, SP-CSAs are composed of two to five principal elements in equal or near-equal molar ratios that form random solid solutions in either a simple face-centered cubic (fcc) or simple body-centered cubic (bcc) crystal lattice structure. Significant suppression of void formation at elevated temperatures has been achieved with increasing compositional complexity in Ni-containing SP-CSAs. In our research, we demonstrated the modification of alloy complexity by increasing the number, the type and the concentration of alloying elements in SP-CSAs.

A group of SP-CSAs (Ni, NiCo, NiFe, NiCoFe, NiCoFeCr, NiCoFeCrMn) irradiated by Ni ions at 773K has been studied by cross-sectional transmission electron microscope (TEM). This study demonstrates the enhancement of radiation tolerance by showing two orders of magnitude of decrease on void swelling with increasing number of alloying elements. The controlling mechanism of defect movements was determined through detailed TEM characterization of defect clusters distributions and Molecular dynamics (MD) simulations. The enhanced swelling resistance is attributed to the tailored interstitial defect cluster motion in the alloys, from a long-range one-dimensional (1-D) mode to a short-range three-dimensional (3-D) mode, which leads to enhanced point defect recombination.

The effect of alloying elements on radiation-induced microstructural evolution has been studied in Ni and Ni-20*X* (*X*=Fe, Cr, Mn and Pd) binary alloys. The 3-D migration mode is identified to be the dominating migration mechanism for interstitial clusters in these binary alloys, contrary to the 1-D mode dominated in dilute alloys. It is found that the solute atomic volume size factor plays a key role in the migration and interaction of defect clusters. The total void swelling generally decreases as the atomic volume factor increases, accompanying with a significantly sluggish interstitial migration and smaller dislocation loop size.

The effects of elemental concentration on radiation tolerance in Ni-Fe alloys have been studied. Void swelling and dislocation loop evolution are both suppressed or delayed with increasing iron concentration. Furthermore, the dominating migration behavior of interstitial clusters shifted from 1-D to 3-D mode with increasing iron concentration. It has been demonstrated that the transition between 1-D and 3-D is a continuous process, and can be quantitatively characterized by the mean free path of the interstitial defect clusters.

This talk demonstrates the enhancement of radiation tolerance in SP-CSAs, and more importantly, reveals its controlling mechanism through a detailed analysis of microstructure characterizations and atomistic computer simulations.

11:10-11:30 (1219276)

Hydrogen Storage Properties of Nano-Crystalline Mg_2Ni Prepared from Compressed 2MgH2-Ni Powder

Khan Darvaish, Shanghai Jiaotong University, China

Limited fossil fuel, climate change and increasingly severe environmental pollution problems, clean energy have been given increasingly widespread attention. The use of clean renewable energy has become an inevitable trend. Hydrogen is a predominant candidate as a future energy carrier for sustainable development. For the wide application of hydrogen-powered fuel cell vehicles, it is of considerable importance to develop a feasible on-board hydrogen storage system. Nevertheless, safe and compact storage of hydrogen in a solid medium is the most demanding and challenging requirement for realizing a hydrogen economy as far as mobile and stationary applications are concerned. Generally, hydrogen can be stored in the form of high-pressure gas, cryogenic liquid, or chemically or physically bonded to a suitable solid-state material. For the safe solid state hydrogen storage, various studies have been carried out, however, Mg-based hydrides stand out due to their high gravimetric storage capacity (7.6wt% for MgH_2), low cost, environmental friendliness, and high natural abundance. Practical applications of Mg-hydrides for stationary or on-board energy sectors are limited due to slow hydrogen absorption kinetics, high thermal stability and very high reaction activity towards oxygen. The sluggish hydrogenation kinetics are due to slow dissociation rate of H_2 molecules on the Mg surface, the low hydrogen diffusion rate on the Mg because it extremely difficult after a MgH_2 layer forms on the surface of Mg because the H_2 diffusion coefficient in MgH_2 ($1.5 \times 10^{-16} m^2/s$) is considerably smaller than Mg ($4 \times 10^{-13} m^2/s$), and formation of Mg/MgH_2 oxides on the surface of Mg/MgH_2. The slow dehydrogenation kinetics is due to the strong bond between Mg and H, the low diffusion rate of H in MgH_2, the high energy required for the nucleation of Mg on the surface of MgH_2, and the combination of hydrogen atoms to form the H_2 molecule on the Mg surface. However, its high decomposition temperature (T>300˚C) is due to the strong ionic characteristics of the Mg-H bond.

We prepared nanocrystalline Mg_2Ni with an average size of 20~50nm was prepared via ball milling of a $2MgH_2$-Ni powder followed by compression under a pressure of 280MPa. The phase component, microstructure, and hydrogen sorption properties were characterized by using X-ray diffraction (XRD), scanning electron microscope (SEM), transmission electron microscope (TEM), pressure-composition-temperature (PCT) and synchronous thermal analyses (DSC/TG). Compared to the non-compressed $2MgH_2$-Ni powder, the compressed $2MgH_2$-Ni pellet shows lower dehydrogenation temperature (290˚C) and a single-

phase Mg_2Ni is obtained after hydrogen desorption. PCT measurements show that the nanocrystalline Mg_2Ni obtained from dehydrogenated $2MgH_2$-Ni pellet has a single step hydrogen absorption and desorption with fairly low absorption (-57.47kJ/mol H_2) and desorption (61.26kJ/mol H_2) enthalpies. It has very fast hydrogen absorption kinetics at 375˚C with about 3.44wt.% hydrogen absorbed in less than 5min. The results gathered in this study show that ball milling followed by compression is an efficient method to produce Mg-based ternary hydrides.

11:30-11:50 (1235446)

Nanoconfinement of Mg by Ultrathin Carbon Layer with Enhanced Hydrogen Storage Properties

Tong Liu, Xiubo Xie, Ming Chen, Miaomiao Hu, Beihang University, China

A facile way has been developed to fabricate ultrathin carbon layer encapsulated air-stable Mg nanoparticles (Mg@C NPs) by methane plasma metal reaction method. Compared with pure Mg NPs, the nanoconfinement of Mg by carbon layer can not only reduce particle size but also prevent Mg from oxidation. By adjust methane from 10 to 300ml, average size of Mg@C NPs reduces from 140 to 60nm and thickness of carbon layer increases from 1 to 4nm. After exposure in air for 3 months, little MgO can be detected in Mg@C NPs. In these Mg@C samples, Mg@C (CH4:50ml) with size of 80nm and ultrathin amorphous carbon shell of 3nm shows the highest hydrogen capacity of 6.3wt% H_2. In comparison, the hydrogen capacities of Mg@C (CH4:10ml) and Mg@C (CH4:300ml) are only 5.4wt% H_2 and 4.3wt% H_2, respectively. Mg@C (CH4:50ml) also displays the highest hydrogenation and dehydrogenation rates which can absorb 4.8wt% H_2 within 10min at 573K and desorb 5.0wt% H_2 within 20min at 623K. The apparent energies for hydrogenation and dehydrogenation of Mg@C (CH4:50ml) are 64.1 and 107.2kJ·mol^{-1}, both smaller than Mg@C (CH4:10ml) of 66.7 and 118.9kJ·mol^{-1} and Mg@C (CH4:300ml) of 67.7 and 137.8kJ·mol^{-1}. The enhanced hydrogen storage properties of Mg@C (CH4 : 50ml) are attributed to smaller particles size and excellent antioxidant properties provided by the ultrathin carbon layer.

M: Renewable Energy Materials and Nuclear Materials: III

Symposium Organizers :

Min Zhu, South China University of Technology, China; Yuan Deng, Beihang University, China; Guanghong Lu, Beihang University, China; Tetsuya Uda, Kyoto University, Japan; Taek-Soo Kim, Korea Institute of Industrial Technology (KITECH), Korea; Dmitri Golberg, Queensland University of Technology, Australia; Assel Aitkaliyeva, University of Florida, USA

Tuesday PM
August 20, 2019

Room: 311(3rd Floor)
Symposium: M

Chairs:
Hongbo Zhou, Beihang University, China
Guanghong Lu, Beihang University, China
JongHyeon Lee, Chungnam National University, Korea
Jing Tang, University of Queensland, Australia

13:30-14:00 Keynote (1233927)

Alternative Ways of Producing Group IV Metals Through a Liquid Copper-Aided Direct Reduction Process of Oxide Feedstocks

JongHyeon Lee, Department of Materials Science and Engineering, Chungnam National University, Korea; Sukcheol Kwon, Vladislav Ri, Wan-Bae Kim, Hwa-Young Woo, Gyu-Seok Lim, HanSik Ryu, Woo-Seok Choi, Department of Materials Science and Engineering, Chungnam National University; Korea; Hayk Nersisyan, Rapidly Solidified Materials Research Center, Chungnam National University, Korea; Young Jun Lee. ZIRON TECH., Co., Ltd., Korea

Direct reduction could significantly simplify the isolation of group IV transition metals from their corresponding oxides (for example TiO_2, ZrO_2, and HfO_2). These metals are typically produced by the Kroll process, but the multiple stages, especially the chlorination step, reduces the effectiveness of the extraction, and increases the cost of the final product and the environmental impact. The main problem of conventional direct reduction of the group IV metal oxide is the higher impurity level than industrial standards, especially gas impurities due to their high oxygen and nitrogen affinities. Here, we report a metal production technology that lowers the oxygen content of Zr to meet the requirements for nuclear-grade metal.
In the first step, Zr-Cu alloy ingots were prepared from a Hf- free ZrO_2 precursor in a molten $CaCl_2$ medium by CaCu reducing agent. The CuZr alloy was further purified by a molten salt electrorefining process to recover pure nuclear-grade Zr in a LiF-Ba_2ZrF_8-based molten salt, the latter of which was fabricated from a waste pickling acid of a Zr clad tube. The purity of the recovered metal satisfied the ASTM B349 specifications for nuclear-grade Zr.
Also, this technology was successfully applied to the preparation of group IV transition metals such as Ti and Hf.

14:00-14:25 Invited (1449109)

Novel Porous Carbon Produced by Elaborately Design of Metal-Organic Frameworks

Jing Tang, University of Queensland, Australia

Thermoelectrics, enabling the interconversion between heat and electricity, become a typical component in the drive for eco-friendly energy technology. The mass-market application demands a high energy conversion efficiency, evaluated by the figure-of-merit (zT), which is proportional to power factor and reciprocal of lattice thermal conductivity. Besides, thermoelectric materials are supposed to be environmentally benign. GeTe is the competent choice to replace the highly toxic Pb-based alloys that are commonly used as mid-temperature thermoelectric materials. Recently, super-high zT over 2.0 for GeTe-based materials has been reported by several research groups. Particularly, our innovative contributions have significantly promoted the advance of high-performance GeTe (Adv. Mater. 2018, 30, 1705942 and Adv. Energy Mater. 2018, 8, 1702333).
Herein, we review the most recent research outcomes in GeTe-based thermoelectric materials. First, we summarize the features of GeTe (i.e., crystal structures, phase transition, multiple sub valence bands, and phonon dispersions), which endow diverse degrees of freedom to manipulate the thermoelectric properties for GeTe. Accordingly, the strategies for enhancing power factor are settled, including alignment of multiple valence bands, resonant distortion of density-of-states, and an increase of band degeneracy induced by slight symmetry reduction. To decrease thermal conductivity, we highlight the methods of strengthening intrinsic phonon-phonon interactions and introducing various lattice imperfections as scattering centers. Then, we overview the current GeTe-based thermoelectric devices, including the technical challenges and the solutions. In the end, we propose possible future directions for developing GeTe.
The significance of this review can be summarized as: (i)The delivered information will bridge the communications among physicists, chemists, and engineers to further enhance the performance of GeTe and to facilitate the establishment of large-scale thermoelectric devices with high conversion efficiency. (ii)The achieved high thermoelectric performance in GeTe-based thermoelectric materials with the rationally developed strategies could serve as references for broader materials to pursue high performance.

14:25-14:45 (1431756)

Non-Destructive Nanoscale 3D Characterization of Energy Materials

Stephen Kelly, Carl Zeiss Microscopy, USA

14:45-15:05 (1235468)

Scale-Up Development of High-Performance Dielectric Films for Compact Capacitors

Daniel Tan, Guangdong Technion Israel Institute of Technology, China

Technology migration from research labs to commercial products has never been easy, which is especially true for transitioning a dielectric material to a compact capacitor that finds great promise in power electronics. This type of transition involves the development of high-performance materials and film processes as well as the scalability of films. The film scale-up processes along with the subsequent metallization and capacitor winding processes are crucial to the fabrication of a reliable capacitor component. A dozen programs were established in the past 10 years for addressing the polymer film requirements for high temperature, high energy density and compactness. Thickness is the third physical parameter in addition to the dielectric constant and the dielectric strength, that provides a satisfactory alternative pathway for the realization of a high-performance compact capacitor. It was found that every micron of film thickness reduction requires substantial technical efforts and cross-disciplinary coordination in the scale-up process. An overview of the developmental efforts on the dielectric materials and polymer films will be provided in this presentation. Several important attempts on scaling up dielectric films and capacitors recently supported by the US government and industry are described. The author’ s scale-up efforts for high temperature polyetherimide films of various thicknesses via the melt extrusion process are illustrated. The successful demonstration of wrinkle-free PEI films in the thickness range of 4 to 10 microns in a commercial-scale is presented.

15:30-16:10 Tea Break

16:10-16:35 Invited (1233605)

Towards Understanding the Influence of Re on H Dissolution and Retention in W by Investigating the Interaction between Dispersed/Aggregated-Re and H

Hongbo Zhou, Fangfei Ma, Fangya Yue, Yuhao Li, Guanghong Lu, Beihang University, China.

Tungsten (W) and W alloys are considered as the most promising candidates for plasma facing materials (PFMs) in future fusion reactors. Rhenium (Re) is not only the typical alloying element but also the main production of transmutation in W-PFMs. The microstructure and mechanical properties of W as well as the behaviors of impurities in W will be influenced by the presence of Re. The deuterium retention in damaged W-3%Re at 750K is two of magnitude lower than that in damaged Re-free W. Therefore, one can expect that Re should have significant effect on the behavior of H isotopes in W. However, little work has focused on this aspect so far. Here, we have systematically investigated the effects of dispersed/aggregated Re on the behaviors of H in W as well as their interaction with point defects using a first-principles method in combination with thermodynamic models. It has been demonstrated that the influence of Re on H is strongly related to the distribution of Re in W. Re will aggregate and form clusters/ Re-rich precipitation phases under high energy ions/neutrons irradiation in W. The influence of Re clusters on H is extraordinary stronger than that of a single Re. The retention of H in W can be significantly suppressed by Re clusters, and their influences will be enhanced with the increasing of the number of Re atoms. On the contrary, it is found that the solution energy of H at most interstitial sites (> 80%) in W-Re sigma phase is much lower than that in pure W. Specifically, the H solution energy at most stable interstitial site in W-Re σ phase is only 0.47eV, ~ 54%lower than that in pure W. This can be attributed to that W-Re sigma phase provides the larger available volume for interstitial H than the pure W, weakening the W-H repulsive interaction. Consequently, our calculations reveal that the Re-rich precipitation can serve as the strong trapping centers for H in W, while dispersed-Re/small Re clusters can be used to suppress H retention. These results provide an important reference to evaluate the influence of Re and other alloying elements on the behaviors of H isotopes in W-PFMs under future fusion conditions.

16:35-16:55 (1232653)

The Recovery of Europium (II) Sulfate as Product of Recycling Waste Fluorescent Lamp Powder

Brajendra Mishra, Mark Strauss, Worcester Polytechnic Institute, United States

Europium is a required element for high technology application such as LEDs, cell phone screens, and laptop displays. The unique chemical properties of europium make it invaluable to these applications. This research shows a process to recovery europium (II) sulfate from waste lamp phosphors to create novel supply of europium. In this process, waste phosphor powder is chemically and physically beneficiated to produce yttrium and europium oxide concentrate. Next, europium (II) sulfate is separated from yttrium by selectively reducing Eu(III) to Eu(II) using zinc powder and precipitating it with sulfuric acid. Cursory experiments were performed to see the effect of pulp density, precipitation time, entrance pH, and stoichiometric ratio of europium to sulfate upon the grade and recovery of europium (II) sulfate. The ideal conditions to maximize grade and recovery of europium (II) sulfate were a 1 hour precipitation time, 10x the stoichiometric ratio of sulfate, 100g/L mixed REO, and the entrance pH equal to 3. The maximum grade of europium sulfate was 93%, and the maximum

recovery was 78%. As a by-product of this separation process, yttrium is recovered by a precipitation step under controlled conditions of pH, temperature and organic to oxide ratio. Both Europium and Yttrium can be recycled into new phosphor production.

16:55-17:15 (1233252)

Thermoelectric Properties of Ag8SiSe6 Argyrodite Near Room Temperature Prepared with Different Quenching Conditions

Qinghui Jiang, Suwei Li, Junyou Yang, Jiwu Xin, Sihui Li, School of Materials Science and Engineering, Huazhong University of Science and Technology, China; Haixue Yan, School of Engineering and Materials Science, Queen Mary University of London, England

Argyrodite compounds, as promosing green thermoelectrics, received much attentations for their much low lattice themal conductivity which may be from low sound velocity, complex crystal structure, liquid-like ions, and lattice anharmonicity. There is a phase transition near 400K for Ag_8SiSe_6, a typical argyrodite compounds. At higher temperature, Ag_8SiSe_6 is face-center-cubic structure, where Ag^+ cations are fully disordered in $[SiSe_6]^{8-}$ anion sublattice which is composed of Se^{2-} anions and $[SiSe_4]^{4-}$ units. At lower temperature, Ag+ cations are localized partially, which leads to the decrease of the electrical conductivity and the increase of Seebeck coefficients. In this work, we first successfully fabricated Ag_8SiSe_6 alloys based thermoelectric bulks with high density (>95%). The processes include melting, annealing, milling and hot press sintering. We discussed the details of the effect of the parameters of these precesses on the phases and crystal structures. By controlling the cooling rates of the ingots, a remarkable improvement of power factor has been achieved in the sample quenched in water owing to the significant reduction in resistivity. In addition, a large amount of nano-precipitated particles and the typical cladding structure confirmed by microstructure analysis may be responsible for the lower resistivity. The Seebeck coefficient, electric conductivity and thermal conductivity at different temperatures are also discussed in details. Its maximum ZT is over 0.7 near room temperature, which makes Ag-Si-Se alloys as a n-type thermoelectric material have a great commercial application instead of Bi_2Te_3 compounds in future.

17:15-17:35 (1235808)

Local Burnup Determination of Irradiated Fuel Using Atom Probe Tomography

Jian Gan, Mukesh Bahhav, Dennis Keiser, Jeffrey Giglio, Idaho National Laboratory, USA; Daniel Jadernas, Studsvik Nuclear AB, Nykoping, Sweden; Ann Leenaers, Sven Van de Berghe, SCK-CEN, Nuclear Materials Science Institute, Belgium

A novel approach is presented to determine the local U-235 burnup in irradiated fuels using isotopic quantification information obtained by Atom Probe Tomography (APT). Knowledge on burnup levels, composition along with distribution of isotopes and 3-D microstructural data of irradiated fuels is essential for nuclear fuel research and development. The microstructural evolution, radioactivity and the physical integrity of the irradiated fuel depend on burnup levels and thus its determination is critical to evaluate fuel performance. In this work, APT is used to quantify the isotopes of U-235, U-236, U-238, Pu-239 and Np-237 for burnup calculation in the irradiated U-7Mo dispersion fuel. This method provides local burnup analysis in the fraction of U-235 fissioned with unprecedented high spatial resolution based on isotopic ratios measured from as-received and irradiated fuels. APT analysis can also be applied to check uranium enrichment and its uniformity for fresh fuel for quality control of fuel fabrication, and the local fission product details in the irradiated fuel. This technique, combined with microstructural characterization using transmission electron microscopy, will help better correlating the local microstructural development with local burnup level. The capability of measuring local burnup is important for advanced characterization of irradiated fuels due to highly heterogeneous microstructure and technical challenges of in-pile irradiation test and post-irradiation examination of nuclear fuels.

M. Renewable Energy Materials and Nuclear Materials: IV

Symposium Organizers :

Min Zhu, South China University of Technology, China; Yuan Deng, Beihang University, China; Guanghong Lu, Beihang University, China; Tetsuya Uda, Kyoto University, Japan; Taek-Soo Kim, Korea Institute of Industrial Technology (KITECH), Korea; Dmitri Golberg, Queensland University of Technology, Australia; Assel Aitkaliyeva, University of Florida, USA

Wednesday AM
August 21, 2019

Room: 311(3rd Floor)
Symposium: M

Chairs:
Renzong Hu, South China University of Technology, China
Xiaoqiu Ye, China Academy of Engineering Physics, China
Tiejun Zhu, Zhejiang University, China
James Stubbins, University of Illinois at Urbana-Champaign, United States

8:30-9:00 Keynote (1228339)

Defective Half-Heusler Thermoelectric Compounds

Tiejun Zhu, Zhejiang University, China

Typical 18-electron half-Heusler (HH) compounds, ZrNiSn and NbFeSb, have been identified as promising high temperature thermoelectric materials. NbCoSb with nominal 19 valence electrons, which is supposed to be metallic, has recently been reported to also exhibit thermoelectric properties of a heavily doped n-type semiconductor. In this talk we experimentally demonstrate that the nominal 19-electron NbCoSb is actually the composite of 18-electron Nb0.8CoSb and impurity phases. Single phase Nb0.8CoSb with intrinsic Nb vacancies possesses improved thermoelectric performance. The similar phenomenon has also been observed in some of other defective 19-electron HH compounds. They all display abnormally low thermal conductivity compared to the normal 18-electron HH. TEM observation indicates a complex and interesting crystal structure, in which the short-range order of vacancies coexists with long range atomic order. This new finding provides important insights into the intrinsic nature of defective HH compounds.

9:00-9:25 Invited (1222513)

Development of Austenitic Oxide Dispersion Strengthened Alloys for Nuclear Applications

Yinbin Miao, Materials Scientist, Chemical and Fuel Cycle Technologies Division, Argonne National Lab, Lemont, USA; Xiang Chen, Research Associate, Advanced Post-Irradiation Examination Department, Idaho National Lab, Idaho Falls, USA; James Stubbins, Donald Biggar Willett Professor, Department of Nuclear, Plasma and Radiological Engineering, University of Illinois at Urbana-Champaign, Urbana, USA

There has been a continuing effort to develop enhanced versions of several types of engineering alloys by strengthening them with a very high number density of very small oxide particles. Most of the recent work has concentrated on ferritic / martensitic ODS alloy development and performance. It is clear that the addition of a fine distribution of nano-oxide dispersoids will provide major improvements in material strength especially at very high temperatures and extend the application temperature range to levels appropriate for advanced nuclear systems. Since the oxide particles are actually ceramics, they should maintain their stability and strengthening capabilities even at very high temperatures. For nuclear applications where atomic displacement damage takes place, the particles also offer a very large amount of internal surface area which can potentially absorb irradiation-induced defects to reduce radiation damage effects.
This process of making metal alloys with dispersed oxide particles has been attempted in a wide variety of metal systems with some success. The current heavy emphasis on developing ODS F/M steels has resulted in a nearly negligible interest in the development of ODS stainless steels. This talk will discuss the possibilities for the development of ODS austenitic steels. Since austenitic stainless steels are currently used for a wide variety of applications in current nuclear reactors and are slated for use in a number of advanced nuclear fission and nuclear fusion reactor systems, the development of ODS austenitic alloys should be of considerable interest. The research work discusses the oxide dispersoid microstructure and mechanical behavior of this class of new alloys for nuclear applications. The talk will also cover recent results on the irradiation behavior of ODS particles and other microstructural features in the ferritic alloys.

9:25-9:50 Invited (1222612)

In-Situ Investigation of Hydrogen Induced Corrosion of Titanium

Xiaoqiu Ye, Xuefeng Wang, Jiliang Wu, Changan Chen, China Academy of Engineering Physics, China

Titanium(Ti) and its alloys have many industrial applications thanks to their excellent corrosion resistance and high specific strength. However, they are potentially susceptible to hydrogen-induced cracking as a consequence of hydrogen absorption. To ensure long term use, a predictive model of hydriding behaviour is desirable and requires detailed understanding. Unlike widely studied thermodynamic properties of the titanium-hydrogen systems, in-situ investigation of hydrogen

induced corrosion of titanium was carried out in the present work by pressure-volume-temperature (PVT) method and hot-stage microscope (HSM) technique. The results show that hydrogen absorption rate of Ti foil at room temperature is very slow, no more than 0.2 H/Ti ratio for 1h. However, when the temperature increasing to 550˚C , the hydrogen absorption rate increased abruptly, with the morphology of Ti foil changing surprisingly: cracks firstly formed on the edge of the sample, and then progresses to the centre part. Thermal stabilities of the surface passivation layers on Ti foil under UHV were investigated using X-ray Photoelectron Spectroscopy (XPS). XPS results show that the C, N and O species on the surface of Ti reduce significantly or even disappear when heated to 700˚C in ultra-high vacuum condition(UHV), thus inducing an appearance of "active" surface with clean metal; while heated to lower than 300˚C the oxygen content on the surface will further increase and the corresponding carbides or nitrides are formed. Among these species, TiO and TiN decompose at 600˚C due to the underlying metal, while TiC decompose at 700˚C . The active surfaces of Ti obtained at 700˚C can be contaminated by oxygen again when cooled down to room temperature in the UHV. The active surface of Ti with clean metal can also be obtained by Ar ion gun sputtering at room temperature. Possible mechanisms of hydrogen induced corrosion of Ti during heating was discussed.

9:50-10:10 (1235239)

The Effect of Location on the Microstructure and Mechanical Properties of Wire Arc Additively Manufactured Nuclear Grade Steel

Chuang Gao, Chuanchu Su, Xizhang Chen, School of Mechanical and Electrical Engineering, Wenzhou University, China; Xiao Chen, School of Mechanical and Electrical Engineering, Wenzhou University & School of Materials Science and Engineering, Liaocheng University, China

The Wire and arc additive manufacturing (WAAM) is a promising process for the fabrication of complex and larger size 9Cr ferritic/martensitic nuclear grade steel components, which are used in the power industries/ nuclear reactor due to good high-temperature performance and excellent corrosion resistance. For this new study, using cold metal transfer (CMT) welding as heat source, 9Cr ferritic/martensitic nuclear grade steel is fabricated by the WAAM technology for the first time. This paper investigated the microstructure and mechanical properties of the additively manufactured 9Cr ferritic/ martensitic component in the different locations. The microstructure mainly consists of untempered martensite. As the height of the deposited wall increases, the microstructures exhibit differences. Positions at different heights have no significant influence on micro hardness and tensile testing results. However, the tensile properties and impact toughness of samples show anisotropy both perpendicular to the build direction and parallel to the build direction. The microstructure variation, defects, the differences of mechanical properties and fracture behavior of samples are also analyzed carefully. The obtained experimental results show that although there are still some shortcomings, it is feasible that using the new additive manufacturing process fabricates 9Cr ferritic/martensitic steel component.

10:10-10:30 (1233354)

Aqueous Asymmetric Supercapacitors Based on Conducting Polymers

Jinzhang Liu, Yi Zhao, Beihang University, China

Supercapacitors are distinguished from ionic batteries for their high power density, yet their drawback is the low energy density, which is about one order of magnitude lower than that of Li-ion battery. The voltage window of a supercapacitor is an important issue determing the energy density. Hence the asymmetric design by using two dissimilar materials as the negative and the positive electrodes, respectively, has received much attention. We have been focusing on redox-active organic molecules, which can be exploited to make supercapacitor electrodes with strong pseudocapacitance. Amino-contained aromatic molecules are electropolymerized and combined with porous activated carbon to make asymmetric supercapacitors with both high specific capacitance and wide voltage window, thus achieving high energy densities. In particular, the electrodeposited poly(diaminonaphthalene) used as the negative electrode shows excellent cycling stability, with a capacitance retention of 103% over 10000 cycles. We studied several newly-syntghesized conducting polymers as the positive electrodes, and performances of different asymmetric cells are investigated. High energy densities up to 55Wh/ kg are achieved. To demonstrate the practical application, several cells in series are used to power LEDs or a mini electric fan.

10:30-10:45 Tea Break

10:45-11:10 Invited (1225650)

Advanced Sn-Based Anode Materials for Li Storage

Renzong Hu, Min Zhu, South China University of Technology, China

The energy density of LIBs is mainly determined by the voltage difference (V) between the cathode and anode, and in particular, the specific capacity (mAh $\cdot g^{-1}$ or mAh$\cdot L^{-1}$) of the electrode materials in suitable potential window. Thus, intense efforts have been devoted to developing high-voltage cathode materials and exploring new high-capacity anode materials to replace the commercial graphite anode that has a low theoretical specific capacity of 372mAh$\cdot g^{-1}$.

The application of a ternary Sn-based alloy (Sn-Co-C) anode has contributed an 30% increase in capacity, and 20% increase in volumetric energy density in Sony's Nexelion battery which introduced firstly in 2005 and then updated in 2011. The reversible specific capacity of the Sn-Co-C ternary anode was around 600mAh·g^{-1} , which could be further increased when the Sn (with theoretical capcity of 994mAh·g^{-1}) is replaced with SnO_2 (1494mAh·g^{-1}). Thus we designed a series ternay SnO_2-M-graphite (M: transition metal, Fe, Co, Mn, Cu, etc) composite. However, two major challenges must be faced for the realization of the full capacity of SnO_2-based anodes. The first one is capacity fading and the short lifetimes induced by large volume changes and particle aggregation upon continued lithiation/delithiation. The second one is the unsatisfactory initial Coulombic efficiency and large irreversible capacity loss, which has to be minimized because it is detrimental to the potential energy density and the cost of LIBs.

In this work, we demonstrate that the nanosize transition metal Mn additives inhibit Sn coarsensing in lithiated SnO_2, resulting in fast interdiffusion kinetics of interdiffusion between Sn and O in the Sn/Li_2O interfaces and thus enabling highly reversible conversion, superior round-trip efficiency, large capacity and long lifetime. We hope that this new ternary SnO_2-based composite could be an alternate high capacity anode material for the current ternary Sn-based alloy anode.

11:10-11:30 (1234166)

Keys for Radiation Tolerance of ODS Steels for Advanced Nuclear Systems

Akihiko Kimura, Peng Song, Jim Gao, Yenjui Huang, Kiyohiro Yabuuchi, Yuuki Yamasaki, Daniel G. Morrall, Kyoto University, Japan; Takanari Okuda, KOBELCO, Japan; Naoko Oono, Hokkaido University, Japan; Yoosung Ha, JAEA, Japan; Peng Dou, Chongqing University, China; Sanghoon Noh, KAERI, Japan

Materials development is essential for realization of advanced nuclear systems where radiation tolerance is demanded for the structural materials to keep their performance during a long term operation. Among the several candidate structural materials of the nuclear systems, oxide dispersion strengthened (ODS) steels, which consist of nano-scaled oxide particles in a high number density and sub-micron sized grains, have been considered to be promising for advanced nuclear systems.

There are several sorts of ODS steels with different Cr contents: (9-12)Cr-ODS ferritic/martensitic steels and (14-16)Cr-ODS ferritic steels with and without Al addition. The former group of ODS steels were developed for applications to sodium cooled fast reactors and fusion reactors, and the latter of ODS steels were for so-called Generation IV nuclear systems. More recently, accident tolerant fuel R&D is progressing to apply high Cr/high Al ferritic ODS steels to fuel cladding of light water reactors because of "Fukushima Incident". It has been considered that the replacement of zirconium alloys cladding with high-performance ferritic steel one may retard the hydrogen generation at a severer accident of nuclear reactors, resulting in a large time lag up to hydrogen explosion.

In this presentation, radiation tolerance mechanisms of ODS steels are introduced in terms of trapping capacity and dislocation sources. Oxides trap radiation defects at the interfaces of nano-scaled ultra-fine oxide particles and matrix and at grain boundaries of sab-micron sized grains. The tolerance to void swelling and He-embrittlement may owe it to this mechanism. As for no loss of elongation mechanism, the suppression of localized deformation can be considered to work as a mechanism, where sub-micron sized grains supply a large number of dislocation sources at grain boundaries as triple points. This mechanism may be workable in most of the cases where embrittlement is accompanied by hardening, like irradiation embrittlement and aging embrittlement.

11:30-11:50 (1249963)

Flexible and Self-Supported Sulfur Cathode for High-Energy-Density Lithium-Sulfur Batteries

Jun Liu, South China University of Technology, China

Lithium–sulfur (Li-S) batteries have attracted much attention in the field of electrochemical energy storage due to their high energy density and low cost. However, the 'shuttle effect' of sulfur cathode, resulting in the poor cyclic performance of batteries, is a big barrier for the development of Li-S batteries. It is critical to design and synthesize novel materials as the sulfur cathode host for Li-S batteries which has high electrical conductivity, large sulfur loading and strong absorb interactions of polysulfides to prevent the 'shuttle effect'. Self-supported nanoarrays with hierarchical voids and rich reaction sites are promising for advanced electrodes of high-performance Li-S batteries. Herein, we have designed a novel sulfur cathode of integrating sulfur, flexible carbon cloth, and metal-organic framework (MOF)-derived N-doped carbon nanoarrays with embedded CoP. These unique flexible nanoarrays with embedded polar CoP nanoparticles not only offer the enough voids for volume expansion to maintain the structural stability during the electrochemical process, but also promote the physical encapsulation and chemical entrapment for all sulfur species. Such designed CC@CoP/C cathodes possess high sulfur loadings (as high as 4.17mg/cm^{-2}) and exhibit large specific capacities at different C-rates. Specially, an outstanding long-term cycling performance could be reached. For example, an ultra-low decay of 0.016% per cycle during the whole 600 cycles at a high current density of 2C is displayed. The current work provides a promising design direction for high-energy-

density Li-S batteries.