

M. Renewable Energy Materials and Nuclear Materials: I

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

Monday PM Room: 311(3rd Floor)
August 19, 2019 Symposium: M

Chairs:

Min Zhu, South China University of Technology, China
James Stubbins, University of Illinois at Urbana-Champaign, United States

13:30-14:00 Keynote (1236362)

Construction of Superlattice-Like Sandwich Structures from 2D Oxide and Hydroxide Nanosheets towards Superior Energy Storage and Conversion

Takayoshi Sasaki, National Institute for Materials Science, Japan

We have developed a variety of transition metal oxide and hydroxide nanosheets via delamination of precursor layered compounds into single layers. The resulting colloidal nanosheets are molecularly thin 2D nanocrystals, extending laterally up to several tens micrometers. Because of their highly redox activity and large surface area, they are promising as a building block for electrode materials and catalysts. One drawback to be overcome is their poorly conducting nature. We combined these oxide and hydroxide nanosheets with graphene oxide (GO) or its reduced form (rGO) into heteroassembled superlattice-like materials through solution-based processes based on electrostatic self assembly.

The oxide nanosheets as well as GO and rGO are negatively charged while hydroxide sheets are positively charged. We can turn their charge by modifying their surface with an appropriate polyelectrolyte, keeping the monodisperse nature. Then such oppositely charged nanosheets were mixed, spontaneously producing bulk-scale flocculates of unique superlattice-like sandwich structures where oxide or hydroxide nanosheets and GO or rGO are alternately stacked at molecular level. We showed that such heteroassembled lamellar composites exhibited superior performance in electrochemical charging/discharging and water electrolysis, showing promise for applications in supercapacitors, Li or Na ion batteries and electrocatalysts.

14:00-14:25 Invited (1217009)

Role of Irradiation and Weld-Induced Post-Irradiation Annealing on Deformation Mechanisms in 304L Stainless Steel

Wharry Janelle, Purdue University, USA; Keyou Mao, Purdue University & Idaho National Laboratory, United States; Cheng Sun, Idaho National Laboratory; Freyer Paula, Westinghouse Electric Company, LLC; Garner Frank, Texas A&M University, USA

This presentation will describe recent advancements in micro-mechanical testing that inform how deformation mechanisms in 304L stainless steels (SS) are affected by the presence of irradiation-induced defects. Austenitic 304L SS is one of the most widely utilized structural alloys in nuclear energy systems, but the role of irradiation on its underlying mechanisms of mechanical deformation remains relatively poorly understood. Now, recent advancement of micro-scale mechanical testing in a scanning electron microscope (SEM), coupled with site-specific transmission electron microscopy (TEM), enables us to precisely determine deformation mechanisms as a function of plastic strain and grain orientation.

We focus on AISI 304L stainless steel irradiated in EBR-II to 20 displacements per atom (dpa) at 415°C, and contain ~3 atomic parts per million (appm) He amounting to 1.5% swelling. A portion of the specimen is laser welded in-hot cell; the laser weld heat affected zone is studied and considered to have undergone post-irradiation annealing (PIA). An archival, virgin specimen is also studied as a control. We conduct nanoindentation testing, then subsequently prepare TEM lamellae from the plastic zone of the nanoindents using site-specific focused ion beam (FIB) milling. TEM investigation reveals nucleation of deformation-induced α' martensite in the irradiated specimen, and metastable ϵ martensite in the PIA specimen. Meanwhile, the unirradiated control specimen exhibits evidence only of dislocation slip; this is unsurprising given that alternative deformation mechanisms such as twinning and martensitic transformation are typically observed only near cryogenic temperatures in austenitic SS. Surface area of irradiation-produced voids contribute sufficient free energy to accommodate the martensitic transformation. The lower population of voids in the PIA material enables ϵ martensite formation, while the higher void number density in the irradiated material causes α' martensite formation. SEM-based micropillar compression tests confirm nanoindentation results. Irradiation damage could enable fundamental, mechanistic studies of deformation mechanisms that are typically only accessible at extremely low temperatures.

14:25-14:50 Invited (1293263)

High-Density Uranium Silicide Fuels – Radiation Response and Oxidation Resistance

Jie Lian, Rensselaer Polytechnic Institute, USA





U_3Si_2 is being considered as a leading form of the accident tolerant fuels for light water reactors due to its excellent thermal conductivity and higher fissile element density. In this talk, the microstructure evolution and radiation response of U_3Si_2 under extensive ion beam irradiation are summarized with the focus on radiation-induced amorphization, grain subdivision, and grain growth. U_3Si_2 is sensitive to ion beam radiation-induced amorphization at room temperature. Above a critical temperature, U_3Si_2 is highly resistant against amorphization, and radiation-induced polygonization and grain subdivision occur. Isothermal annealing was performed on pre-amorphized U_3Si_2 , leading to the formation of high-density nano-sized silicide. The critical doses for radiation-induced amorphization and grain subdivision and the kinetics of the grain coarsening are determined, providing experimental data for the development and validation of the MARMOT fuel performance models.

In addition, U_3Si_2 is prone to oxidation at low temperatures under synthetic air and steam conditions. Innovative fuel design and fabrication are required for the development of the high-density silicide fuels with enhanced oxidation and water corrosion resistance. Monolithic and composite U_3Si_2 fuels with sintering additives are fabricated by spark plasma sintering (SPS), and the microstructure and phase behavior of the SPS-densified silicide fuels are characterized and correlated with the sintering process. Dynamic oxidation and mechanical tests of the densified fuels are also performed and compared with the silicide fuels fabricated by conventional sintering. The concepts of using chemical doping and sintering additives for developing U_3Si_2 fuels with enhanced oxidation and corrosion resistance are also highlighted.

14:50-15:10 (1221029)

Dehydration-Hydration Behaviors of Lanthanum Compounds as Potential Thermochemical Heat Storage Materials

Naoyuki Hatada, Kunihiro Shizume, Kazuaki Toyoura, Tetsuya Uda, Kyoto University, Japan

Thermal energy storage based on chemical reactions (thermochemical heat storage) is a prospective technology for the reduction of fossil-fuel consumption by storing and using waste heat. For widespread application, a critical challenge is to find appropriate reversible reactions that occur below 250°C , where abundant low-grade waste heat and solar energy might be available. Previously proposed reactions include dehydration-hydration reactions of alkaline-earth compounds such as $Mg(OH)_2$, $CaCl_2 \cdot nH_2O$, and $CaSO_4 \cdot 1/2H_2O$. However, there is still need to find materials satisfying all of the following criteria: high energy density, adequate storage temperature for low-grade waste heat, sufficient reversibility of reactions, non-corrosiveness, low cost, etc. It should be noted that most of rare-earth compounds

except for $La(OH)_3$ have been left uninvestigated as thermochemical heat storage materials to date while the prices of yttrium, lanthanum and cerium have dropped due to oversupply. Therefore, we have investigated dehydration-hydration behaviors of several lanthanum compounds, namely, $La(OH)_3$, $La_2(SO_4)_3 \cdot H_2O$, $La_2(SO_4)_3(OH)_4$, and $ALa(SO_4)_2 \cdot xH_2O$ ($A=Na, K, Rb$), as potential thermochemical heat storage materials.

Thermogravimetry revealed that $La(OH)_3$ and $La_2(SO_4)_3 \cdot H_2O$ reversibly dehydrate/hydrate on heating / cooling at $50\sim 400^\circ\text{C}$ under humidified argon atmospheres (water vapor pressure: $0.12\sim 0.23$ atm). Especially, the reactions of $La_2(SO_4)_3 \cdot H_2O$ proceeded in the temperature range from 50 to 250°C with remarkably small thermal hysteresis of less than 50°C at the heating/cooling rate of $20^\circ\text{C}/\text{min}$, and thus it emerges as a new candidate system for thermal energy storage. By contrast, the other compounds dehydrated on heating but hardly rehydrated on cooling.

Detailed study on $La_2(SO_4)_3$ was then conducted. High-temperature X-ray diffraction analysis and first-principles molecular dynamics simulation revealed that the dehydration/hydration reactions proceed through an unusual mechanism for sulfates: water molecules are removed from, or inserted in $La_2(SO_4)_3 \cdot xH_2O$ with progressive change in hydration number x without phase change. In addition, a characteristic microstructure of $La_2(SO_4)_3$ polycrystalline particles consisting of 200nm -thick fine platy grains was found to facilitate the fast hydration reaction, by thermogravimetry, transmission electron microscope and gas adsorption studies. The standard enthalpy change of the dehydration reaction of $La_2(SO_4)_3 \cdot H_2O$ was assessed to be $91\text{kJ}/\text{mol}$, or $154\text{kJ}/\text{kg}$ -monohydrate. This value is comparable to those of typical phase change materials (PCM) and renders the need for further enhancement of energy density.

15:10-15:30 (1221996)

$NiCo_2S_4/Ni_3S_2$ Heterostructure on Nickel Foam as Self Supporting Electrodes for Water Splitting

Weiji Dai, Ye Pan, Southeast University, China

Nowadays, the increasing consumption of nonrenewable fossil fuels, such as coal, petroleum and natural gas has caused a series of severe environmental problems, ranging from air and water pollution to global warming. Therefore, the development of new type energy with environmental friendly, high efficiency and sustainable development, such as solar energy and wind energy, as well as hydrogen energy, is a significant and urgent task for the scientific community. Among this, with the zero carbon emission and high energy density output, hydrogen has been regarded as an ideal renewable resource to replace the increasingly depleted fossil fuels. Furthermore, water splitting technology has widely recognized as a promising and appealing strategy to convert electrical energy into renewable



hydrogen energy. Therefore, the development of high efficiency and earth abundant electrocatalysts materials for the two half reactions of water splitting: the hydrogen evolution reaction (HER) at the cathode and the oxygen evolution reaction (OER) at the anode is the uppermost challenge. To date, the most efficient HER catalysts are platinum (Pt)-based noble metal materials and the state-of-the-art OER catalysts are iridium (Ir) and ruthenium (Ru)-based oxides, however, the scarce abundance and high cost severely limited their large-scale applications. Great efforts have been devoted to developing transition metal-based electrocatalysts for HER and OER. Herein, we report the controllable synthesis of $\text{NiCo}_2\text{S}_4/\text{Ni}_3\text{S}_2$ Heterostructure on Nickel foam and their application as an efficient bifunctional electrocatalyst for overall water splitting. The $\text{NiCo}_2\text{S}_4/\text{Ni}_3\text{S}_2$ heterostructure is achieved by the facile one-step hydrothermal approach without preparation of any precursor. The resultant $\text{NiCo}_2\text{S}_4/\text{Ni}_3\text{S}_2$ electrode exhibits as an effective bifunctional electrocatalyst, to achieve an current density of $10 \text{ mA}\cdot\text{cm}^{-2}$ for HER and OER it need overpotentials of only 167 and 280mV respectively in 1M KOH solution. Such enhanced electrocatalytic performance can be credited to (i) the interface effect of $\text{NiCo}_2\text{S}_4/\text{Ni}_3\text{S}_2$ Heterostructure, (ii) the flower like morphology of $\text{NiCo}_2\text{S}_4/\text{Ni}_3\text{S}_2$ could expose massive active sites. This work not only provides a new efficient and stable catalyst for overall water splitting, but also proposes an interface design principle for Nickel Foam based high-performance water splitting electrocatalysts materials.

15:30-16:10 Tea Break

16:10-16:35 Invited (1222518)

Neutron Irradiation Behavior of Fe-Cr Alloys, from Model to Engineering Alloy Compositions

Weiyang Chen, Argonne National Lab, Lemont, USA; *Xiang Liu*, Idaho National Lab, Idaho Falls, USA; *Huan Yan*, *Hoon Lee*, *James Stubbins*, Department of Nuclear, Plasma and Radiological Engineering, University of Illinois at Urbana-Champaign, Urbana, USA

A number of alloys ranging from simple binary and ternary Fe-Cr alloys to commercial ferritic/martensitic alloys were irradiated in the Advanced Test Reactor at Idaho National Lab over a range of displacement doses from 0.01dpa to 10dpa at nominal irradiation temperatures of 300°C, 450°C and 550°C. The intent of this large irradiation matrix was to develop an understanding of the behavior of these alloy systems by building on the response of simple alloy systems up to very complex systems. The irradiations included specimens for microstructural examination as well as tensile testing.

This talk will discuss the findings of microstructural

behavior and its relationship to mechanical properties performance for a range of alloys and irradiation conditions. This includes a presentation of the understanding of the development of the α' phase (a Cr-rich Fe-Cr phase) which is not found in heavy ion irradiations of the same materials, and is difficult to identify in experimental techniques that rely on diffraction scattering analysis. The relationship between materials composition and irradiation conditions for the formation of this phase are still in dispute, as is the equilibrium phase boundary.

The talk will also cover some in situ tensile tests of certain of these alloy conditions to show the advantages of dynamic straining to elucidate which microstructural features are playing a role in the deformation process and to what extent. Plans for future testing will also be discussed.

16:35-16:55 (1235366)

Effect of Phase Composition and Local Crystal Structure on Transport Properties of Solid Solutions $\text{ZrO}_2\text{-Gd}_2\text{O}_3$

Filipp Milovich, *Tabachkova*, National University of Science and Technology "MISIS", Russian Federation; *Mihail Borik*, *Elena Lomonova*, *Valentina Myzina*, *Alexey Kulebyakin*, Prokhorov General Physics Institute, Russian Academy of Sciences, Russia; *Polina Ryabochkina*, *Tatyana Volkova*, Ogarev Mordovia State University, Republic of Mordovia, Russia; *Ekaterina Agarkova*, Institute of Solid State Physics, Russian Academy of Sciences, Russia

Currently, the use of materials based on zirconia as a solid electrolyte for solid oxide fuel cells (SOFC) is associated with the need to solve a number of scientific and technological problems. The production of materials with high conductivity in the range of average temperatures (500~700°C) and the increase in the stability of the electrophysical characteristics of solid electrolyte at operating temperatures for a long time are some of these issues. In accordance with this, the identifying of various factors, such as phase composition and local crystal structure, affecting the magnitude of oxygen-ionic conductivity of zirconia-based solid solutions, is a relevant research topic.

Comprehensive studies of the phase composition and local structure of zirconium dioxide crystals stabilized by gadolinium oxide in a wide range of compositions from 2.7 to 38mol.% were performed and the effect of Gd_2O_3 on the transport characteristics of crystals of these solid solutions was established. The presence of transformable t and untransformable t' tetragonal phases was established in crystals of zirconia partially stabilized by gadolinium oxide, with a concentration of 2.7 and 3.6mol.%, and their crystal structure parameters were determined. The presence of a twin structure formed during the transition of the high-temperature





cubic phase to the tetragonal phase is shown in ZrO_2 crystals with a content of 8mol.% Gd_2O_3 by transmission electron microscopy and Raman spectroscopy. It was established that the twin structure is absent with the same content of yttrium oxide in ZrO_2 -8mol.% Y_2O_3 crystals, and the structure of the crystals corresponds to the structure of the t'' -phase. Studies of the features of local crystal structure ZrO_2 - Gd_2O_3 were carried out using optical spectroscopy methods. Eu_2O_3 was used as a spectroscopic probe. It has been established that the local structure of the ZrO_2 - Gd_2O_3 solid solutions is determined mainly by the concentration of stabilizing oxides Gd_2O_3 . It was shown that the decrease in ionic conductivity in the concentration range of stabilizing oxides above 12mol.% Gd_2O_3 is due to the increase in the relative fraction of Gd^{3+} cations with oxygen vacancy in the nearest crystalline surroundings, and in the concentration range above 20mol.% Gd_2O_3 the formation of two anionic ions vacancies in the nearest crystalline surroundings of Gd^{3+} ions.

The work was carried out with financial support in part from the RSF (№ 18-79-00323).

16:55-17:15 (122362)

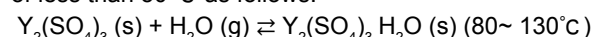
Reversible Hydration-Dehydration Reaction of Yttrium Sulfate as a New Candidate of Thermal Energy Storage Material for Low-Temperature Waste Heat.

Kunihiko Shizume, Naoyuki Hatada, Shoko Yasui, Tetsuya Uda, Kyoto University, Japan

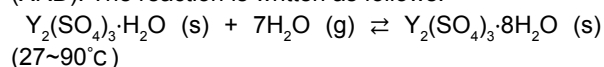
Thermal energy storage based on chemical reactions (thermochemical heat storage) is a prospective technology for the reduction of fossil fuel consumption by storing and reusing industrial waste heat. For widespread application, a critical challenge is to find appropriate reversible reactions which occur below 250°C where abundant low-grade waste heat might be available. Hydration (endothermic)-dehydration (exothermic) reaction cycle of inorganic solids with water vapor is one of the practical reaction systems due to its safety and easy storage of water. However, many hydration reactions of inorganic solids are slower compared with their dehydration reactions when their reaction temperatures are about 300°C or less. Exceptionally, hydration reactions of calcium sulfate $CaSO_4$ and lanthanum sulfate $La_2(SO_4)_3$ can proceed promptly even by exposure to air by water insertion into the pore in their crystal structure. However, they form hydrates with only small hydration numbers such as hemihydrate $CaSO_4 \cdot 1/2H_2O$ and monohydrate $La_2(SO_4)_3 \cdot H_2O$. Therefore, the enthalpy changes of the reactions are not large enough for practical application. In this work, we have focused on yttrium sulfate $Y_2(SO_4)_3$ as a new candidate material. Dehydration reaction of yttrium sulfate octahydrate $Y_2(SO_4)_3 \cdot 8H_2O$ has been reported to complete below 200°C, but rehydration

behavior of the anhydrate is unknown. If the anhydrate reacts with water vapor rapidly to form the hydrates $Y_2(SO_4)_3 \cdot nH_2O$ with large hydration number n , it will be a prospective candidate for thermochemical heat storage material.

We conducted thermogravimetry (TG) on $Y_2(SO_4)_3 \cdot 8H_2O$ during heating-cooling cycles under a humidified argon atmosphere (Ar-1%~2% H_2O). It revealed that $Y_2(SO_4)_3 \cdot 8H_2O$ dehydrated to $Y_2(SO_4)_3$ at between 150 to 270°C during heating at a rate of 20°C·min⁻¹, and then during cooling to 27°C, $Y_2(SO_4)_3$ rehydrated to form $Y_2(SO_4)_3 \cdot nH_2O$ where n increased step by step with the range from 0 to 6. At least two hydration/dehydration reaction processes were observed at different reaction temperature ranges when heating/cooling rate was 1°C·min⁻¹. At between 80 to 130°C, hydration number varied from 0 to approximately 1 with small thermal hysteresis of less than 50 °C as follows:



This hydration/dehydration reaction temperature range is narrower than that of $La_2(SO_4)_3$ (80~250°C) and nearly equal to that of $CaSO_4$ (70~120°C). At lower temperature range, further hydration of $Y_2(SO_4)_3 \cdot H_2O$ proceeded. The hydration number reached about 6 at below 30°C on cooling process, and the partial formation of $Y_2(SO_4)_3 \cdot 8H_2O$ was confirmed by X-ray diffraction (XRD). The reaction is written as follows:



It is interesting that hydration number reached as large as 8 without any high water vapor partial pressure treatments. In fact, $La_2(SO_4)_3 \cdot 9H_2O$ and $CaSO_4 \cdot 2H_2O$ are stable hydrates, but can not be formed from their anhydrate under the same atmosphere (Ar-1%~2% H_2O). Therefore, if the hydration/dehydration reaction between $Y_2(SO_4)_3$ and $Y_2(SO_4)_3 \cdot 8H_2O$ is applied to thermochemical heat storage, higher heat storage density is expected than those of other candidates. The mechanisms of the reaction will be discussed on the basis of the change of crystal structure and microstructure of $Y_2(SO_4)_3 \cdot nH_2O$ during hydration/dehydration reaction revealed by high temperature XRD and gas adsorption measurements.

17:15-17:30 (1221384)

Ordered Mesoporous Carbon Supporting Well-Dispersed Active Co Nanoclusters for Low Temperature CO₂ Methanation

Feng Li, Chunxia Zhao, Hang Li, Wen Chen, State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, School of Materials Science and Engineering, Wuhan University of Technology, China; Yunxia Yang, The Commonwealth Scientific and Industrial Research Organization, Australia

An energy efficient process must be developed for utilizing CO₂ as a carbon source to produce commodity



chemicals aligned to industrial needs because of the serious environmental problems and resources limitation. The Sabatier reaction (also known as CO₂ methanation) reduces CO₂ with H₂, over a catalyst, to produce methane at elevated temperatures and pressures. A high-efficiency CO₂ methanation catalyst is the key of this reaction. At present, Ni-based metal oxide supported catalysts such as Ni/Al₂O₃, Ni/TiO₂, Ni/SiO₂ and Ni/CeO₂, are easily deactivated at high temperature and humidity. So, it is necessary to study new types of low-temperature catalysts and expand the diversity of catalyst support materials. In comparison, cobalt based catalyst exhibits almost the same methanation activity as Ni catalyst, but it has lower activation energy. Thus it is possible that cobalt is applied to low temperature CO₂ methanation. With respect to catalytic supports, carbon materials, including CNTs, graphene, AC, mesoporous carbon etc, have different chemistry and structures from metal oxides. However, there are relatively few studies on CO₂ methanation catalysts based on carbon materials. Ordered mesoporous carbon, CMK-3, has a two-dimensional hexagonal mesoporous structure and

a large specific surface area which could provide a good environment to highly disperse catalysts. In our work, Co@CMK-3 catalyst with well-dispersed Co nanoclusters on the channels of ordered mesoporous carbon was synthesized by impregnation method with Co(NO₃)₂ as Co source and CMK-3 as support and then were activated in situ under methanation reaction conditions at 350°C. The prepared Co@CMK-3 catalysts have high specific surface area of 957m²/g and uniform pore size of 3.61nm. As a result, a CO₂ conversion rate of 16.22% is obtained by this catalyst at 300°C and 30bar. Then, the influences of CMK-3 surface modification and Ru, Co co-loading on the catalytic activity of CO₂ methanation are investigated. It is found that The acid-pretreated CMK-3 can promote the low-temperature catalytic performance of the composite catalyst, and the CO₂ conversion rate is 37.17% at 300°C and 30bar. Ru and Co co-loading can also significantly improve the low temperature catalytic performance, and the CO₂ conversion rate is increased to 45.01% at the same reaction condition.



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/Martensite 12Cr-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 manufacturing 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-20X (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 Mg₂Ni 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 MgH₂), 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 H₂ molecules on the Mg surface, the low hydrogen diffusion rate on the Mg because it extremely difficult after a MgH₂ layer forms on the surface of Mg because the H₂ diffusion coefficient in MgH₂ ($1.5 \times 10^{-16} \text{m}^2/\text{s}$) is considerably smaller than Mg ($4 \times 10^{-13} \text{m}^2/\text{s}$), and formation of Mg/MgH₂ oxides on the surface of Mg/MgH₂. The slow dehydrogenation kinetics is due to the strong bond between Mg and H, the low diffusion rate of H in MgH₂, the high energy required for the nucleation of Mg on the surface of MgH₂, and the combination of hydrogen atoms to form the H₂ molecule on the Mg surface. However, its high decomposition temperature ($T > 300^\circ\text{C}$) is due to the strong ionic characteristics of the Mg-H bond.

We prepared nanocrystalline Mg₂Ni with an average size of 20~50nm was prepared via ball milling of a 2MgH₂-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 2MgH₂-Ni powder, the compressed 2MgH₂-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 $375^\circ C$ 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, $Mg@C$ ($CH_4:50ml$) 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 $Mg@C$ ($CH_4:10ml$) and $Mg@C$ ($CH_4:300ml$) are only 5.4wt% H_2 and 4.3wt% H_2 , respectively. $Mg@C$ ($CH_4:50ml$) 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 $Mg@C$ ($CH_4:50ml$) are 64.1 and 107.2kJ·mol⁻¹, both smaller than $Mg@C$ ($CH_4:10ml$) of 66.7 and 118.9kJ·mol⁻¹ and $Mg@C$ ($CH_4:300ml$) of 67.7 and 137.8kJ·mol⁻¹. The enhanced hydrogen storage properties of $Mg@C$ ($CH_4 : 50ml$) are attributed to smaller particles size and excellent antioxidant properties provided by the ultrathin carbon layer.

Tuesday AM | August 20, 2019



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 Room: 311(3rd Floor)
August 20, 2019 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, $\sim 54\%$ 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 Ag_8SiSe_6 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 promising green thermoelectrics, received much attention for their much low lattice thermal 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 $[\text{SiSe}_6]^{8-}$ anion sublattice which is composed of Se^{2-} anions and $[\text{SiSe}_4]^{4-}$ 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 processes 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 Room: 311(3rd Floor)
August 21, 2019 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 Nb_{0.8}CoSb and impurity phases. Single phase Nb_{0.8}CoSb 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

Jin Zhang 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 determining 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-synthesized 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·g⁻¹ or mAh·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·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 $600\text{mAh}\cdot\text{g}^{-1}$, which could be further increased when the Sn (with theoretical capacity of $994\text{mAh}\cdot\text{g}^{-1}$) is replaced with SnO_2 ($1494\text{mAh}\cdot\text{g}^{-1}$). Thus we designed a series ternary 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 coarsening in lithiated SnO_2 , resulting in fast interdiffusion kinetics of interdiffusion between Sn and O in the $\text{Sn}/\text{Li}_2\text{O}$ 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 sub-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 $4.17\text{mg}/\text{cm}^2$) 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.

Wednesday AM | August: 21, 2019



M. Renewable Energy Materials and Nuclear Materials: V

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 PM Room: 311(3rd Floor)
August 21, 2019 Symposium: M

Chairs:

Young-Joo Eo, Korea Institute of Energy Research, Korea
Ajayan Vinu, University of Newcastle, Australia

13:30-14:00 Keynote (1234718)

TiFe and Related Alloys for Energy Storage

Etsuo Akiba, Rika Hayashi, Haiwen Li, Makoto Arita, Zenji Horita, Kaveh Edalati, Kyushu University, Japan

TiFe was reported in 1974 by Reilly and Wiswall. The alloy has the appropriate hydrogen equilibrium pressure at room temperature that is almost same as that of LaNi₅. The hydrogen capacity is 1.8~1.9wt% that is higher than LaNi₅. For stationary applications the cost is the critical issue. TiFe is the least expensive hydrogen absorbing alloy as far as the authors know. However, initial activation of TiFe needs hydrogen pressure of 30MPa and temperature at 400°C at the same time. This is the serious roadblock to apply realistic applications, especially large-scale hydrogen storage.

There have been various attempts to solve this roadblock. We have already been very much successful in introducing super plastic deformation to TiFe. Diffusion of surface elements of TiFe makes hydrogen pass through the surface oxide layers. Of course, huge defects are introduced and they are also thought to contribute for easy activation.

In this paper, we showed the effect of the third element addition to the TiFe. TiFe_{0.8}x_{0.2} (x= V, Cr, Mn, Co, Ni, Zr, Nb, Sn) are prepared using the arc melting method. Evacuation at 150°C for 2 hours was enough for activation for every TiFe_{0.8}x_{0.2} alloy. However, the heat of 150°C is almost impossible for large scale application considering the cost and design of heat exchanger. It was found that some of the alloys could be activated by evacuation at 30°C for 2 hours but some could not. The surface analysis using XPS has been done with heating from room temperature to 150°C under vacuum. The surface was covered by carbon but carbon existed just on the surface. The alloy that could not be activated at 30°C has thicker oxide layers, which is one of the reasons for difficulty in activation. The alloy TiFe_{0.8}Co_{0.2} that could

not be activated near room temperature is pseudo-binary alloy. In other words, it is pure solid solution. TiFe_{0.8}Cr_{0.2} consists of three phases such as TiFe, Ti and the Laves phase. Co-existence of the active phase near the surface to decompose hydrogen molecule to atoms is other reason of easiness of activation.

14:00-14:25 Invited (1263222)

Advanced Nanoporous Nitrides for Energy and Environmental Applications

Ajayan Vinu, University of Newcastle, Australia

Mesoporous carbon nitrides (MCN) with large surface areas and uniform pore diameters are unique semiconducting materials and exhibit highly versatile structural and excellent physicochemical properties which find them applications in diverse fields such as metal free catalysis, photocatalytic water splitting, energy storage and conversion, gas adsorption, separation, and even sensing. Although there have been series of mesoporous boron nitride or carbon nitride materials with C₃N₄ stoichiometry reported, only a little attention has been given to the mesoporous materials with C₃N₅, C₃N₆, C₃N₇, etc even though they have unique band structure. In this talk, I will present the preparation, structural and morphological control, and the functionalization of highly ordered and graphitic carbon nitride materials with tunable nitrogen contents. The relation between the structural parameters and the performance of these materials in various applications including catalysis, sensing, and carbon capture and energy storage will be demonstrated. In the second part of the talk, the fabrication of various nanoporous films including carbons, nitrides, semiconducting nanostructures, and biomolecules with tunable macroporosity, thickness, and morphology will be presented. These porous films have been fabricated by using P123 block copolymer and polystyrene spheres as templates, and utilized for sensing. For example, nanoporous CN film offers the superior affinities for toxic acid molecules but the selectivity can be totally reversed for basic molecule after treatment with UV. The application of these fascinating materials for carbon capture, water splitting, oxygen reduction reaction will also be presented.

14:25-14:50 Invited (1233917)

Development of Commercialization Technology of CIGS Thin Film Solar Cell at KIER

Young-Joo Eo, Korea Institute of Energy Research, Korea

Solar energy has attention as a renewable and alternative energy source for the further sustainable development. A silicon solar cell producing electricity from solar energy has been conventionally used, however the material cost has been still the first problem for the supply of global energy demand. A chalcogenide Cu(In, Ga)Se₂ (CIGS) solar cell is one of the most promising alternatives due





to the potential of low-cost fabrication technique and high efficiency among all the thin film solar cells. The technological development of fabrication method for CIGS solar cell has resulted in record-breaking efficiency improvement, which can realize the highest efficiency of 23% in polycrystalline thin film CIGS solar cells by a three-stage vacuum-based process. However, since it is the complicated and expensive method for commercial fabrication, the simple process with low cost are required as well as high efficiency. To address these concerns, commercialization technology of CIGS thin film solar cell has been researched at KIER (Korea Institute of Energy Research) for the last 10 years and achieved many promising results. Here, we introduce the recent development of large area of CIGS thin film solar cell at KIER including Roll to Roll equipment and process, and its application toward building integrated photovoltaics (BIPV).

14:50-15:10 (1235114)

Materialization of High Grade Tantalum Metal from End of Life Ta Scrap

Kyoung-Tae Park, Taek-Soo Kim, Korea Institute of Industrial Technology, Korea; Jae-Hong Lim, Korea Institute of Industrial Technology & Kroea University, Korea; Bon-Woo Koo, Eco-Recycling Co., Korea; Soong-Ju Oh, Kroea University, Korea

Tantalum (Ta) is a refractory metal with atomic number 73, atomic weight of 180.95g/mol, density of 16.6g/cm³ and a high melting point of 3017°C. From refractory characteristics, it shows excellent chemical and physical stability at elevated temperatures. Demand of Ta metal and related compounds is growing with the growth of the electronics and chemical industries. However, Ta ores are classified as conflict minerals due to which Ta production is strictly regulated. To ensure smooth supply demand balance, it is necessary to recycle Ta from the currently available Ta end of life products.

This work consists of two parts; in which first part deals with the extraction of Ta from Ta end of life springs and the later part deals with its materialization. Ta was first converted to K₂TaF₇ by hydrometallurgical process followed by metallothermic reaction to obtain pure Ta powder. Later, Ta ingot, TaCu and TaC were manufactured from extracted Ta powder using electron

beam melting (EBM), spark plasma sintering (SPS), and self-propagating high temperature synthesis (SHS) respectively. Detailed microstructural, structural and compositional analysis of all extracted and materialized Ta products were performed. Moreover, the ideal conditions necessary for the extraction of Ta from Ta scrap and its materialization are also discussed in detail.

15:10-15:30 (1235394)

Retarded Recrystallization of Helium-Exposed Tungsten

Wangguo Guo, Shiwei Wang, Long Cheng, Yue Yuan, Guanghong Lu, Beihang University, China; Gregory De Temmerman, ITER Organization, China

It has been recognized that impurity such as helium (He) from fusion edge plasma could affect recrystallization kinetics. In view of ITER operations, where recrystallization poses serious issues, it is important to understand the necessary conditions for retarded recrystallization to occur and identify the mechanisms at play. In this work, a combined experimental and modelling approach is used to study the effect of He plasma and ion implantation on the recrystallization kinetics of W.

He plasma exposure was observed to have a moderate retarding effect on recrystallization of W. The recrystallization temperature of W was increased by about 50K after He plasma exposure. And He ion implantation showed a significant retarding effect on recrystallization of W. The recrystallization temperature of W was increased by more than 400K. The retarding effect requires only tens of appm He and it is suggested that a deeper He distribution in W bulk is favourable for the retarding effect. The affected depth was limited to He range.

The retarding effect is attributed to the pinning effect of He bubble or cluster on grain boundary migration and is confirmed by transmission electron microscope observation. Molecular dynamics simulation shows that grain boundary migration could be impeded by a cluster of few He atoms at elevated temperatures.

This study demonstrates that He in W leads to significant changes in the kinetics of recrystallization and grain growth. The implications of plasma and particle induced retarded recrystallization on the operational budget of the ITER divertor will be discussed.



M. Renewable Energy Materials and Nuclear Materials

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

August 19-21, 2019

Room: Exhibition Area (3rd Floor)

M-1: Compositional and Structural Optimization of ZrFe₂ Based Alloys for High Pressure Hydrogen Storage Application(1226368)

Min Zhu, Hui Wang, Chao Zhou, School of Materials Science and Engineering, South China University of Technology, Guangdong Provincial Key Laboratory of Advance Energy Storage Materials, China

Hydrogen is an ideal energy carrier without causing any pollution. However, the lack of effective and safe hydrogen storage technology limits the large-scale application of hydrogen energy. In addition to the widely known gaseous-, solid-, and liquid-state hydrogen storage systems, the gas-solid hybrid hydrogen storage mode combines the high pressure gaseous hydrogen storage with materials-based solid-state hydrogen storage. Therefore, the hybrid hydrogen tank has higher gravimetric or volumetric hydrogen density compared with conventional hydrogen storage techniques. Thus it is feasible to reduce the volume and operating pressure (to 35~45MPa) of high-pressure hydrogen tank without the loss of hydrogen capacity, and the safety of hydrogen storage system could be also improved.

To match the fast hydrogen charging and discharging performances of hybrid hydrogen tank within the working pressure range, it demands hydrogen storage alloys with high equilibrium pressure, fast kinetics, low hydride formation enthalpy (less than 20kJ·mol⁻¹ H₂) and high cycle ability. Meanwhile, the small hysteresis coefficient (Hf) between absorption and desorption is also one of the criteria to weigh the performance of high-pressure hydrogen storage alloys.

ZrFe₂ alloy has great potential as high-pressure hydrogen storage medium because of its high equilibrium pressure and fast kinetics at ambient temperature. Nevertheless, its ultrahigh equilibrium pressure and low hydrogen capacity hinder its further application. To improve the thermodynamic properties and hydrogen storage performances of ZrFe₂, we study the alloying with Cr, Mn, V, Ti elements and its effect on the structure and hydrogen storage behaviors of ZrFe₂. The dependence of lattice constant, electron concentration, and the volume modulus on the composition (stoichiometry,

atomic size ratio of A-/B- site elements) of alloys, and the corresponding effects on the de-/hydriding plateau characteristics were systematically investigated. A series of ternary and quaternary alloys have been prepared by arc-melting, their hydrogen storage properties including the capacity, equilibrium pressure, hydrogen sorption rate have been evaluated.

M-2: Effect of Heat Treatment on M23C6 Carbide Precipitation and Its Effect on Tensile Properties of Alloy 690 Tubes (1230655)

Taehyuk Lee, Korea Institute of Geoscience and Mineral Resources, Korea; Jonghyeon Lee, Chungnam National University, Korea

Alloy 690, a nickel-based alloy having high chromium content (27~31wt.%), was developed as a replacement for alloy 690 in the steam generators of PWRs in NPPs, and is now widely used owing to its excellent resistance to SCC, pitting corrosion, and corrosion fatigue in aggressive primary water environments. These special properties are dependent on the size and distribution of precipitates in the matrix. Generally, under the conditions of heat treatment or during high-temperature service, M23C6, as a typical carbide commonly precipitates at the grain boundary in alloy 690. The precipitation behavior then could be affected by the alloy composition (such as carbon content) and heat treatment conditions. Hence, it is very important to study carbide precipitation behavior according to the heat treatment conditions, such as solution annealing and thermal aging and its effect on mechanical properties of alloy 690. In this study, we investigated the effect of solution annealing and aging treatment on the intergranular carbide precipitation behavior of alloy 690 tubes for steam generators. The carbides precipitated on the grain boundaries were identified as chromium-rich M23C6 carbide, which has a cube-cube orientation relationship with the matrix on one side of neighboring grains. The carbide precipitation behavior is closely related with the interaction between the solubility of carbon in Ni-based matrix and diffusion of alloying elements. The ultimate tensile strength and elongation of the solution annealed alloy 690 tubes at 300°C are 638.8±12.4MPa and 43.2±4.2%, respectively. In the early stage of precipitation, the ultimate tensile strength increased to 720.4±13.5MPa. The carbides function as reinforcement in alloy 690 and provide strength enhancement with aging time reached 15 hours. However, when the aging time passed 15 hours, this property gradually decreased to 710.6±12.6MPa due to the low bonding strength between the carbide and matrix.

M-3: Comparison of Different Interatomic Potentials for Tensile Simulation of α -Fe at 723K (1233376)

Heng Rui, Huiping Zhu, Baochen Chang, Ting Zhou,





Fenglei Niu, Yan Ma, North China Electric Power University, China

The mechanical properties of structural materials which are mainly iron-based materials in nuclear power plants affecting the safe operation severely. Hence, it is necessary to study the mechanical properties and microstructure evolution of materials under different working conditions. The molecular dynamics (MD) simulation technology can reveal the microscopic dynamic process of materials and calculate the relevant mechanical parameters. However, the accuracy of the simulation bases on the reliability of the used interatomic potentials. Thus, the interatomic potentials used for the MD simulation need to be verified by testing their capability in relevant material properties. This paper using MD method to compare different interatomic potentials for tensile simulation of body-centered cubic (bcc) iron in high temperature, and determine a suitable interatomic potential for subsequent in-depth research. Considering the high temperature of the material under actual working conditions, the stretching temperature was set to 723K and compared with the room temperature. Through the simulated stress-strain curves, the tensile strength and yield strain of different potential models at different temperatures were calculated. Open Visualization Tool (OVITO) software was used for visualizing the microstructure evolution, and the local structure around each atom was resolved by using the common neighbor analysis (CNA) technique. Meanwhile, Dislocation analysis (DXA) was applied to analyze the dislocations during tensile loading. The results showed that the tensile strength and yield strain were both reduced with the increasing temperature, the phase transformation is advanced and the phase transformation process is increased during the stretching at 723K, but no significant influence on the formation of dislocations was found. At the start of stretching, the body-centered cubic (bcc) structure remained intact. After reaching the yield strength, the phase transition occurred and the new phase of face-centered cubic (fcc) structure increased. The $1/2\langle 111 \rangle$ dislocations were generated and migrated subsequently. Besides, different interatomic potentials had different performances in predicting the stress-strain curves and microstructure variation. The details were discussed in the full paper.

M-4: Current Status and Development Trend of Impact Limiter Filling Materials for Nuclear Spent Fuel Transport Cask(1233715)

Youdong Xing, Siyi Yang, Yukun An, Ertuan Zhao, Zhongfang Li, Pengfei Zhang, Shandong University of Technology, China

With the widespread use of nuclear fuel, the transportation of nuclear spent fuel is also particularly important. In China or other countries, nuclear spent fuel is carried out by transport casks. In order to ensure the safety of the

transport cask during lifting and transportation, impact limiters must be installed at top and end of the cask to avoid unpredictable consequences caused by fallen leakage spent fuel. The impact limiter acts to absorb energy, control overload and ensure structural integrity, consisting of the outer cladding material and the inner filler material. The filling material is an important part of the impact limiter energy absorption.

The traditional filler material of the impact limiter is mainly wood. In addition, polyurethane foam and honeycomb aluminum material also have the case of being an impact limiter filling material; all of the above three materials have good energy absorption and light weight characteristics, which are suitable for impact limiters, however, the above materials also have defects. The wood has texture, which leads to the directionality of mechanical properties, also it has perishable defect. Polyurethane foam has flammability and low strength, and energy absorption needs large size. Honeycomb aluminum materials have unidirectional mechanical properties, and the manufacturing process of honeycomb aluminum materials is complicated.

As an important part of the impact limiter, how to make it have excellent energy absorption performance, light weight and fire resistance is the focus of research on filling materials. Our team aims to apply two kinds of metal materials (bi-directional corrugated honeycomb aluminum, aluminum foam) as the filling material for the impact limiter. Between them, the bi-directional corrugated honeycomb aluminum material is made as the nuclear fuel storage cask impact limiter filling material has been used in other country like USA without China. The bi-directional corrugated honeycomb aluminum has mechanical properties in two directions, and its weight is lighter than that of the same volume of aluminum. It implies superb energy absorption characteristics after researched. We aims to design and optimize the bi-directional corrugated honeycomb aluminum material to make it have better use characteristics. Additionally, our team creatively proposed to use aluminum foam as an impact limiter filling material, and launched a new application for aluminum foam. In the new direction, the next step is to study and manufacture large foam aluminum blocks with more uniform structure and better energy absorption characteristic. Through the above work, we will do our utmost to research and manufacture the impact limiter filling materials and denote our passion.

M-5: Indium Recovery from Indium-Tin Scrap by Electrorefining in Molten Fluoride Salt(1235073)

Hyun-gyu Lee, Sang-Hoon Choi, Jae-Jin Sim, Kyoung-Tae Park, Korea Institute for Rare Metals, Korea Institute of Industrial Technology, Korea; Hyun-gyu Lee, Sang-Hoon Choi, Soong-Keun Hyun, Department of Advanced Materials Engineering, In-Ha University, Korea



The essentiality of indium in electronic devices has increased many fold during recent past. At the same time indium is rare in natural abundance indium is obtained as a byproduct of zinc metal refining so that the need for recycling of indium has increased dramatically in the near past. Out of other recycling methods, molten salts based electrorefining holds promising future because it provides high conductivity, purity and eco-friendly process. General methods of molten salt electrorefining presents that solid anode and cathode is adapted and handled to get refined metal, but in this study indium and tin is used. Impure scrap containing indium-tin alloy shows lower melting temperature than electrolyte, LiF-KF system, so electrorefining specially carried out using molten anode(In-Sn impure) and cathode(purified indium) materials. Herein, we report electrorefining of indium at the tungsten and molybdenum electrode as anode and cathode, respectively. Process temperature was held at 700°C and electrolyte is molten LiF-KF eutectic (49~51mol.%). Contents of InF₃, initiative compounds was controlled for reducing polarization of potential in electrolytic cell. Chemical stability between fluoride electrolyte and materials used in this experiments such as In-Sn alloy, alumina crucible was pre-analyzed before electrolysis. Concentration of InF₃ was changed from 3wt% to 7wt% and it was found that the electrochemical reduction of indium at the cathode site and then it was directly move into the bottom crucible as a liquid phase. Cyclic voltammetry(CV) was performed to evaluate the electrochemical behavior of the In electrorefining. Mo was used as a working electrode in conjunction with a tungsten rod as counter electrode Ni wire Electrode was used as a pseudo-reference electrode, serving only to monitor and control the potential of working electrode during the experiments. The cathode was molybdenum metal. Electrochemical measurements were performed using a potentiostat/galvanostat. To get the In deposition, chronopotentiometry (CP) analysis was performed to compare the variation of potential for various applied current densities at the cathode during electrolysis of the In-Sn impure. It was observed that recovery rate of indium increases by increasing time. As a result, In-Sn alloy was recycled into pure In with low levels of impurities.

M-6: 2-Step Degradation of Hydrogen Permeability Through Pd-53mol%Cu Alloy Membrane with B2 Crystal Structure at Low Temperature(1235500)

Hiroshi Yukawa, Suzuki Asuka, Nagoya University, Japan; Hideki Araki, Mizuno Masataka, Sugita Kazuki, Osaka University, Japan; Higemoto Wataru, Japan Atomic Energy Agency, Japan

Pd-53mol%Cu (Pd-40wt%Cu) alloy membrane with B2 crystal structure is widely used as hydrogen separation membrane. The activation energy for hydrogen

permeation is much smaller for Pd-53mol%Cu alloy than ordinary Pd-Ag alloys (e.g., Pd-25wt%Ag) with fcc crystal structure, indicating that Pd-Cu alloy membrane has a potential to show higher hydrogen permeability than Pd-Ag alloy membrane at low temperature, e.g., room temperature. However, the temperature dependence of hydrogen permeability for Pd-Cu alloy membrane have not been investigated in detail especially below about 250°C. In this study, the hydrogen permeability of Pd-53mol%Cu alloy membrane at low temperature region has been investigated in a fundamental manner.

A thin foil of Pd-53mol%Cu alloy with a thickness of 20µm is prepared. XRD analysis is performed in order to conform the sample is composed of a single phase with B2 crystal structure. The hydrogen permeation tests are performed from 350°C down to room temperature. During the test, the hydrogen pressures at feed and permeation sides of the membrane are kept constant of 0.10MPa and 0.01MPa, respectively.

The the hydrogen permeability at 350°C is in good agreement with previous study. The hydrogen permeability decreases with decreasing temperature and obeys Arrhenius-type relation above 200°C. However, the hydrogen permeability declines more and deviates from the linear relationship below about 150°C. It is found that the hydrogen permeability at room temperature decreases about one order of magnitude in two steps during 4 days after cooling down to room temperature. Such a slow and large decrement in hydrogen permeability at low temperature for Pd-Cu alloy membrane has not been reported. It is noted that the hydrogen permeability recovers to the original value when the the sample cell is heated up to 350°C again.

M-7: Effects of Glass Chemistry and Additives in Ag Paste on Fire-Through Contact Formation onto Boron Emitters of n-type Si Solar Cells(1235573)

Sung-Hu Kim, Hee-Soo Kim, Ji-Gun Park, Joo-Youl Huh, Korea University, Korea

N-type Si wafers have higher efficiency potentials compared to p-type Si wafers owing to higher carrier lifetime and the absence of light induced degradation. The solar cells based on n-type Si wafers are commonly realized by forming boron emitters. However, it has long been known that the conventional Ag pastes used for contacting phosphorous emitter are not capable to reliably contact boron emitters, leading to contact resistances above $5 \times 10^{-2} \text{ohm-cm}^2$. This problem has been partially resolved by adding a small amount of Al to the Ag paste. Although the addition of Al to Ag paste was reported to produce boron emitter contacts with specific contact resistances below $1 \times 10^{-2} \text{ohm-cm}^2$, it can cause other detrimental effects, such as shunting behavior and higher line resistivity. Recently, a significant progress in Ag paste has been made by replacing the conventional PbO-based glass frit with TeO₂-based glass frit, which





enables to fabricate high-quality ohmic contacts to the phosphorous emitter with a sheet resistance of $\sim 100\text{ohm/sq}$. In this study, we used Ag paste containing tellurite glass frit to search a possibility to contact boron emitters without adding Al. By varying the tellurite glass chemistry and adding inorganic additives to Ag paste, we examined the contact microstructure and contact properties. In the presentation, we will discuss the roles of the glass chemistry and additives in the contact firing reactions for boron emitter contacts based on the contact microstructure observations and contact resistance measurements.

M-8: Effect of Ball Milling Time on the Thermoelectric Properties of Bi-Sb-Te alloys with Dispersion of Cu (1235704)

Seok min Yoon, Chul Hee Lee, May Likha Lwin, Sharief Pathan, Soon Jlk Hong, Kongju National University, Korea

Thermoelectric materials are capable of converting waste heat into electricity and vice versa. They are used in power generation and cooling devices; which are adverse advantageous such as low maintenance and environment friendly. Bi-Sb-Te thermoelectric materials have been used for room temperature applications. However, the energy conversion efficiency of the commercialized products is still below about 10%, most of the studies focused on increasing thermoelectric performance of the existing materials.

It has been reported that the addition of a small amount of Cu to the Bi-Sb-Te thermoelectric material reduces the lattice thermal conductivity and significantly improves the electrical conductivity, thereby improving the thermoelectric performance.

In order to effectively disperse the Cu into $\text{Bi}_{0.5}\text{Sb}_{1.5}\text{Te}_3$ powder, we have utilized low energy ball milling with various milling time. Then as-prepared powder was consolidated using Spark Plasma Sintering process. (SPS)

The crystal structure of BST-Cu powder and bulks were analyzed by X-ray diffraction (XRD). The microstructure and chemical composition of BST-Cu samples were characterized using Scanning Electron Microscope (SEM) and Electron probe micro-analyzer (EPMA) techniques respectively. The result indicate that electrical conductivity increased with milling time while Seebeck coefficient decreased. The thermal conductivity decreased with increasing milling time, as a result, ZT was improved.

M-9: Monolayer MoS_2 on Nanoporous Graphene as a Electrocatalyst for Hydrogen Evolution Reaction (1444935)

Yongzheng Zhang, Fujita Takeshi, Kochi University of Technology, Japan

2D layered materials have attracted much attention in recent years due to their remarkable properties and potential for highly active catalysts. MoS_2 , two-dimensional layered materials, is highly stable, active, nano-structured and shows promising activity for hydrogen evolution reaction (HER). However, the 2D electrocatalysts usually suffer from lower photoelectrochemical efficiency because of the challenges in effectively utilizing the 2D electrocatalysts in three-dimensional electrodes with a reserved surface area and 2D electronic properties. The efficient electrons, as well as proton transport processes in the electrocatalysts, are the key factors for HER activity. Graphene is regarded as superior electron mobility and excellent electronic behavior material for modification of conduction. In addition, graphene could be used as an efficient and low-cost cocatalyst for electrocatalytic reactions because of its high specific surface area and good electron transfer abilities. Herein, we report that MoS_2 / nanoporous graphene hybrid catalysts of monolayer MoS_2 sheets coating on nanoporous graphene with the high surface area are fabricated and applied for HER. The fabrication process of 3D nanoporous graphene is shown in the Scheme. And the BET surface area of synthesized nanoporous graphene was above $600\text{m}^2\cdot\text{g}^{-1}$. MoS_2 was deposited on nanoporous graphene by chemical vapor deposition (CVD) method. Different deposited time and temperature were studied. By controlling time and temperature, monolayer MoS_2 with different loading amount were obtained. The HER test results showed that the onset potential is -80mV with the Tafel slope of $60\text{mV}/\text{dec}$ for best $\text{MoS}_2/\text{graphene}$ sample.

M-10: Corrosion model Study of Cu Cr Zr Alloy for Fusion Reactor (1222647)

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As a fusion of divertor heat sink and the first wall material of copper, Cu Cr Zr alloy under the condition of the running of the fusion, will contact with the pile of high temperature and high pressure in the cooling water, which corrosion occurs, the Cu Cr Zr alloy corrosion products will be on the surface of the cooling water, washed down with cooling water migration, and will eventually deposition on the surface of the other parts of the cooling circuit. These corrosion products are irradiated and thus become part of activated corrosion products, which may be irradiated by factory workers inspecting or maintaining cooling loop equipment. After experiments, all the test specimens were analyzed and examined by weight change method to determine the corrosion mechanism and factors affecting the corrosion rate. The model was established by referring to the inherent model and verified by comparing the experimental data. The result of the experiment shows:



In the flowing water, the corrosion weight of Cu Cr Zr changes linearly with time, and in the continuous water, the corrosion weight changes exponentially with time. Then referenc grey model, and build corrosion model in the flowing water and in the continuous water, which means that the corrosion behavior of Cu Cr Zr alloys in different water environments was studied by grey model. And the model was verified by comparing with the experimental data .

