

Energy Harvesting & Storage

Room Naupaka Salon 1-3 - Session EH-WeP

Energy Harvesting and Storage Poster Session

EH-WeP-1 Spintronic Diode as a Signal Detector and RF Energy Harvester, *Andrei Slavin*, Oakland University

The spin-torque magnetic diode (STMD) effect [1] is a quadratic rectification effect of the input microwave current $I_{RF}(t)$ in a magneto-resistive nano-junction, which is commonly observed in a traditional regime of operation of an STMD, when the magnetization of the “free” layer lies *in-plane*, and when the frequency f_s of the current $I_{RF}(t)$ is close to the ferromagnetic resonance (FMR) frequency f_0 of the junction. It was demonstrated theoretically in [2] that in an STMD, biased by an *out-of-plane* static magnetic field, a novel dynamical regime of STMD operation characterized by large-angle out-of-plane magnetization precession can be realized.

It was demonstrated experimentally in [3] that the out-of-plane magnetization precession regime in an STMD predicted in [2] can be realized without *any bias magnetic field*, if an STMD “free” layer has a *perpendicular magnetic anisotropy*. It was further shown in [3] that the developed bias-free STMD provides sufficient dc voltage to power a practical nanodevice – a black phosphorus photosensor.

Here we present an analytical and numerical theory explaining the performance of such a bias-free STMD with perpendicular magnetic anisotropy [4]. We show that such a device can operate as a broadband energy harvester capable of converting incident RF power into a DC power with a conversion efficiency of ~5%.

References

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- [2] V. Prokopenko, I. N. Krivorotov, E. Bankowski et al., *J. Appl. Phys.*, Vol. 111, p.123904 (2012).
- [3] B. Fang, M. Carpentieri, S. Louis et al., *Phys. Rev. Appl.*, Vol. 11, p.014022 (2019).
- [4] P. Yu. Artemchuk, O. V. Prokopenko, E. N. Bankowski et al., *AIP Advances.*, Vol. 11, p. 025234 (2021).

EH-WeP-2 Strain Imaging of a LiTi_2O_4 Anode in a Li-Ion Battery, *Keiji Takata*, Kansai University, Japan

Li-ion batteries have advantages including high energy density, high output voltage, and the absence of the memory effect, and so they are recognized as promising candidates for energy storage. These advantages are mainly provided by the lowest electrode potential of Li^+/Li and low density of Li, which are -3.04 V and 0.534 g/cm³, respectively. Li-ion batteries have advanced a great deal through the use of intercalation and have been applied in portable electronic devices and electric vehicles.

Li-ion batteries operate through the migration of Li ions between the electrodes. Therefore, non-destructive observation of the migration with high spatial resolution is important.

When charging and discharging, Li-ions are extracted or inserted into electrode materials, which generally causes changes in volume. An atomic force microscope (AFM) can detect and image these volume changes through current collectors with high spatial resolution, which enables us to investigate Li-ion migration without destruction.

Here, we present our results of LiTi_2O_4 . LiTi_2O_4 is an anode material with high safety having a theoretical capacity of 160 mA h g⁻¹ (from LiTi_2O_4 to $\text{Li}_2\text{Ti}_2\text{O}_4$). The phase change from spinel to rock-salt lead to very small volume changes. Therefore, it might be difficult to observe the Li migration by this method. Cathode of observed samples was layered LiCoO_2 , and electrolyte and separator are commonly used materials. AFM detects surface displacements synchronizing the charging/discharging cycle, and provides strain images along with topography.

The strain images consist of dark regions that any strain was not detected and bright regions that relatively constant strains were detected. We considered these images together with the frequency dependence of the images and impedance spectroscopy, and concluded that the dark regions were LiTi_2O_4 particles and the bright regions resulted from electrolyte flux induced by the gradient of Li-ion concentration in the interspace of the particles. The gradient of Li-ion concentration and electrolyte flux in the interspace were generated by the charging/discharging.

Electric fields, the electrolyte flux, and diffusion move Li ions from one electrode to another electrode. This electrolyte flux is one of the most important issues for increasing the energy density of lithium ion batteries.

Reference s :

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EH-WeP-3 A Novel Doping Strategy of PTAA for High-Performance Inverted Perovskite Solar Cell, *Jihyeon Heo, H. Park, H. Park*, Hanyang University, Korea

Organic-inorganic hybrid halide perovskite solar cells (PSCs) have achieved great developments with their high-power conversion efficiency (PCE) surpassing 25.8%. Among various research to maximize the performance of PSCs, a modification of charge transport materials plays an important role to attain such a high-performance of PSC. Particularly, doping engineering can enhance the charge extraction/transport capability of the charge transport layer. Although organic hole transport materials (HTM) including small molecules such as 2,2',7,7'-tetrakis(N,N-di-p-methoxyphenylamine)-9,9'-spirobifluorene (spiro-OMeTAD) and conducting polymers such as poly(3-hexylthiophene-2,5-diyl) (P3HT) and Poly[bis(4-phenyl)(2,4,6-trimethylphenyl)amine] (PTAA) are advantageous with high-quality thin films by a simple solution process, an additional doping process is necessary due to their inherent low hole mobility. Therefore, a search for suitable p-type dopants and their fabrication methods for organic HTM should be further studied. In this work, we propose a simple interfacial doping (ID) strategy of PTAA/F4-TCNQ double layer structure with the application of a new solvent 2-butanone. Through this approach, the optoelectrical performance with high power conversion efficiency of 20.67% (p-i-n structure) is achieved and the reproducibility of PTAA-based PSCs is improved with significantly reduced process time compared to the existing solution blend doping (SBD) method. To compare the SBD and ID strategies, both doping methods are analyzed from an electrochemical and morphological viewpoint. As a result, it is confirmed that the ID method improves the thin film properties of PTAA, and the maximized dispersion of F4-TCNQ by 2-butanone achieves effective doping of PTAA, enabling the realization of high-performance PSCs.

EH-WeP-4 The Role of Artificial Intelligence in Minimizing Analysis Errors, Illustrated with EXAFS, Nanoindentation, and Core Level Photoemission, *Jeff Terry*, Illinois Institute of Technology

We have developed artificial intelligence based methodology that can be utilized to reliably analyze experimental results from Extended X-ray Absorption Fine Structure (EXAFS) measurements. This development will help to address the reproducibility problems that slow research progress and inhibit effective tech transfer and manufacturing innovation in these scientific disciplines. A machine learning approach was applied to the analysis of extended X-ray absorption fine structure (EXAFS) spectroscopy measurements collected using a synchrotron radiation facility. Specifically, a genetic algorithm was developed for fitting of the measured spectra to extract the relevant structural parameters. The current approach relies on a human analyst to suggest a potential set of chemical compounds in the form of feff.inp input files that may be present. The algorithm then attempts to determine the best structural paths from these compounds that are present in the experimental measurement. The automated analysis looks for the primary EXAFS path contributors from the potential compounds. It calculates a goodness of fit value that can be used to identify the chemical moieties present. The analysis package is called EXAFS Neo and is open source written in Python. It requires the use of Larch and Feff for calculating the initial EXAFS paths. We have recently extended the code to make use of Feff8.5lite so it can calculate the paths needed for populating the analysis from within the EXAFS Neo package. We have expanded the use of the base genetic algorithm software to fitting of Nanoindentation, X-ray astronomy data, and to the analysis of core level photoemission. The publication describing the analysis package and where to obtain the software can be downloaded at: <https://doi.org/10.1016/j.apsusc.2021.149059> or by contacting the speaker.

Wednesday Afternoon, December 14, 2022

EH-WeP-5 In Situ Cryo-Xps Analysis of Intercalation Mechanism in Aqueous Zn-MnO₂ Batteries, *Bhuvana M. Sivakumar, H. Chang, K. Hankins, M. Fayette, V. Shutthanandan, V. Murugesan, D. Choi, X. Li, D. Reed*, Pacific Northwest National Lab

Aqueous Zinc ion batteries (ZIB) based on Zn²⁺ intercalation chemistry is gaining attention as large scale energy storage system due to zinc's high capacity (820 mA h g⁻¹), high abundance and stability along with lower material costs. However, a comprehensive understanding of the principles governing Zn-MnO₂ electrochemistry has not yet been achieved. In particular, the identity of intercalating cationic species (i.e. Zn²⁺ and/or H⁺) and subsequent redox evolution in MnO₂ cathode material is still not clear. Towards understanding the electrochemical changes in the MnO₂ cathode (such as oxidation changes at metal centers) during the battery cycling process, we employed *in situ* cryogenic x-ray photoelectron spectroscopy (cryo-XPS) technique. Our unique *in situ* coin cell setup coupled with cryo-XPS characterization uniquely reveals the chemical identity and distribution of active participants in MnO₂ cathode under various charge and discharge conditions without the need for disruptive sample preparations such as solvent washing or Ar sputtering. By preserving the interface, we observed the broadening of Zn 2p core spectra indicating the evolution of Zn-O and Zn-SO₄ bonding environment during long term cycling process (up to 200 cycles). Similarly, the Mn 2p core spectra reveal the emergence of Mn³⁺ from parent Mn⁴⁺ indicating the Zn intercalation induced redox reactions within cathode material. These new molecular-level insights about the intercalation mechanism and subsequent redox state changes will be discussed based on electronic states evolutions within MnO₂ cathodes.

EH-WeP-6 High-Generating Electrical Power of Chemo-Mechanical Energy Harvesters from Carbon Nanotube Yarn Twist, *Seongjae Oh*, Department of Energy Science Sungkyunkwan University, Republic of Korea; *S. Kim*, Department of Advanced Textile R&D Korea Institute of Industrial Technology, Republic of Korea

The ocean covers 70% of the Earth, and monitoring the ocean conditions (wave height, wave frequency, temperature, pH, etc.) that play an important role in modern life is emerging as an important technology. In the ocean, it is difficult to use secondary batteries or supercapacitors because the ocean has infinitely wide space and fluidity, so research on energy harvesting for self-powered is required. In this regard, research on chemo-mechanical harvesters that converts mechanical energy in the ocean into electrical energy has been recently conducted, and expectations for the possibility of using an actual self-powered system are growing.

Among chemical mechanical harvesters, a carbon nanotube (CNT) based chemo-mechanical harvester was reported in 2017[1]. The chemo-mechanical harvester showed remarkable harvesting performance of frequency normalized peak power or highest peak power between a few Hz and 600 Hz compared to other types. This harvester used a coiled CNT yarn made by highly twisting a CNT yarn. As stretching the coiled CNT yarn, the density of the coiled CNT yarn increases. When the density of the coiled CNT yarn increases, it is to escape the ions of the electrochemical double layer formed on the surface of the CNT inside the coiled CNT yarn, just like water comes out when a wet towel is pulled out. In this way, the mechanical contraction is converted into electrical energy. In this work, to improve the performance of this harvester, we propose a novel internal structure that can facilitate ion access inside the coiled CNT yarn and maximize the density change when the coiled CNT yarn is stretched[2]. The coiled CNT yarn with a novel internal structure has four times the peak power and more than twice the efficiency compared to the performance reported in 2017[1]. This structure opened up the possibility to further improve the performance of the harvester and it was analyzed by molecular dynamics modeling. Our results are expected to contribute to the implementation of self-powered IoT systems in the ocean.

Ref.

[1] S. H. Kim et. al, "Harvesting electrical energy from carbon nanotube yarn twist" *Science* 357, 773-778 (2017)

[2] S. Oh et. al, "Chemo-mechanical energy harvesters with enhanced intrinsic electrochemical capacitance in carbon nanotube yarns" *Advanced science* accepted (2022)

EH-WeP-7 TOF-SIMS Analysis for Power Semiconductors, *Jaeyeong Lee, Y. Jeong, H. Moon, J. Jin*, Korea Basic Science Institute, Korea (Democratic People's Republic of)

Power semiconductors convert, control, and distribute power in electronic devices, which increases battery life and reduces power usage, which is very important for improving the efficiency of energy harvesting devices.

Power semiconductors are being applied in various energy harvesting fields such as batteries for electric vehicles and solar power generation, and the demand is increasing due to the rapid growth of mobile devices such as smartphones. Among them, power semiconductors using Silicon Carbide (SiC) are attracting attention due to their small size and stability against high temperature and high voltage, but they are experiencing difficulties in developing more diverse devices due to the advanced technology required for production. In this study, we have conducted analysis for Power semiconductor using Time of Flight Secondary Ion Mass Spectrometry (TOF-SIMS). Using TOF-SIMS, it is possible to check the behavior of component ions by depth of the metal-oxide-semiconductor field-effect transistor (MOSFET) device through depth profile analysis as well as the distribution of ion components on the surface of the device. By comparing the TOF-SIMS data of a device that failed due to exposure to harsh environments such as high temperature and high humidity with that of a normal device, it was possible to check where the change occurred in the case of a failure and the change in components. In Figure 1, the failed device was analyzed using TOF-SIMS. Ti⁺ and Al⁺ were mainly detected at the interface of the junction, and Si⁺ ions, an insulating film component, were observed at the interface of the gate pad. In addition, a lot of Si⁻ and P⁻ ions were detected at the defective site. The distribution of Si⁺ in the underlying layer of Al⁺ ions indicates that the wire bonding lift occurred at the junction of the Al metal and the underlying Si layer.

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