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המחלקה למדע והנדסה של חומרים

אלה שמתאהבים בבעיה
הם אלה שממציאים לה פתרון

Synthesis and Performance of Pt/Mo_2C Nanotube Catalyst for Oxygen Reduction Reaction

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Abstract

Our work investigates new ways of increasing the oxygen reduction reaction (ORR) catalyticactivity without harming the durability of the catalyst. Recent studies have focused on molybdenum carbide (Mo_2C) as a platinum support instead of the traditional carbon black. Mo_2C shows greater stability in ORR catalysis, has a stronger connection to Pt than carbon and shows Pt-like ORR catalytic performance giving it the ability to function as a catalyst without Pt as well. With all these great factors, Mo_2C still lacks in stability and undergoes corrosion in acidic ORR conditions.Previous studies show that the addition of Ta to Mo when synthesizing the carbide improves its stability. Therefore, in our research we used Mo_2C and Mo_2C+15 mol% Ta nano tubes as supports for Pt catalysts, testing their corrosion stability and ORR kinetics, while comparing the results to supports that do not have nano scale morphology. Both supports were synthesised via a salt flux method, and the platinum was deposited via borohydride reduction method. The ORR analysis reveals that the addition of Tantalum decreases the ORR kinetics for Pt Mo_2C supported catalysts with nanotube morphology and the corrosion resistance for those supports increased. A comparison to former studies indicates that downscaling the morphology to nano scale results in a significant increase in electrochemically active surface aria (ECSA), and an improve in ORR kinetics as well.

Ar–Annealing of Vertically Aligned Carbon Nanotubes for Homogeneity Enhancement

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Abstract

CNTs are one of the most promising materials in nowadays technologies. They have extraordinary properties, including remarkable mechanical properties, and high electrical and heat conductance. CNTs have great potential for large scale applications in many fields such as thin-film transistors, energy storage, and composite materials. However, this potential was not fulfilled yet because of three main challenges: poor dispersion, chemical inertness, and orientation loss. Using vertically aligned carbon nanotubes (VACNT) architecture, poor dispersion and orientation loss can be solved. Nevertheless, VACNT present a new problem of difference in coating accessibility between the center and the peripheries. To increase accessibility to the VACNT center without damaging the architecture, a dry surface treatment was chosen – argon (Ar) annealing. This treatment should enhance the uniformity of the nanotubes by disposing amorphous carbon and decreasing the oxygen content and eventually enhance the homogeneity of further coating.

In this work, we studied the effect of Ar-annealing on VACNTs structure, chemical content, and morphological properties, using RAMAN, XPS, and SEM analysis respectively.

The results have shown that the oxygen content was decreased overall. The oxygen gradient was also decreased suggesting enhanced homogeneity. In addition, the aromaticity and the structure of the tubes wasn't preserved.

This technique could improve the quality and performance of VACNT based composites thus optimizing their based devices. Furthermore, these findings may contribute to the understanding of thermal treatments effect on VACNTs and inspire further research that will help utilizing them in the industry.

Revealing Structural Trends of n-Alkanethiolate Self-Assembled Monolayers on Bismuth Thin Films

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Abstract

Bismuth is an exotic semimetal with a long Fermi wavelength, which makes it ideal for the probing of quantum confining effects. This paper presents an initial structural characterization of n-alkanethiols self-assembled monolayers formed on bismuth thin films, performed by static contact angle measurements, X-ray Photoelectron Spectroscopy (XPS), and Scanning Electron Microscopy (SEM). The contact angle results reveal the existence of three structural regimes in the order of formed SAMs: pseudo-forming (C6-C8), liquid-like (C9-C12), and solid-like (C14-C18), where the solid-like has a high hydrophobic behavior. In addition, we found that lowering the substrate's roughness enhances the SAMs' density but simultaneously detracts from their hydrophobicity. This discrepancy probably hinges upon the incompatibility of the template-stripping step under these given conditions, which is proved by the observation of pinholes under SEM imaging. Furthermore, we optimized the conditions of ammonium sulfide treatment, which aims to remove the bismuth's native oxide. We confirmed its efficacy through an XPS survey scan, which exposed a Bi_2O_3 peak attenuation after the treatment. The appearance of the Bi_2S_3 peak indicates the replacement of the native oxide by Bi_2S_3 coating.

Predicting The Metallicity of Compounds Using a Machine Learning Approach

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Abstract
A machine learning model was developed to successfully classify inorganic compounds of metals and nonmetals using a minimal set of 3 structure-based and lattice features. This classification model was created using an artificial neural network (ANN) trained on the Materials Project (MP) database (DB) of density functional theory (DFT) computations. The network used the binary cross entropy cost function and gradient descent optimization algorithm to perform its supervised learning process. The created machine learning tool can help in the screening of solid-phase inorganic compounds, speed up long DFT calculations, and focus synthesis efforts for novel and newly developed materials.

Exploring The Capability of Geometrical Prediction of Cleavage in Single Crystals

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Abstract

Cleavage is a common and important physical property of a crystalline materials. It describes the ability of a single crystal to break easily along a specific plane. A wide variety of industries use crystalline materials and thus could benefit from understanding their cleavage related properties. Acquiring a reliable data about cleavage is critical for understanding brittle fracture, plasticity and strength of crystalline materials and that way predict and prevent catastrophic failures. The prediction of promising cleavage planes in materials in this project was preformed using GALOCS (GAp LOcations in Crystal Structure), a geometrical based program previously written using MATLAB[1]. GALOCS calculations were based on the of the average electron density within a specific plane that depends on the crystallographic structure of the material. The main goal of this projects was to search for materials with the potential of having special and non-trivial predicted cleavage planes in order to research their cleavage properties practically in the future. The results given by GALOCS were analyzed using a graphical illustration of the value of the planar gap. This project final findings were two crystals, BaY_2F_8, and $Au_2Cs_2X_6$ $(X = Cl, Br, I)$. The cleavage plane found for BaY_2F_8 is (100), and the cleavage planes found for cubic $Au_2Cs_2X_6$ were (100) and (110), and for tetragonal $Au_2Cs_2X_6$ were (110) and (001).

Free-standing Perovskite Membranes by Epitaxial Growth on a Sacrificial Layer Followed by Selective Etching

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Abstract

We grow an epitaxial water-soluble $Sr_3Al_2O_6$ thin films to be used as sacrificial layers for future synthesis of free-standing perovskite membranes. We used the pulse laser deposition technique with in-situ monitoring by reflection high energy electron diffraction (RHEED). This method provides a general approach for producing **2**D crystalline membranes of perovskite oxides with a broad range of physical and chemical properties. Our process allows integration with a wide range of applications such as high-efficiency capacitors and solar cells. The release of the membrane by selective etching of the sacrificial layer is less destructive than the standard physical methods. The sample retains its structural quality after the membrane is released.

We have faced a few challenges during the project; we describe how we overcome them. Initially, we successfully synthesized a $Sr_3Al_2O_6$ pellet. We then used it to grow an epitaxial $Sr_3Al_2O_6$ water-soluble sacrificial layer by Pulsed laser deposition. We were able to preserve the step-and-terrace structure of the $SrTiO_3$ substrate obtained using a detailed etching and annealing process. Subsequently, we successfully grew a praseodymium cerium copper oxide thin film on top of the sacrificial layer. The final step was the release of the membranes and transferring them to arbitrary substrates. This last step is still in an optimization process. There is a need for further study and optimization of the release of the free-standing membranes and the transfer to arbitrary substrates.

Our work solves the problem of how to efficiently synthesize atomically smooth $Sr_3Al_2O_6$ films, paving the way for exploring incorporating 2D crystalline perovskite membranes with heterostructures in semiconductors and layered compounds.

Calcific Aortic Valve Microstructure and Chemical Characterization Utilizing Tomography and Microscopy Methods

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Abstract

The aortic valve, located between the left ventricle and the aorta, is responsible for maintaining an outward unidirectional flow. A common aortic valve progressive disease the calcific aortic valve disease (CAVD). This disease is characterized by calcification growth in the aortic valve cusps leading to thickening and stiffening of their tissues. Eventually, CAVD will lead to aortic stenosis and malfunction that ultimately lead to the valve's replacement.

In this project, our goal was to examine the microstructure and the chemical compositions of the calcium deposits. Towards that goal, the microstructure was investigated using computed tomography (CT) scans and reverse calcification technique (RCT) that recreate the different calcification growth stages. Utilizing the RCT, the initiation sites of the calcification were predicted, and additional insightful observations of the calcification development patterns were exemplified. This further extends the predictive capabilities of RCT, and with further studies validating the calcification progression rates, it may aid in the decision of whether an intervention is required for each patient.

In addition, a chemical characterization process using scanning electron microscopy (SEM-EDS) and X-ray Photoelectron Spectroscopy (XPS) was done in order to determine the elements and compounds that exists in the calcification. The results showed that the calcification consists mainly of the elements oxygen, calcium, phosphorus and carbon and different calcium phosphate compounds.

This approach was examined in its ability to enhance the current known calcium deposits formation aspects in-part by inspecting its detailed heterogeneous structure.

Hydrogen Gas Sensing Using Electrostatically Formed Nanowire

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Abstract

This project deals with hydrogen gas sensing using an electrostatically formed nanowire (EFN) device with a palladium (Pd) layer in contact with a silicon dioxide (SiO_2) layer, while focusing on the special interaction between Pd and hydrogen gas. As a result of this unique interaction, the device is highly sensitive to hydrogen gas presence and has a great potential as a hydrogen gas sensor. In the project, a new mathematical model is suggested in order to link between the theoretical simulations and real device measurements. This link allows an accurate assessment of the hydrogen concentration in the environment of the sensor, as well as the assessment of the optimal working voltage range to provide a wide detection range. The model relays on the fact that hydrogen gas is absorbed to the Pd\SiO_2 interface and changes the work function of the Pd. The hydrogen gas is absorbed to the interface as a dipole layer and changes the dimensions of the EFN. Therefore, the current measured through the device changes as a function of the hydrogen concentration. After composing the model, it was validated using real device measurements and device simulations, and a dynamic working voltage map was created. From this map, the predicted optimal working range can be extracted, as well as the range in which the device does not function at all.

Electron-Beam-Induced Photoresist Shrinkage Trends

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Abstract

Scanning Electron Microscopy (SEM) is frequently used as a method for process monitoring and control in the semiconductor industry. The method utilizes electron-beam for detection of defectivity and for metrology in the chip manufacturing line. Each lithography step performed on silicon wafers in chip manufacturing process requires the use of photoresist (PR) materials. These PRs are electrons sensitive. Interaction with electrons can result in PR dimension changes which might affect chip performance and manufacturing process yield.
This work aims to examine and quantify PR shrinkage under varying SEM imaging conditions, in order to gain understanding of shrinkage dominant factors, and define the required application envelope that will enable defectivity and metrology monitoring with minimal trace.
To serve this purpose, SEM exposures were performed on a stripe patterned ArFi PR layer, which was implemented on a silicon wafer. In each set of exposures, single electron-beam parameter was changed while the other maintained constant. In such a manner, the shrinkage effects of electron dose, probe current, acceleration voltage and pixel illumination time were differentiated. Thereafter, the SEM trace was evaluated using Atomic Force Microscopy imaging, and PR shrinkage magnitude was measured.
Several trends were identified. The higher the electron-beam acceleration voltage was, the more severe was the PR shrinkage. Shrinkage enhancement was also detected when electron dose was increased in a high enough acceleration voltage. When voltage was low, saturation in shrinkage was observed, even though dose was raised. Pixel time and probe current variation was not observed as an effecting factor on PR shrinkage. Therefore, it is reasonable to conclude that minimal SEM trace can be achieved in low acceleration voltages and small electron doses. With regard to pixel illumination time and probe current, additional studies have to be conducted for trends to be determined.

Development and Fabrication of a Novel Microfluidic Device Using Photolithography

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Abstract

Here we develop a novel microfluidic glass cell for measurements within an optical tweezer device, using photolithography. The main landmarks in this work are the creation of photoresist structures on top of two glasses with different thicknesses, capillary manufacturing for micropipette aspiration and gluing & alignment methods. In addition, a specialized holder for the new microfluidic device was designed and manufactured. The motivation of this project is the need to combine two different methods of experimental measurement in one glass cell: Microfluidics, and Micropipette Aspiration. Combining micro-pipette aspiration within a micro-fluidic device will allow greater experimental flexibility for learning about the processes that occur at cell membranes and understanding of membrane fusion during infection of enveloped viruses.

Controlled Dielectric Breakdown Based Solid State Nanopores for Molecular Junctions Fabrication

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Abstract

Our study presents first steps in a novel molecular ensemble junctions (MEJ) fabrication process, based on metalized nano-sized pores perforated by controlled dielectric breakdown (CDB). Beside its relative simplicity to operate and its low cost, this perforating method can result in a wide range of relatively low diameter nanopores (from a few nanometers to tens of nanometers). Thus, after nanopores metallization, this method allows for a conductive channel formation with a cross sectional size in the order of magnitude of the Fermi wavelength of Bismuth, which is the intended metal for this device. As a result, quantum phenomena of electron transfer (such as electron interference), which are highly significant for the nano-electronics field, are suggested to be observed. In the first part of our work, a multiple micro and nano fabrication steps process has been developed for creating micron-scaled solid-state membranes (made of Silicon Nitride) which the pores are "drilled" on. Next step involves the fabrication of the pores themselves, focusing on optimizing the fabrication process by studying different approaches for applying the CDB method and performing post-CDB pore-shape enhancement processes for adjusting the nanopores shape to our application. Finally, we attempt to characterize our system with both Scanning Electron Microscopy and electrical measurements, for a better observation of our system feasibility. Our results demonstrate our ability to fabricate CDB based nano-sized pores, enhance their shape in voltage and etching based processes, and construct a metallic channel inside of them with a cross sectional radius of a few tens of nanometers. This study also indicates our process difficulties, as lack of repetitivity and nanopores delocalization, which are suggested to be addressed by different approaches which are already investigated in our lab.

Print Mechanical Properties Evaluation by Nano-Scratch and Development of Real-Time Scratch Analysis.

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Abstract

Polymeric thin films are used in various applications and in the print industry. A print is an ink-substrate system with additional functional layers, and high scratch durability is a desired property. The most common method to characterize scratches is with scratch tester using the critical loads method. The project objectives were to present a new approach for mechanical properties characterization of ink layer using scratch tests, compare the scratch resistance of different ink formulations, and present a new set-up for real-time scratch analysis. Four samples were printed with different ink formulations on Polyethylene terephthalate substrate with no additional layers. The first sample is HP Indigo's Electroink® (IE), and the second is IE with a crosslinker. The other two samples have different resins and one of them had been thermally treated (PEM and PEM+TT). The samples were tested using a Tritech -Anton Paar nano-scratch instrument and the scratches were recorded using the in-situ set-up. The failure modes and critical loads were examined using a scanning electron microscope and optical microscope. Critical loads analysis was also performed using the in-situ method and compared to the optical ex-situ method. During the scratch, cohesive and adhesive failures can develop. The thermal treatment and crosslinker addition improved the print resistance both to cohesive and adhesive failures. IE samples show higher resistance to crack formation, high plasticity, and higher elastic modulus compared to the PEM samples, but lower resistance to delamination considering the thickness. The mechanical properties characterization presented, show good sensitivity to changes in the ink formulation and suggest different ink's durability mechanisms. The in-situ method shows good accuracy in detecting the critical loads and the elastic recovery can be seen. The method can be used to analyze the material's scratch resistance in a quicker and more statistical characterization.

Detection and Modeling Gold Nanoparticles Inserted into Plant Cells

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Abstract

Nanotechnology which consists of a matter with dimensions in the nanoscale, opened up a huge potential for innovative developments in medicine in different research fields, like: drug delivery, gene therapy, biosensing. For medicine, this new technology brings many advantages, such as: greater cell specificity, sensitivity and efficiency. Gold nanoparticles (i.e. AuNPs) are well known due to their double role as drug carriers for targeted delivery of therapeutics into the cell as well as biomolecule nanoprobes detection and monitoring target molecules. Gold nanoparticles are very popular due to great characteristics, like: biocompatibility, different shapes, narrow size distribution, surface modifications are simple, high surface area to volume ratio, non-cytotoxic.

This work investigates drug delivery to cells by gold nanoparticles. By inserting AuNPs in a size about 30(nm) into cells which conjugate with DNA strands, it is expected that for complementary DNA strands a hybridization event will occur on the AuNP. This event can be detected by a unique electrical impedance signal. These electrical characteristics are monitored by electrical impedance spectroscopy in the low frequency range consists of 4Hz to 5MHz. The experiment is based on a comparison between non-complementary DNA strands to a complementary DNA strands which are mixed (separately) with DNA-AuNPs conjugates. The results show that different signal of impedance is obtained for the sample contains complementary DNA strands, meaning that hybridization event has occurred. Hence, specificity is achieved in the binding of two complementary DNA strands. Another finding is that heating/cooling cycle and frequency are two factors which affect hybridization event.

Examination of Fibrin and Thrombin Hydrogel - A Working Protocol.

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Abstract
Natural polypeptide-based hydrogels are potentially good candidates for tissue engineering and drug delivery as they meet the desired functionality, reversibility, sterilizability and biocompatibility for biological and biomedical uses. Hydrogels are considered a viscoelastic material who show behavior somewhere between that of an ideal liquid (viscous) and ideal solid (elastic) able to store part of the energy transferred to it through a deformation as elastic energy. In this research a Fibrin hydrogel was polymerized using Thrombin and PBS for hydrolyzation. The best polymerization conditions were examined in additional to the mechanical characteristics using a rheometer. A rheometer monitors the deformation of the hydrogel in response to applied force using different rates and duration of the force/displacement applied.
In this research, the rheometer was used based on rotational forces using small oscillatory movement. The final setup was changed by using different geometries (plates with changing radiuses) and gaps (final distance from the sample). When starting the rheometer characterization, the torque applied can be determined by final strain% applied on the gel (also known as the oscillation amplitude) or the frequency at which the plate will turn (i.e., how many times a second the plate turns).
According to the results, a protocol was written including the best polymerization conditions of the hydrogel, basic steps needed to operate the machine and specific instructions on how to use it as the analytical tool for mechanical characterization of the Fibrin.

A Study by Evolutionary Algorithms Simulations to find new Bismuth Oxide Phases

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Abstract

In this research project the phase space of 1-1 ratio Bismuth oxide is investigated using the USPEX (universal structure predictor: evolutionary xtallography) evolutionary algorithm code and VASP (Vienna Ab Initio Simulation Package) ab initio calculations. new undiscovered Bi_xO_x structures are found which are predicated by our calculations to exhibit lower enthalpy of formation than any other previously known structure.