New Horizons in Coatings and Thin Films
Room Royal Palm 1-3 - Session F3

2D Materials: Synthesis, Characterization, and Applications

Moderators: Haitao Liu, University of Pittsburgh, USA, Jiaxing Huang, Northwestern University, Liping Wang, Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences

2:10pm **F3-3 Tunable MoS_2 and MoS_2-based Electrocatalysts by Hot-injection Method for Hydrogen Evolution Reaction***, **Chia-Ling Wu**, P Huang, S Brahma, J Huang,* National Cheng Kung University, Taiwan*; S Wang,* Southern Taiwan University of Science and Technology, Taiwan

Hydrogen has been considered as one of the most promising renewable energy for production and storage to replace petroleum-based energy. The 2D structure and the presence of several effective active sites make MoS_2 an excellent electrocatalyst for hydrogen evolution reaction (HER). However, the most common syntheses nowadays are not only expensive but also time-consuming. Here, we report an efficient, fast and tunable hot-injection method to prepare MoS_2 and MoS_2-MoO_2 composite with/without tributyl phosphate (TBP). MoO_3 with oleic acid (OA) and S powder with oleylamine (OLA) are used as Mo- and S- precursor, respectively. With increasing reaction temperature and time, OA reorganize the octahedral units of MoO_3 and gradually turn into low valence of Mo. Fourier transform infrared spectroscopy (FT-IR) clearly shows the increase/decrease of the intensity of M=O and 2Mo-O bond vibrations. After injecting S-precursor, OLA first reduces Mo-precursor to MoO_2, and then S atoms replace O atoms to form MoS_2. The addition of a drop of tributyl phosphate (TBP) as surfactant in Mo-precursor significantly accelerate the production of MoS_2 via MoO_2 as the intermediate phase ($MoO_3 \rightarrow MoO_2 \rightarrow MoS_2$). The X-ray diffraction (XRD) (Fig.1) shows that the peaks of MoS_2 dominate by adding TBP, and the peaks of MoS_2 and MoO_2 are equal without adding TBP. Scanning electron microscope (SEM) shows the uniform layer like morphology of nanoscale MoS_2. Transmission electron microscopy (TEM) confirms the existence of few-layer MoS_2 with abundant edge sites (Fig.2) and the core-shell MoS_2-MoO_2 structure (Fig.3), respectively. HR-TEM image shows the MoS_2 (002) plane and d-spacing is measured as 0.62 nm. This simple, flexible and tunable synthesis has large potential for the production of MoS_2 and MoS_2-MoO_2 composite. High purity of MoS_2 and MoS_2-MoO_2 composite can combine with other materials for energy conversion and storage. The detailed electrochemical properties on HER will be reported in future.

2:30pm **F3-4 High-throughput Combinatorial Synthesis and Multimodal X-ray Analysis of Co-based Ternary Alloys***, **Janak Thapa**, C Gross, V Hegde, L Ward, S Naghavi, C Wolverton, Y Chung, M Bedzyk,* Northwestern University, USA

Cobalt-based superalloys have excellent high temperature properties such as creep resistance and chemical inertness during applications at elevated temperatures. Potential applications include high performance jet engine turbine blades and ultra-supercritical steam driven power plants. In this work, we undertook efforts to begin filling in the database gap of Co-based ternary systems. Such a database will facilitate the design and development of Co-based superalloys. We have observed new phases in previously empty regions. We use the naturally scalable techniques of photolithography, DC magnetron sputtering, and high-flux X-ray analysis for high-throughput studies. Gamma and gamma-prime phases, which are essential for high-temperature applications of conventional superalloys, are also being identified. High-throughput DFT is being employed to efficiently determine crystal structures based on X-ray data. These phase diagrams will provide a foundation of understanding to accelerate the creation and implementation of novel Co-based superalloys, and potentially other alloy systems.

2:50pm **F3-5 Development and Characterisation of Cost-Effective Graphene Oxide-Nickel Nanocomposite Coatings***, S Qi, X Li, **Hanshan Dong**,* The University of Birmingham, UK

Graphene is a very attractive new carbon-based coating material due to its extraordinary mechanical, thermal, chemical and optical properties. Notwithstanding the fact that some nano/micro scale studies have shown the potential of graphene as tribological and anti-corrosion coatings on Cu and Ni, its application for coatings on other metallic materials has yet to be fully explored. This is mainly due to the high cost and low yield of pristine graphene produced by exfoliation and the difficulties in transferring CVD-grown graphene films onto 3D real engineering surfaces with necessary bonding. Hence, how to cost-effectively deposit large-area graphene coatings on metallic materials for corrosion and wear protection is a scientifically interesting and technologically important research area.

One possible solution is to use relatively low-cost graphene oxide (GO) in metallic matrix composite. In this work, a nickel/GO composite coating was deposited on steel using a purposely developed electrochemical deposition method to ensure homogenous distribution of GO in the matrix. The deposited Ni/GO coatings were fully characterised using XRD, FIB/SEM, Raman and TEM; their mechanical and tribological properties were evaluated using nano-indentation and friction/wear testing. The thermal stability of the Ni/GO coatings was investigated by thermal annealing at 100, 200, 40 and 600ºC for 30min.

The experimental results reveal that transparent and silk-like graphene oxide sheets are randomly distributed in the Ni matrix. As a result, the hardness and Young's module of Ni coating can be increased by 56% and 29% respectively due to the reinforcement and refinement of the matrix by GO sheets; the coefficient of friction is reduced from 0.6 for Ni to 0.4 for the Ni/GO nanocomposites and the wear rate is reduced by about 90%. Most importantly, the thermal stability of Ni coating can be significantly improved by adding GO. For example, when annealed at 400ºC for 30min, while the hardness of Ni coating was reduced by 36% no appreciable reduction in hardness was observed for the Ni/GO nanocomposite coatings.

3:10pm **F3-6 Fabrication of Functional Graphene Reinforced Polyurethane Nanocomposite Coatings with Regular Textures for Corrosion Inhibition***, **Wenjie Zhao**,* Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, China

In order to further enhance its anti-corrosion properties as a surface coating for protecting various materials from corrosion, polyurethane (PU) needs to be modified by adjusting the chemical composition and interface structure. In this work, a series of functionalized graphene (FG) reinforced PU nanocomposite coatings with regular texture were fabricated using a replication method. The structural and morphological properties of the as-prepared PU composite coatings were characterized by Fourier transform infrared spectroscopy, Raman spectroscopy, X-ray photoelectron spectrometer, transmission electron microscopy, scanning electron microscopy and atomic force microscopy. Results showed that FG was dispersed homogeneously in the PU matrix after chemical modification. Moreover, the morphology of the obtained coatings showed a circular cone with a diameter of 8 µm spaced 8, 6 and 4 µm apart, respectively. Most importantly, the presence of surface texture and well-dispersed FG effectively enhanced the anti-corrosion properties of the textured FG/PU composite coating. It is attributed to the hydrophobicity and barrier effect of the obtained coatings, which not only reduce the contact and interaction between water and the surfaces, but also increase the tortuosity of the corrosive medium diffusion pathway.

3:30pm **F3-7 Structure and Tribological Properties of TiSiCN Coatings Incorporated with Layered Structure of MAX Phase in Artificial Seawater***, **Jinlong Li**, Y Wang, C Dang, L Wang, Q Xue,* Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, China

The TiSiCN coatings were fabricated on Ti6Al4V alloy by arc ion plating at 500 º C. In order to obtain a MAX phase with like graphic layered structure, the different bias voltages were employed during the deposition of the TiSiCN coating. The structure of the TiSiCN coating were characterized using Scanning electron microscopy, X-ray diffraction, X-ray photoelectron spectroscopy and Transmission electron microscopy. The hardness and tribological properties of the TiSiCN coating were evaluated by nanoindentation, potentiostat and ball-on-plate wear tests. All TiSiCN coating shows a coupled structure of a TiN nanocystallite / Si_3N_4 amorphous. When the negative bias voltage increases to 100 V, some Ti_3SiC_2 MAX phase with a like graphic layered structure also is found in the TiSiCN coating. The TiSiCN coating has a higher hardness of 40 GPa. The MAX phase with a layered structure contributes to significantly decrease of the friction coefficient and wear rate of the TiSiCN coating. The imposed protection potential has a positive effect on protecting the coating from electrochemical corrosion. However, the cracks inside the coating will accelerate the coating failure.

3:50pm **F3-8 Graphene: Improving Material Performance by Keeping the Surface Cleaning***, **Haitao Liu**,* University of Pittsburgh, USA

Recent studies showed that graphitic materials can be easily contaminated by airborne and waterborne hydrocarbons. In this talk, I will discuss ways to protect a graphitic surface from airborne contamination. It was shown that a monolayer thick of water film significantly slows down the adsorption of airborne hydrocarbon. The water-protected graphitic surface showed extreme high electrochemical activity; the measured heterogeneous electron transfer rate is even higher than that of a Pt electrode.These results highlight the potential to achieve intrinsic material properties of graphitic materials under ambient environments.

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