Studies of Dynamic Material Interfaces in Extreme Environments

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The scattering of atomic and molecular beams from well-characterized surfaces is an incisive method for studying the dynamics of gas-surface interactions, providing precise information on energy and momentum transfer as well as complex reaction mechanisms. Scanning probe measurements provide a powerful complement to scattering data as SPM measurements give a direct route to the visualization and spectroscopic characterization of interfacial atomic and nanosystems. This AFOSR program is examining critical aspects of the chemical and physical behavior of dynamic material interfaces operating in extreme environments. Extreme conditions encompass high and low temperature regimes, high velocity gas flows, optical and charged particle illumination, and severe oxidative environments where interfacial aerodynamic performance (energy and momentum transfer characteristics), morphological change, and chemical stability need to be assessed and quantified.

We will report at this year's meeting on several achievements: (i) Our newest scattering instrument which combines supersonic beam surface interactions with *in situ* STM visualization is now fully operational, as shown in a comprehensive study of graphite oxidation [1,2], now examining GaAs oxidation [3] and N_2 dissociation. In support of aerothermodynamic calculations, we have conducted scattering experiments where we monitor velocity and angle distributions for energy transfer of atmospheric gasses, important for calculating aerodynamic drag, heating of the flight surface, and boundary layer heat transport. We have measured the energy exchange of a monoenergetic molecular beam of N_2 colliding with the SiC(0001) surface. This was done at different incident angles and with incident N_2 energies between 100 and 850 meV and surface temperatures of 600 K and 1200 K. We also compared the experimental results with those of a monoenergetic atomic beam of Ne, which helps elicit information about how internal degrees of freedom affect energy exchange with the surface. We are in the process of comparing the experimental results with MD simulations. We have also extended our studies of energetic interactions with ice [4], including embedding of neutral species into crystalline, amorphous, and porous ice. This is an important new mechanism for understanding gas-surface energy & momentum exchange in high velocity gas flows with ice and thin molecular films. Moreover, we have demonstrated a new method for the separation of isotopologues and isotopes [5]. We use the threshold for molecular or atomic embedding into ice as a gateway filter for the preferential absorption of heavier species. This isotope selectivity during deposition may open new routes for *in-situ* isotopic materials engineering. Finally, we continue to innovate precision elastic and inelastic neutral helium atom scattering as an insightful and unique tool for probing, *in situ*, the structure and dynamics of complex interfaces [6].

Selected Recent Publications

1. Atomically-Resolved Oxidative Erosion and Ablation of Basal Plane HOPG Graphite Using Supersonic Beams of O_2 with Scanning Tunneling Microscopy Visualization, Ross Edel, Tim Grabnic, Bryan Wiggins, and S. J. Sibener, *J. Phys. Chem. C* 122, 14706-14713 (2018).
2. Chemical Dynamics Simulations and Scattering Experiments for O_2 Collisions with Graphite, Moumita Majumder, K. D. Gibson, S. J. Sibener, and William L. Hase, *J. Phys. Chem. C* 122, 16048-16059 (2018).
3. Room Temperature Oxidation of GaAs(110) Using High Translational Energy Molecular Beams of O_2 Visualized by STM, *Surface Science* 692, 121516/1-7 (2020).
4. Sticking Probability of High-Energy Methane on Ices of Astrophysical Interest, Rebecca S. Thompson, Michelle R. Brann, and S. J. Sibener, *J. Phys. Chem. C* 123, 17855-17863 (2019)
5. A New Method of Isotope Enrichment and Separation: Preferential Embedding of Heavier Isotopes of Xe into Amorphous Solid Water, K. D. Gibson and S. J. Sibener, *PCCP* 23, 7902-7907 (2021).
6. Material Properties Particularly Suited to be Measured with Helium Scattering: Selected Examples from 2D Materials, van der Waals Heterostructures, Glassy Materials, Catalytic Substrates,Topological Insulators and Superconducting Radio Frequency Materials, Bodil Holst, Gil Alexandrowicz, Nadav Avidor, Giorgio Benedek, Gianangelo Bracco, Wolfgang Ernst, Daniel Farías, Andrew Jardine, Kim Lefmann, James Manson, Roberto Marquardt, Salvador Miret-Artes, Steven J. Sibener, Justin Wells, Anton Tamtögl, and Bill Allison, *PCCP* 23, 7653 - 7672 (2021).