RESEARCH OBJECTIVES AND SUMMARY OF RESEARCH

The general purpose of our research program is to study problems relating to the atomic, molecular, and electronic processes occurring at gas-solid interfaces. Examples of these processes are: thermionic emission, surface ionization, adsorption, absorption, oxidation, catalysis by metals, electrode processes in electrical discharges, and the scattering of molecular beams from solid surfaces. Such processes are encountered in thermionic energy converters, ion propulsion engines, high-speed flight, and high-temperature nuclear reactors. At present, we are concentrating on the following problems.

1. Oxidation of Metals at High Temperature and Low Pressure

We have developed a quasi-equilibrium model of the reaction of gaseous O\textsubscript{2} with various solids (W, Mo, and C) at high temperature and low pressure where the reaction products (oxides) are volatile. Considering the simplicity of the model, the calculated evaporation rates of the various volatile products agree surprisingly well with existing mass-spectrometric data on these reactions, especially when we account for the fact that not all of the impinging molecules are equilibrated to the surface. We have recently computed the rate of "erosion" of tungsten by volatile oxidation and the results provide a semiquantitative explanation of experimental data. We are now considering other gas-solid systems (e.g., halogen-tungsten) and are attempting to gain a clearer understanding of the adsorption probability, which appears to be the rate-controlling factor. We are considering possible experimental techniques for measuring the adsorption probability as a function of pressure and temperature.

2. Adsorption of Gases and Vapors on Solid Surfaces

The objective of this study is to contribute to the development of a theory of adsorption of gases or vapors on solid surfaces. Our major effort has been directed toward obtaining experimental data on both the energy and dipole moment of the adsorption bond between the adsorbate and the substrate. The energy is determined from residence-time measurements based on a modulated molecular-beam technique, whereas the dipole moment is inferred from thermionic and contact-potential measurements of the change in work function during adsorption. To obtain surfaces that are both clean and well-defined, single-crystal specimens are employed, together with ultrahigh vacuum techniques. During the past year, we have constructed an apparatus for detecting surface impurities by Auger electron spectroscopy. This technique will also enable us to measure the concentration of the adsorbate on the surface.

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3. Adsorption, Permeation, and Desorption Processes for Gases Dissolved in Metals

We have constructed an experimental apparatus for measuring the spatial and speed distributions of H$_2$ desorbing from various metals; these data should lead to a better understanding of the process of "activated adsorption." Preliminary measurements for the desorption of H$_2$ and D$_2$ from nickel show that the spatial distributions are substantially narrower than the commonly assumed form of diffuse re-emission. We hope to develop a satisfactory explanation of the mechanism responsible for this nondiffuse desorption process, and our first step will be to improve experimental apparatus so that we may be certain that the surfaces of the single-crystal nickel samples are truly monocrystalline and are extremely pure (i.e., not contaminated by carbon, oxygen, sulphur, etc.). We propose to utilize LEED and Auger techniques in these experiments.

4. Catalytic Reactions at Gas-Solid Interfaces

The quasi-thermodynamic approach to heterogeneous reactions has also been applied to catalytic reactions, such as hydrogen dissociation and ammonia decomposition. In the future we plan to utilize molecular-beam and mass-spectrometric techniques to determine the kinetics of these reactions and others on catalysts having well-defined crystal structure and chemical composition, as determined by LEED and Auger techniques.

5. Scattering of Gas Atoms and Molecules from Solid Surfaces

We are employing modulated molecular-beam techniques to investigate the collisions of gas atoms and molecules with solid surfaces. The principal goal is to determine the dependence of energy and momentum transfer on the properties of the gas and the solid, and on the structure and composition of the surface. Data have been obtained for the scattering of rare gases and atmospheric gases from the (110) face of a tungsten crystal. The W(110) surface was intentionally contaminated with O$_2$ for the purpose of determining the sensitivity of the scattering pattern to the degree of surface contamination. These results illustrate the potential usefulness of low-energy molecular scattering (LEMS) as a technique for studying both the properties of solid surfaces and the dynamics of gas-solid collisions. At present, we are examining the possibility of using molecular-beam scattering as a means of determining the faceting of solid surfaces at high temperature.

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