Electronic Structures of Solids and Their Surfaces

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Research Scope and Objectives

The main objective of this effort is to improve the understanding of the electronic interactions among atoms in metals, alloys, metal oxides, and in certain compounds, some of which are technological materials. It is especially important to learn about differences between the interactions in the bulk of such solids and interactions at the surfaces, and interaction of surfaces with adsorbates in order to study the heterogeneous physico-chemical phenomena at the interface. These studies are being carrried out mainly through photoelectron spectroscopy with conventional photon sources as well as synchrotron radiation at the NSLS. Studies are also being made of the geometrical and electronic structures of condensed matter with emphasis on the systematics of the density of unoccupied states of elements, and structure and dynamic behavior of metal complexes in solution. This work, an application of x-ray absorption near-edge structure (XANES) extended x-ray absorption fine structure (EXAFS), has been carried out during visits at the Stanford SSRL and it will be pursued further at the NSLS. The results are directly related to certain aspects of the chemical reactivity, kinetics and mechanism.

Description of Research Effort

Our current effort has been centered on synchrotron spectroscopy at the National Synchrotron Light Source (NSLS). The first U-7 experiment at the NSLS involves the study of carbon films, in particular the use of carbon K-edge spectroscopy to investigate the "transition" of hydrogenated amorphous carbon prepared *in situ* by glow-discharge on Nb backing to graphitic carbon; and graphitic to carbidic "transition" of carbon layers on niobium (110). It is found that upon annealing hydrogen gas was evolved and the disorder amorphous film became order graphitic microcrystalline as indicated by the EXAFS results. The photoemission and near-edge structure also show that energy bands characteristic of graphite structure were formed as a result of heating (500-600°C). Annealing with high temperature results in the formation of thin graphite layers of NbC (as shown by photoemission measurements). The near-edge structure clearly shows the presence of narrow and high density of unoccupied carbon p states. This may be evidence for p_z orbitals of carbon perpendicular to the surface predicted by theory (Feibelman). This research is relevant to the study of catalytic behavior of carbon on metal surfaces.

A second carbon K-edge experiment involves the adsorption of hydrocarbons on transition metal surfaces. The absorption spectrum near the carbon edge reveals molecular orbital structures of definite symmetry which may be determined using the polarization dependence of the absorption cross section. From this the angular orientation of the molecule with respect to the surfce may be learned. We have found the orientation of C_2H_2 and C_2H_4 on Ni(111) by this method. Other metal + adsorbate systems will be investigated soon.

Future Research

In the future, efforts will be directed to:

(a) interaction of organic molecules with metal surfaces using synchrotron radiation (K-edge absorption of low z elements) at the NSLS VUV ring,

(b) charge redistribution upon compound formation and dissolution of heavier elements at the NSLS x-ray ring and other national facilities.