

Preface

It has been recognized for many years that the understanding and exploitation of solid state phenomena depend largely on the ability to accurately describe the microscopic structures of surfaces and interfaces, and to define correlations between those structures and physical and chemical phenomena of interest. Only during the last decade have experimental and theoretical tools been developed that make it possible to investigate surface structure and related surface phenomena in the required detail.

There has been a trend in technology to place increased emphasis on the use of materials in *thin-film form*, where the surface-to-volume ratio is large, and where solid-solid and solid-gas interfaces are prevalent. For example, in technologies that use magnetic films in recording devices, or microminiaturized semiconductor devices in large-scale-integrated circuits, the functional performance of those devices depends crucially on the ability to control the physical and chemical processes at surfaces and interfaces. In another example, continued efforts to increase the performance of FET devices rely on an understanding of the role of electron traps in such devices.

The papers in this issue present a cross section of the many aspects of surface science currently being studied within IBM and elsewhere. Several papers are directed toward fundamental aspects of these technologies. The two papers by DiMaria, Hunter, Serrano, and Young are concerned with the characterization and location of electron traps associated with the ion implantation of Al into SiO₂. Raider and Flitsch have studied the nature and chemical composition of the interface between Si substrates and a thin oxide overlayer. Ludeke reports on the electronic structure and surface states of ternary alloys of semiconductors.

Chuang and Wandelt are concerned with an analysis of the techniques used to examine the nature of interfaces between Ni and Fe films. Diffusion of material across such interfaces is relevant to the properties of metallic heterojunctions, and their studies may also help us to understand the preferential segregation of certain components of an alloy at a surface. Brundle presents a detailed study of the chemical reaction, at very low coverage, of CO and O₂ with Fe surfaces, which may serve as a prototype of early stages of corrosion chemistry for transition metals. Winters, for ethane on tungsten, and Demuth, for acetylene and ethylene on several metals, are concerned with the chemisorption and reaction of simple hydrocarbons on metal surfaces. These studies are of fundamental interest in surface chemistry and, more specifically, have relevance for the understanding of heterogeneous catalysis.

Finally, Simonyi, Graczyk, and Torrance are concerned with the preparation and properties of single-crystal films of the organic charge transfer system (NMP) (TCNQ). This system is one of a small group of organic materials with reasonably high electrical conductivity. Preparation in well characterized thin-film form should provide a unique means of studying and exploiting the unusual electrical properties of these organic materials.

In all these studies, many of the recently developed surface-sensitive spectroscopies have played a critical role. Thus, low energy electron diffraction, LEED, which makes it possible to determine geometrical order on a surface, is used in the work reported by Brundle, Winters, and Ludeke. X-Ray photoelectron spectroscopy, XPS, which leads to characterization of chemical composition and features of the chemical environment, such as oxidation states at or near a surface, is used by Raider and Flitsch to describe not only the composition but also the nature of the bonding of Si with Si and of Si with O at the SiO₂-Si interface. Ultraviolet photoelectron spectroscopy, UPS, and XPS can also elucidate fine details of the electronic structure resulting from the chemical bonds that are formed by chemisorbed species. These approaches are used by Brundle (XPS) and Demuth (UPS). Electron loss spectroscopy, ELS, is used by Ludeke to probe the nature of electronic surface states in InGaAs and GaSbAs alloys. Secondary-ion mass spectroscopy, SIMS, an especially sensitive surface spectroscopy, is used by DiMaria et al. to help determine the location of ion-implanted Al in SiO₂. The use of Auger electron spectroscopy, AES, to determine the chemical composition of an interface is assessed by Chuang and Wandelt, and experimental artifacts are separated from the actual features of the surface.

Another exciting feature of surface science is that theoretical developments have also progressed rapidly in recent years. This is reflected in the two purely theoretical papers on chemisorption, one using localized molecular orbital theory and the other, band theory. The paper by Bauschlicher, Bagus, and Schaefer represents a complete and comprehensive study of the potentials and limitations of the molecular orbital cluster approach to chemisorption. It demonstrates that methods for the determination of the electronic structure and bonding of molecules can be applied to the analysis of many features of chemical bonding at a surface. The paper by Pandey focuses on the consequence of the direct and indirect interactions between adsorbed atoms on surfaces for monolayer and greater coverages, and shows that a tight-binding-derived surface bond structure can successfully model and permit the interpretation of observed UPS spectra. Molecular orbital theory also plays a key role in the work of Demuth in his interpretation of the conformational changes that occur when a molecule is chemisorbed. From these papers, it is clear that theory can be expected to have, very soon, a major impact on electronic structure problems at surfaces.

ERIC KAY
IBM Research Laboratory
San Jose, California