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Grant DE-FG02-86ER45239

Final Report

Project titles:

Atomic and electronic structure of metals and alloys

Rare earths, ultrathin films and surface alloys

The results of the work done under DOE sponsorship are summarized in the list of publications at the end of this narrative. Here we give a brief description of the nature and the significance of the accomplishments.

Most of the goals set at the beginning of the period have been achieved and several new results have been obtained in the process. The project has been very productive: 47 refereed publications in little more than 5 years constitute a sustained substantial achievement. While confined to the area of surfaces and thin films, the project has covered a wide range of physical properties and different materials: rare earths, bulk and surface alloys, metal surfaces, magnetism and, especially, atomic and electronic structure of ultrathin films.

Notable achievements include the first ever *quantitative* studies of the atomic structure of *clean* rare-earth surfaces—Tb(0001), Tb(11 $\bar{2}$ 0), Gd(0001) and Gd(11 $\bar{2}$ 0). The basal planes exhibit reconstructions similar to those of other hexagonal close-packed metals, in contrast to some theoretical results that had predicted otherwise. The (11 $\bar{2}$ 0) surfaces exhibit not only perpendicular, but also parallel relaxations. These studies are not easy: the surfaces of the rare-earth metals are extraordinarily reactive and therefore very difficult to prepare and to keep in the clean state. But knowledge of the atomic and the electronic structure of these surfaces are of great scientific interest, because it provides the basic information necessary to understand the exotic optical and magnetic effects exhibited by these materials.

We have also carried out the first structure determination of surface alloys, in particular, the structure of Cu{001}c(2 $\times$ 2)-Au and Cu{001}c(2 $\times$ 2)-Pd. This kind of work

requires the use of a surface-sensitive probe such as low-energy electron diffraction in its *quantitative* mode. (We note in passing that the number of laboratories which have the competence and the expertise to use this probe quantitatively is limited to only four or five in the United States.) Surface alloys are interesting from a scientific viewpoint in studies of chemisorption and chemical reactivities, and are potentially useful in tests of catalytic activity.

Perhaps the most important achievement of the whole project lies, however, in the application of quantitative low-energy electron diffraction to the study of ultrathin films. We have pioneered this kind of work and have demonstrated its usefulness in a number of studies of metal-on-metal films, particularly magnetic metals on nonmagnetic substrates, e.g., Fe on Ag{001}, Fe on Ru(0001), Fe on Rh{001}, Co on Rh{001}, etc. This activity, which was also supported by the National Science Foundation, has far-reaching scientific and technological ramifications which are presently being picked up by a number of laboratories in Europe and in Japan. Ultrathin films are films involving only a few atomic layers, from one to, say, twenty layers. We have demonstrated that quantitative low-energy electron diffraction can determine the interlayer spacings in the "bulk" as well as in the surface of the ultrathin film. This is an accomplishment which cannot be done with the "classical" experimental techniques used in the past for the study of thin films (e.g., high-energy electron diffraction), and which even today cannot be easily done with many other surface-sensitive techniques. Once the interlayer spacings are known, one can determine the strains in the film if one knows the equilibrium (i.e., the unstrained) structure. This information is useful if one wants to understand why some of the properties of ultrathin films are different (as indeed they often are) from those of bulk macroscopic samples of the same material. It is particularly useful if the film has the structure of a metastable phase, i.e., a phase that is not normally encountered in nature at room temperature—such is the case, for example, for films of face-centered cubic Fe grown on Cu{001}, for films of face-centered cubic Mn grown on Pd{001}, for films of body-centered cubic Co grown on semiconductor or alloy surfaces, etc.

Publications of work sponsored by DOE
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1. "Structural and electronic properties of a surface alloy of Pd and Cu on Cu{001}", by S.H. Lu, Z.Q. Wang, S.C. Wu, C.K.C. Lok, J. Quinn, Y.S. Li, D. Tian, F. Jona and P.M. Marcus, Phys. Rev. B **37**, 4296 (1988).
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