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Grant DE-FG02-86ER45239

Continuation Proposal

1/1/93 - 12/31/93

Table of contents

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Project title:

Rare earths, ultrathin films and surface alloys

I. Performance report

The scope of the project was drastically reduced following the cuts to the budget—from a requested total of \$610,687 over three years to a total of \$62,000 per year over two years.

We have nevertheless pursued some of the goals set in last year's renewal proposal and have succeeded in reaching several of them.

In the area of the rare earths we have published the results of experiments on Tb samples that we have already discussed in the last progress report. To summarize the basic facts in this area: reproducible work with Tb (and, we believe, with all late rare-earth metals) can only be done by starting from ultrapure bulk material and by developing appropriate cleaning procedures for the preparation of clean surfaces. Such procedures are not always obvious because even bulk impurities present in the bulk at the 20 to 30 ppm level, such as iron, segregate on the surface rapidly and massively during the unavoidable annealing treatments of a surface that has been subjected to ion bombardments. We started from ultrapure material prepared in the Ames-Iowa laboratory and further purified by solid-state electrotransport at the University of Birmingham in England, and we developed the appropriate surface-cleaning procedures for both the basal plane and the $(11\bar{2}0)$ surface of Tb. The structure of both surfaces was found to be relaxed: the (0001) surface is contracted by 3.9% in the first and expanded by 1.4% in the second interlayer spacing; the $(11\bar{2}0)$ surface is contracted by 3.3% in the first layer and exhibits an interesting change in registry not heretofore detected on hcp $(11\bar{2}0)$ surfaces. The latter result is particularly significant in view of the observations by the Liverpool group of radical structure reconstructions on $(11\bar{2}0)$ surfaces of Y, Gd, Ho and Er.

Thin films of several rare earths, namely, Gd, Tb, Dy, Ho and Er, were grown on a W{110} substrate in ultrahigh vacuum. Such thin films are widely grown and studied in several laboratories around the world in order to determine and understand the physical and chemical properties of rare-earth surfaces, the main justification being that thin films grown *in situ* are likely to be purer and cleaner, at least for a limited time, than bulk material. We found that such films are indeed purer than bulk material, if we can extrapolate from the case of Tb for which we have now extensive experience, but the crystallinity, i.e., the long-range order, is less developed in the films than in bulk single crystals. This information is important to keep in mind by the workers who routinely infer the properties (especially the *structure-sensitive* properties) of bulk rare-earth crystals from thin-film studies.

In the area of thin and ultrathin films we have carried out several studies of epitaxial systems involving Cu, Fe and Mn on Fe and Pt, Cu, and Pd substrates, respectively. Particularly noteworthy are: the results of growth of a metastable body-centered-cubic (bcc) structure of copper, and of growth of ultrathin films of enormously strained (8 to 9%) face-centered-cubic (fcc) copper; the preparation of ultrathin films of metastable fcc manganese and of a new, as yet unknown, crystalline phase of manganese; and the growth of bcc iron in the {110} orientation over five or six layers of fcc iron pseudomorphic with a Cu{111} substrate. The significance of these results lies in two facts. One is the *discovery* of new, metastable and heretofore unknown crystalline phases whose physical and chemical properties may turn out to be both scientifically interesting and technologically useful. The other fact, perhaps even more important, is the demonstration of our ability to determine and characterize *quantitatively* both the bulk and the surface atomic structure of films with thicknesses of only 8 or 10 atomic layers. We would like to point out that there are not many experimental techniques, in addition to quantitative LEED as used by us, that can provide this information, and none of them has been consistently used, so far, for this particular purpose. We believe that this work, which we intend to continue and to intensify, will have a notable impact on the science and the applications of epitaxial growth.

Two other projects that had been started in the period covered by the preceding Grant have now been completed and published. They concern the study of possible ferromagnetism in $4d$ elements such as Rh (and Ru), and the study of relativistic effects in the electron band structure of Cu{111}.

II. Plans for the following year

We plan to continue the studies of the atomic structure of rare-earth surfaces. We will not pursue the photoemission investigations that we intended to do last year for the elucidation of the electron structure, because the financial cuts that we have suffered have cancelled our presence at beamline U7 at the National Synchrotron Light Source. But with regard to the atomic structure we have the distinction of being the only group in the world with the facilities and the know-how to shed light on this long-standing problem which many scientists would like to see solved (see,e.g., the review of F.P. Netzer and J.A.D. Matthew in Rep. Prog. Phys. 49, 621 (1986)).

The most puzzling problem in this area is the contrast between the reports by the Liverpool group of structure reconstructions on the $(11\bar{2}0)$ surfaces of Y, Gd, Ho and Er on the one hand and our own experience with the $(11\bar{2}0)$ surfaces of other rare earths on the other. We have tried (and shall try again) to reproduce the Liverpool results on the Gd surface, but we could only find the (more reasonable and expected) result of relaxation that we had already determined on the corresponding Tb surface. We will prepare samples of Er, for investigations of both the (0001) and the $(11\bar{2}0)$ surface (we have already obtained an ultrapure crystal of Er from Dr. David Fort of the University of Alabama in England), and we will carry out appropriate LEED and AES experiments and associated intensity analyses for both surfaces. It is important to establish whether the reconstruction of the $(11\bar{2}0)$ surface is reproducible, in which case it will be useful and necessary to understand why it occurs, or whether the reconstruction found in Liverpool was an artifact of that experiment, in which case it will be instructive to understand what produced that artifact. We will also examine a sample of $Y(11\bar{2}0)$ that was lent to us by the Liverpool group—the very sample on which that group found the structure reconstruction.

We will continue and intensify the work on ultrathin films. Support for this work is shared between DOE and NSF. (Originally, the distinction between the two supporting Grants was made on the basis of type of material, the DOE support being predominantly for noble-metal work and NSF for transition-metal research, hence studies of epitaxial systems such as Fe on Cu or Mn on Pd are naturally shared.) As pointed out in the preceding section, research on the epitaxial growth of ultrathin films is an extremely "hot" subject, at the present time, in the U.S., Japan and Germany, owing to the potential for novel and favorable properties in ultrathin films of metastable phases—phases which are not normally encountered in nature in bulk form. Our plans include continuation of presently ongoing studies of Fe on Ag{001} and Ag{111}, and of Fe on Au{001} and Au{111}, as well as initiation of new projects including ultrathin films of Co on Au, Ag, Rh, Ru, and possibly Ni and Cu substrates.

III. Personnel

In 1992, no students were supported by the present Grant. One post-doctoral fellow (Dr. Tony Begley) was supported in 1992 and will be supported with the continuation Grant in 1993.

IV. Publications of work sponsored by DOE

Papers appeared in print since the last progress report:

1. "Ultrathin films of Rh on Au{001} and Rh on Ag{001}: growth mode and magnetism", by H. Li, S.C. Wu, D. Tian, Y.S. Li, J. Quinn and F. Jona, Phys. Rev. B **44**, 1438 (1991).
2. "Large strains in the epitaxy of Cu on Pt{001}", by Y.S. Li, J. Quinn, H. Li, D. Tian, F. Jona and P.M. Marcus, Phys. Rev. B **44**, 8261 (1991).
3. "Surface relaxation on Tb(0001)", by J. Quinn, Y.S. Li and F. Jona, Surf. Sci. **257**, L647 (1991).
4. "Relativistic effects in the electron band structure of Cu{111}", by S.C. Wu, H. Li, Y.S. Li, D. Tian and F. Jona, Phys. Rev. B **44**, 13308 (1991).
5. "Surface state on clean Tb(0001)", by S.C. Wu, H. Li, Y.S. Li, D. Tian, J. Quinn, F. Jona and D. Fort, Phys. Rev. B **44**, 13720 (1991).
6. "Electronic properties of body-centered-tetragonal copper", by H. Li, S.C. Wu, J. Quinn, Y.S. Li, D. Tian and F. Jona, Journal of Physics: Condensed Matter **3**, 7193 (1991).
7. "Atomic and electronic structure of thin films of Mn on Pd{111}", by D. Tian, S.C. Wu, F. Jona and P.M. Marcus, Phys. Rev. B **45**, 3749 (1992).
8. "Atomic and electronic properties of ultrathin films of Gd, Tb, Dy, Ho and Er", by H.Li, D. Tian, J. Quinn, Y.S. Li and S.C. Wu, Phys. Rev. B **45**, 3853 (1992).
9. "Re-examination of the electron band structure of Tb along $\Gamma\Delta A$", by S.C. Wu, H. Li, Y.S. Li, J. Quinn, D. Tian, F. Jona, D. Fort and N.E. Christensen, Phys. Rev. B **45**, 8867 (1992).
10. "Structure of ultrahin films of Fe on Cu{111} and and Cu{110}", by D. Tian, F. Jona and P.M. Marcus, Phys. Rev. B **45**, 11216 (1992).
11. "New metastable phase of Mn by epitaxy on Cu{111}" by D. Tian, A.M. Begley and F. Jona, Surf. Sci. **273**, L393 (1992).
12. "Atomic structure of Tb(11$\bar{2}$0)", by Y.S. Li, J. Quinn, F. Jona, and P.M. Marcus, Phys. Rev. B **46**, 4830 (1992).

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