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A. Introduction

Within the framework of a DOE National Laboratory/EPSCoR-state partnership, investigations by researchers at Louisiana State University and Oak Ridge National Laboratory were focused on revealing the unique nanophase properties of alloy thin-films and bimetallic surfaces. Employing a number of experimental preparation techniques and characterization probes (synchrotron-based angle-resolved and valence/core-level PES and variable-temperature STM/STS), the goal of this program was to elucidate of the interconnecting physical and chemical properties of a variety of alloy surfaces and thin-films, specifically, determining the correlation between atomic structure/composition, electronic structure, and catalytic/chemisorption properties of these nanoscale material systems. The research is currently centered on three parallel areas: 1) Surface atomic and electronic structure of clean and modified intermetallic alloys 2) Surface atomic, electronic, magnetic structure of heteroepitaxially grown bulk-immiscible alloys and 3) Surface chemistry of bimetallic and oxide thin-film alloys.

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B. Overview

Throughout the period this grant, the research program progressed well and proceeded, more or less as planned. We have basically "stayed on course" with the research topics that were outlined in the original proposal. However, as new results/ideas emerged, we branched out to include other topics, which were deemed relevant to the scope of the original research proposal. As outlined in more detail below, a major focus was on elucidating the physical and chemical properties of heteroepitaxially grown metal-on-metal thin-film alloy systems, namely, experimentally determining the atomic and electronic structure of certain thin-film transition-noble metal combinations. The interest in these bimetallic systems is that, whereas in the bulk they are immiscible, at the surface they form 2-D surface alloys. Because of the reduced dimensionality, these unique nanophase materials elicit novel properties that are not found in the bulk, and thus present new material opportunities to the "miniaturization" of the technological world. Employing scanning tunneling microscopy (STM) and synchrotron-based, angle-resolved photoemission (ARUPS), we have characterized the unique surface overlayers, alloying, and de-alloying atomic structures and, correspondingly, the consequent changes in the surface atomic structure. A key finding from these systems is substrate-adlayer *sp-d* hybridization and reduced-dimensionality that results from the formation of prepared nanostructures. In addition to this major thrust area, elucidating surface atomic and electronic structure of various intermetallic alloys and thin-film insulators were also pursued. From these latter studies, a key outcome was the elucidation of a new nanophase of alumina. Specific details of all studies are outlined below.

As part of this DOE National Laboratory/EPSCoR-state partnership, collaborative efforts between Oak Ridge National Laboratory (ORNL) and Louisiana State University were undertaken in many parts of this research program. This included trips by both PI and graduate students to ORNL to conduct surface atomic structural studies on a variety of intermetallic alloy surfaces. Both STM and low-energy electron diffraction (LEED) studies have been performed at ORNL (Division of Condensed Matter) on various crystallographic surfaces of FeAl and NiAl. In addition, the primary ORNL contact (D. Zehner) was a part, at least in the analysis and interpretation of data, of most of the experiments conducted at Louisiana State University.

The success of this research program has been, in part, due to participation of excellent graduate and undergraduate students. Two specific graduate students (Dustin Hite and Orhan Kizilkaya) worked, by and large, full-time on projects directly related to the contents of this grant. They also traveled to ORNL and conducted research using facilities there. Having the a research experience was Both of these graduate students have now received Ph.D. degrees based on the research related to this project. Concerning undergraduates, Edward Bruster, a minority student from Grambling State University (a HBSC institution), also conducted research efforts this summer as an undergraduate intern. Jerry Taylor, an undergraduate student from LSU, also was directly involved in research pertaining to this grant. In addition to these graduate students, there are various other graduate and undergraduate students (not paid from the grant), who have assisted in various experiments up to this point.

Overall, we believe that this DOE Laboratory/EPSCoR S&T program has been a great success. As a testament, we have made numerous presentation at conferences, published a series of papers (with more in the works), and have helped to educate many graduate and undergraduate students through research opportunities.

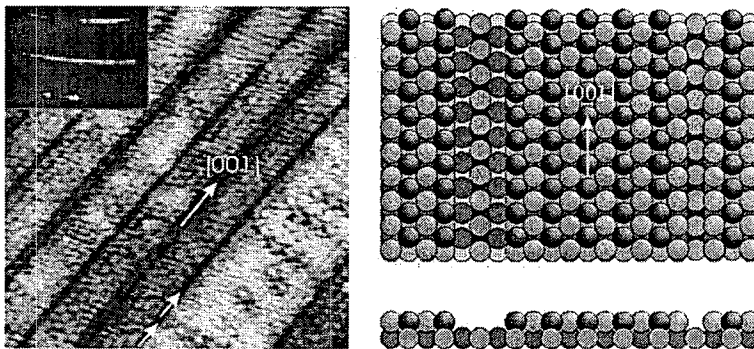
C. Research Accomplishments:

C.1: Surface atomic and electronic structure of clean intermetallic alloy : FeAl

The physical and chemical properties of the intermetallic alloys in high technology applications such as corrosion resistance, oxidation, and catalytic activity depend on the structure and the composition of the surface layer. By changing the stoichiometry of the alloy, a new material can be readily developed and the new structure of the alloy can show unprecedented physical and chemical properties. In order to modify these properties, a detailed understanding of the atomic and the electronic structure of metal alloys is required. In particular, transition metal aluminides, e.g. NiAl, CoAl, and FeAl, have attracted considerable interest due to their unique properties such as high melting points, enhanced corrosion resistance, relatively low density, and utility as soft magnetic materials. These transition metal aluminides are ordered intermetallic alloys, wherein the electronic structure is dictated by the degree of charge transfer from Al to the transition metal, and hybridization between Al *sp* and transition metal *d*-states play essential roles in bonding.

In this research program, we have focused on determining the surface atomic and electronic structure of low-index faces of FeAl, in particular the (110), (210), and (310). It is well known that surfaces of solids can differ significantly from the bulk in regard to the atomic and electronic structure. In addition to the geometrical reordering in the surface, metal alloy surfaces can exhibit a deviation in chemical composition. Surface atoms may have chemically different atomic neighbors compared to those in the bulk and this leads to a chemical reordering in the surface. When the chemical reordering is not stoichiometric (not preserving the quantity of constituents present in the bulk) due to segregation of one of the constituents to the surface, new ordered/disordered phases emerge in the surface/surface selvage. This leads to a "surface" phase diagram which can be radically different from its bulk phase diagram counterpart. STM and angle-resolved photoemission (ARPES) techniques have proven to be indispensable for revealing the atomic and electronic structure of these novel surface alloy phases.

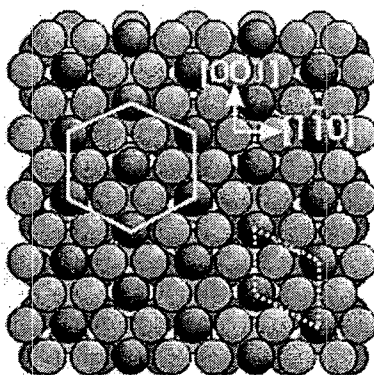
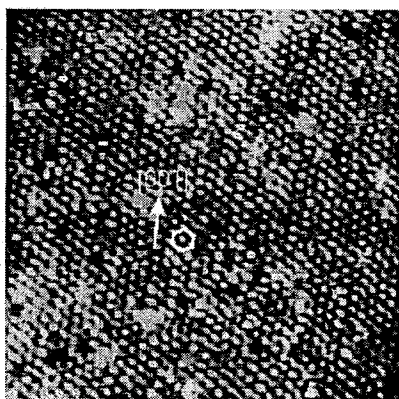
As an example of this phenomena, we have studied the surface electronic and atomic structure of FeAl(110) as a function of near surface concentration of the bimetallic constituents. Regarding the atomic structure, preferential sputtering of Al results in a decrease of the stoichiometric composition in the near surface region. Subsequent annealing then restores the near surface concentration through Al segregation. For example when the sputtered FeAl(110) surface is annealed to 600-800 °C, there is an increase in the Al at the surface. Correspondingly, our STM results indicate that the ensuing increased compressive stress along the $[1\bar{1}0]$ direction is relieved through the formation of strain-relieving missing row reconstruction (see above figure). Again, this surface phase results from a slightly larger Al concentration as compared to the bulk and the reconstruction results from relief of the compressive stress



[left] STM image of FeAl(110) ($200 \times 200 \text{ \AA}^2$, $I_t = 3.33 \text{ nA}$, $V_t = -0.01 \text{ mV}$) shows a missing row like reconstruction (see arrows) [right] The models show top and side view of the missing row reconstructed phase.

at the surface.

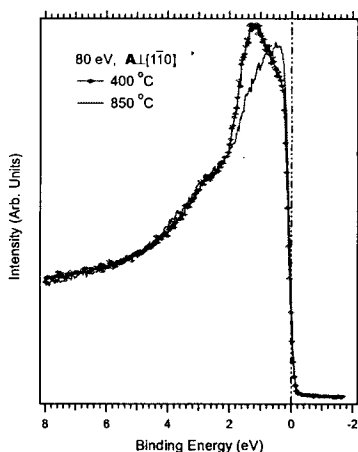
However, this surface structural phase is metastable. Upon annealing above 850 °C, the surface undergoes another type of reconstruction. In this case the surface stoichiometry is FeAl_2 , wherein the larger surface concentration arises through Al bulk segregation to the surface. As seen in the STM image below, the lowest energy atomic structure of this novel surface phase



[left] STM image ($150 \times 150 \text{ \AA}^2$, $I_t = 5.41 \text{ nA}$, $V_t = 30.2 \text{ mV}$) of $\text{FeAl}(110)$ surface after annealing to 850 °C. **[right]** Ball model displays Fe atoms surrounded by six Al atoms and a unit cell of FeAl_2 stoichiometry.

is nearly incommensurate with the underlying lattice. The details of the atomic structure of this incommensurate phase are seen in the STM image below. A quasi-hexagonal arrangement of atoms is atomically resolved in the image. The structural model of the ordered quasi-hexagonal overlayer which has a unit mesh containing two Al and one Fe atoms is also displayed (see left fig.).

In addition to employing STM to resolved the atomistic structural properties of the various surface phases, ARPES has been used to elucidate the surface electronic structure of the bimetallic surfaces. The increased Al concentration on the surface after annealing above 850 °C modifies the surface potential. This modification is expected to cause increased hybridization between the Fe d and Al p -states. It is pointed out in the previous studies that Fe- e_g orbitals



EDCs of clean $\text{FeAl}(110)$ for bulk and incommensurate surface (850 °C) collected at normal emission and $\text{Al}[110]$ geometry.

provide bonding between the Fe atoms and Fe- t_{2g} orbitals bond to the Al atoms [28,29]. Therefore, it makes sense that in the hybridization scenario between the Al and Fe atoms, the Fe d -bands which are close to Fermi level and possess the t_{2g} symmetry should be affected. The figure at left shows two photoemission spectra for bulk terminated (400 °C) and incommensurate (850 °C - as in the STM image shown above) phase surfaces at a photon energy of 80 eV. The distinctive features are the diminished intensity of the Σ_1 state at 1.25 eV and intensified peak feature of the Σ_3 state at 0.6 eV on the photoemission spectrum of the incommensurate phase compared to photoemission spectrum of the bulk terminated surface. This difference is due to the increased hybridization of the Fe d -band with the Al p -band in the FeAl_2 phase. Specifically, it is presumed that the Al p admixed with the symmetry forbidden Σ_3 -state. In addition, core-level spectra from the of the Al- $2p$ and Fe- $3p$ confirm the STM and valence photoemission results.

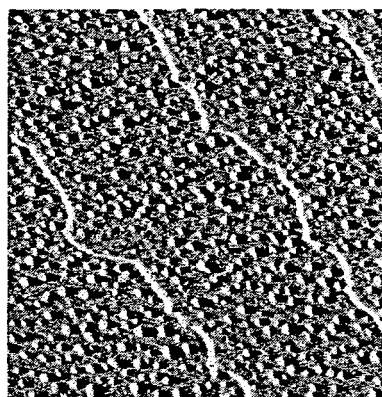
C.2: Surface atomic and electronic structure of heteroepitaxially grown bulk-immiscible alloys

Metal films grown on metal and semiconductor substrates have been studied for decades mainly due to a wide variety of resulting technological applications, including semiconductor heterostructure devices, magnetic spin valves, and heterogeneous catalysis. In order to fully take advantage of the applicability and full functionality of these heteroepitaxial systems, a fundamental understanding of the atomic-scale processes and resultant electronic structures is warranted. In particular, as structures and devices are fabricated with ever-decreasing scales, quantum mechanical effects play an ever-increasing role. In fact, many of these widely used technological applications of thin films remain poorly understood on a fundamental level. Motivated by the desire to understand these heteroepitaxial systems on a fundamental level, the investigations in this research program were aimed at correlating the surface morphology and resultant electronic structure of a unique class of heteroepitaxial systems in the initial stages of growth. Particularly, the focus was on systems that deviate from the traditional growth modes of epitaxy, exhibiting surface confined alloy formation (Ag/Cu(110), Ag/Ni(110), Co/Cu(110)), subsurface growth (Ni/Ag(100), Co/Ag(100)) and reactive epitaxy (Be/Si(111)). In many of the systems studied, it is found that bulk-immiscible surface alloys are exclusively confined to the outer most surface layer, thus giving rise to two-dimensional alloy phases for which there is no three-dimensional analog. As a result, new and technologically advantageous properties emerge, e.g. enhancement of catalytic reactivity and selectivity.

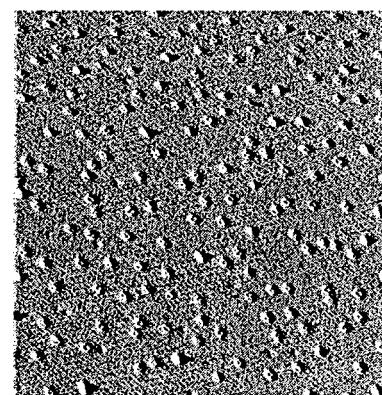
Important findings from this study were 1) the role of surface stress/strain in the formation of nanostructured surface alloys, 2) the identification of *sp-d* hybridization in noble-transition metal surface alloys and 2) the novel “electronic dimensionality” found in these types of surface confined surface alloy system. In what follows, a short summary of a few select systems will be outlined in greater detail.

One system which we have focused on is the determination of the growth morphology and electronic structure of Ni/Ag(100). This is a unique system because the surface morphology deviates drastically from usual growth modes, exhibiting subsurface growth. This growth is strongly dependent on temperature and as a result so is the surface magnetism of the Ni. When deposited at or below room temperature, submonolayer coverages of Ni grow in the form of randomly distributed nanoclusters that are approximately 30 Å in diameter and 1 to 2 atomic layers thick (see figure at right). Once annealed to 150°C, these nanoclusters diffuse into the subsurface region of the Ag(100) substrate forming embedded nanoclusters capped by at least one Ag layer (Fig. 1, bottom). These surface morphological studies were conducted at ORNL. This phenomena of Ni “sinking” beneath the substrate surface is predicted from simple free energy arguments. Namely since the surface free energy of Ni ($\gamma_{\text{Ni}} = 1.9 \text{ J/m}^2$) is greater than that of Ag ($\gamma_{\text{Ag}} = 1.3 \text{ J/m}^2$), upon reaching thermodynamic equilibrium through annealing, Ag

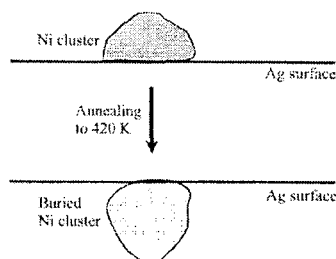
1000 × 1000 Å²



1000 × 1000 Å²



STM images of Ni/Ag(100) (see text for details)



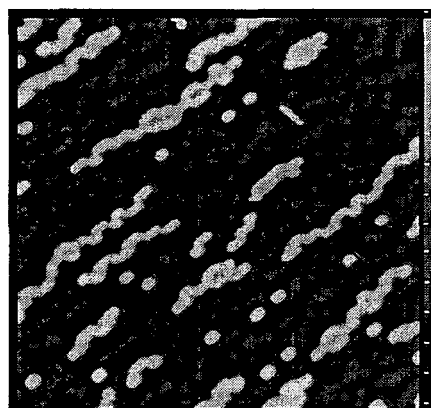
Schematic depiction of the "sinking" Ni nanoclusters. **[Upper]** Volmer Weber growth mode results from deposition of Ni on Ag(100) at room temperature. **[lower]** Annealing the Ni/Ag(100) system to 420 K leads to a subsurface "surfactant-like" growth morphology

from the bulk covers over the Ni cluster. Based on this result, the question then becomes: what is the electronic nature of the Ni nanoclusters? At CAMD we performed ARUPS experiments that show the dramatic changes in the electronic structure as a result of the different surface structure, clusters on top vs. embedded clusters. The photoemission results show very narrow, non-dispersive *d*-bands of Ni for the case where of Ni clusters on the surface (Figure below, left). In the case of embedded clusters, the Ni *d*-bands show a three-dimensional-like dispersion and increased width (Figure below, right). This increase in *d*-band width is a result of the increased coordination and hybridization of the embedded nanoclusters with the substrate. Based on numerous theoretical papers and the fact that the observed changes in the Ni *d*-bands tend to balance out the majority/minority band

filling in the subsurface growth regime, our conjecture is that the surface magnetism of the Ni is relatively large in the un-annealed system and significantly reduced once the clusters have become embedded.

As can be seen from this example, the main focus and objective of this research project has been correlating the atomic structure with the resultant electronic structure. The main tools used to investigate the morphological structures is scanning tunneling microscopy (STM), while the electronic structures have been characterized using synchrotron-based, angle-resolved photoemission spectroscopy (SR-ARPES). Using these two extremely powerful techniques, a wealth of information has been assimilated regarding the highly hybridized metallic bonding and electronic dimensionality associated with the increased coordination in surface alloy formation.

One more system which illustrates the invaluable combination of STM and ARPES is Ag/Cu(110). In this case, clear correlation between atomic scale structure and electronic structure has been elucidated. From STM studies, it is known that for subsurface coverages of Ag on Cu(110), atomic Ag-wires form on the surface. This can be seen in the STM images (see right). Here de-alloyed zigzag chains of Ag dimers and trimers are imaged bright yellow. These Ag nanowires appear 1-D in atomic structure, but their electronic structure is more complicated.



STM images of Ag deposited on Cu(110) after deposition of ~ 0.4 ML (200 \AA^2) The [001]-direction is along the chains from bottom-left to top-right.

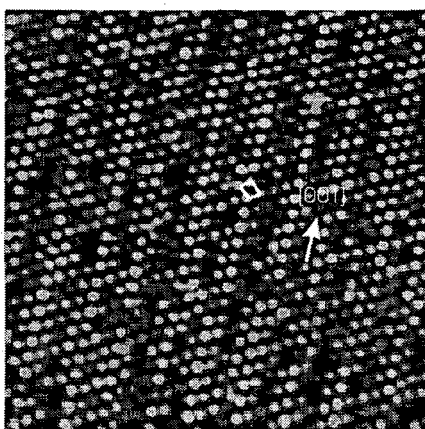
Synchrotron-based photoemission was used to identify both the nature of the bonding and the electronic dimensionality of various structural phases. In the case of Ag/Cu(110), it was found that the Ag-nanowires induce new electronic states at the surface. These so-called surface resonances occur due to the breaking of symmetry of the bulk and unique anisotropic structure of the "Ag-wires". As shown in the figure at below, photoemission reveals that for this polarization of light, a new Cu state emerges (B) due to the bonding/hybridization with the Ag. State B is derived from the Cu Σ_4 band, however it is observed in "forbidden" photoemission geometry because of the reduced symmetry of the

surface. Band structure calculations reveal that this is due to a $sp-d$ hybridization between the Cu and Ag nanostructure. In addition, ARPES spectroscopy reveals that the “electronic dimensionality” differs depending if the states are aligned with the Ag chains or perpendicular to them. From the dispersion of the Ag d -bands as a function of photon energy it was found that the Ag states along the chains were 1-D like, whereas perpendicular to the chains, due to the strong Ag- $d +$ Cu- sp hybridization, the Ag states were 2-D like. This is very important conclusion, that is, in these types of nanostructures the “electronic dimensionality” can be grossly different along different bonding directions.

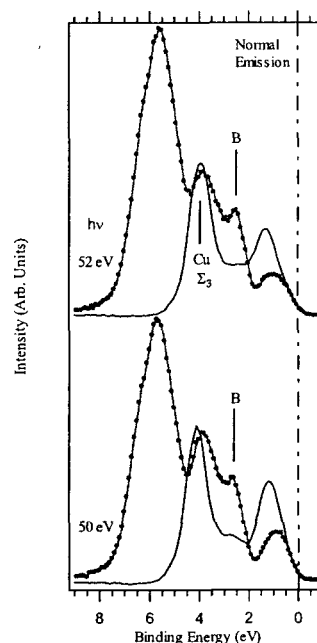
C.3: Surface chemistry of oxides

Due to their importance in a broad range of technological applications such as catalytic supports, microelectronics devices, and metal ceramic-based sensors, studies of oxide surfaces continue to draw considerable attention. Among the oxides, alumina has been the focus of numerous studies due to its desirable physical and chemical properties. Bulk alumina gives rise to several phases, all of which are comprised of a close packed oxygen sub-lattice. The differences in occupancy of tetrahedral and/or octahedral coordination determine the crystal phase of alumina, and consequently, the overall properties. Despite years of investigation, developing a fundamental understanding of their complex surface/thin-film electronic and atomic properties has been hindered by the lack of high quality oxide surfaces that can be probed with standard surface/thin-film techniques.

In this research program we have focused physical and chemical properties of a number of oxide surfaces. For example, the chemisorption of S, Cl, and O on TiO_2 (in collaboration with



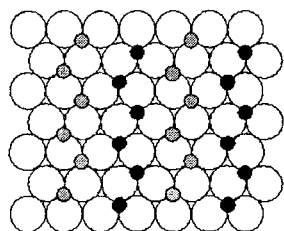
STM image ($70 \times 70 \text{ nm}^2$) of oxidized FeAl(110) surface. The surface exposed to 1000 L of O_2 at 850°C . Unit mesh of oxide structure ($18.6 \times 19.6 \text{ \AA}$) is shown with solid line.



EDCs of clean Cu(110) (black) and Ag/Cu(110) with a coverage of 0.6 ML (red).

U. Diebold from Tulane University) and growth of NiO and TaO_x (in collaboration with C. Ventrice from U. of New Orleans). However, the system which has revealed the most interest has been alumina grown on FeAl surfaces. Specifically, the oxidation behavior of FeAl(110) was studied to elucidate the atomic and electronic structure of the ultrathin oxide film. A well-ordered Al_2O_3 phase is formed after exposing the surface to 1000L of oxygen at 850°C . STM images of this ordered oxide film were recorded after the sample was recooled to room temperature. The large area STM (see left) scan shows a regular and nearly hexagonal superstructure pattern. The spot-spot distance of the superstructure is measured to be 19 \AA . This saturation coverage (1000L O_2) of STM image shows that the thin alumina, Al_2O_3 , has a flat and homogeneous morphology. However, there is a small lateral disorder exhibited perpendicular to the $[001]$ direction. Although not shown, STM reveals that the

alumina oxide is only approximately 0.8 nm thick, thus this is a true 2-D oxide. Moreover, STM also revealed a zigzag-stripe atomic structure consistent with of an even mix of octahedrally and tetrahedrally coordinated Al ions (i.e. κ - Al_2O_3). As shown in the model at left, this indicates that this is indeed a unique phase of alumina due to its 2D nature.

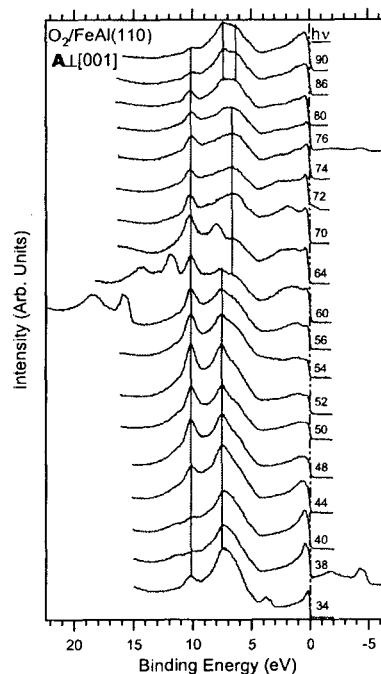


Schematic drawing of the A plane of the kappa alumina structure. Octahedral atoms are black and tetrahedral ones are in gray color.

In addition to the structural studies done by STM and LEED, core-level spectroscopy was used to determine both chemical information of the oxide and structure at the buried interface. The figure below shows an example. An important fact which emerged was the formation of an Al interfacial layer between the oxide film and the substrate was also

found as a weak shoulder in the XPS.

Valence ARPES experiments revealed a two dimensional electronic structure was found from the dispersion behavior of the electronic states. The ARPES spectra (shown at right) as a function of photon energy revealed that a true 2-D band structure. The photoemission spectra of the oxide film also showed an enhanced intensity in the band gap of bulk oxide. Either a sub-oxide or a defect state has been proposed as the source of this peak. This latter observation is quite interesting; specifically, it confirms the assessment that the electronic properties of this 2D oxide are indeed quite different from the corresponding phases of bulk alumina.



EDCs of $\text{Al}_2\text{O}_3/\text{FeAl}(110)$ collected at normal emission indicate lack of dispersion as function of photon energies.

D. Publications/Presentations:

A vital part of this research project has been dissemination of information through published journal articles and conference/scientific conferences. Below a list of these can be found

Conference/scientific conference presentations:

1. "Photoemission and STM studies of oxide thin films on FeAl(110)" O. Kizilkaya, D.A. Hite, D. M. Zehner, and P. T. Sprunger, 2003 Physical Electronic Conference, Cornell University, June 16, 2003
2. "Electronic and atomic structure of clean and oxidized FeAl(110) surface" O. Kizilkaya, D. A. Hite, D. M. Zehner, and P. T. Sprunger, 2003 March Meeting of the American Physical Society, Austin, Texas, March 5, 2003.
3. "The electronic and atomic structure of Ag/Cu(110) and Ag/Cu(100)" O. Kizilkaya, D. A. Hite, R. L. Kurtz, and P. T. Sprunger, 2003 March Meeting of the American Physical Society, Austin, Texas, March 5, 2003.

4. "Dimensionality Investigation of an Alloy-dealloy Phase Transition on Ag/Cu(110)", O. Kizilkaya, D. A. Hite, J. Choi and P. T. Sprunger, AVS 48th International Symposium, San Francisco, California, November, 2, 2001.
5. "Surface Reconstruction STM Studies of Clean and Oxidized Low Index FeAl Surfaces", O. Kizilkaya, D. A. Hite, D. M. Zehner and P. T. Sprunger, AVS 48th International Symposium, San Francisco, California, November, 2, 2001.
6. "Electronic Structure of Surface-Confined Alloys in Bulk-Immiscible Systems", D. A. Hite and P. T. Sprunger, in competition for the Nottingham Prize, 61st Annual Physical Electronic Conference, Taos, New Mexico, June 12, 2001.
7. "Electronic and Atomic structure of bimetallic thin-film alloys", Phillip Sprunger, Dustin A. Hite, Orhan Kizilkaya, M. Sackler Colloquium of the National Academy of Sciences on "Nanoscience - Underlying Physical Concepts and Phenomena." , Washington DC, May 19, 2001.
8. "Electronic Structure of Surface-Confined Alloys in Bulk-Immiscible Systems", D. A. Hite, O. Kizilkaya, S. -J. Tang, and P. T. Sprunger, 7th Annual CAMD Users' Meeting, Baton Rouge, Louisiana, April 20, 2001.
9. "STM Study of Be/Si(111) - (7 x 7)", D. A. Hite and P. T. Sprunger, 2001 March Meeting of the American Physical Society, Seattle, Washington, March 12, 2001.
10. "Surface Resonances in Ag/Cu(110)", D. A. Hite, O. Kizilkaya, Jaewu Choi, and P. T. Sprunger, 2001 March Meeting of the American Physical Society, Seattle, Washington, March 15, 2001.
11. "Temperature Dependent Adsorption of Oxygen on TiO₂(110): a Photoemission Study", H. Geisler, E. L. Hebenstreit, W. Hebenstreit, M. Li, U. Diebold, S. N. Thornburg, C. A. Ventrice, Jr., D. A. Hite, and P. T. Sprunger, 47th International Symposium of the American Vacuum Society, Boston, Massachusetts, October 5, 2000.
12. "Adsorption of S and Cl on TiO₂(110) Studied by Ultra-violet Photoelectron Spectroscopy", E. L. Hebenstreit, W. Hebenstreit, U. Diebold, H. Geisler, D. A. Hite, P. T. Sprunger, S. N. Thornburg, and C. A. Ventrice, Jr., 47th International Symposium of the American Vacuum Society, Boston, Massachusetts, October 3, 2000.
13. "Electronic Structure of Ag/Ni(110) and Ag/Cu(110): Dimensionality and Hybridization in the Submonolayer Regime", D. A. Hite, O. Kizilkaya, and P. T. Sprunger, 60th Physical Electronics Conference, Baton Rouge, Louisiana, June 23, 2000.
14. "Atomic and Electronic Structure of Ni/Ag(100) and Ag/Ni(110)", D. A. Hite and P. T. Sprunger, 46th International Symposium of the American Vacuum Society, Seattle, Washington, October, 27, 1999.
15. "Atomic and Electronic Structure of Ag/Ni(110): Dimensionality of the Surface Alloy and Overlayer Phases", D. A. Hite, S. -J. Tang and P. T. Sprunger, 1999 Centennial Meeting of the American Physical Society, Atlanta, Georgia, March 22, 1999.
16. "Growth Morphology and Electronic Structure of Epitaxial NiO Films: NiO(100)/Ag(100) and NiO(111)/Au(111)", C. A. Ventrice, Jr., M. M. Howard, B. R. King, P. S. Robbert, H. Geisler, D. A. Hite, and P. T. Sprunger, 1999 Centennial Meeting

of the American Physical Society, Atlanta, Georgia, March 23, 1999.

17. "Atomic and Electronic properties of thin-film Alloy Surfaces", P.T. Sprunger, *invited talk*, Materials Research Society Fall Meeting, Boston MA, Nov. 1998.

Published papers

1. "Formation of aluminum oxide thin films on FeAl(110) studied by STM", O. Kizilkaya, D. A. Hite, D. M. Zehner, and P. T. Sprunger, *Surface Science* 529, 223 (2003).
2. "Reactive epitaxy of beryllium on Si(111)-(7 × 7)", D. A. Hite, S. -J. Tang, and P. T. Sprunger, *Chemical Physics Letters* 367, 129 (2003).
3. "The adsorption of elemental chlorine on TiO₂(110) studied with scanning tunneling microscopy and photoemission spectroscopy", E. L. D. Hebenstreit, W. Hebenstreit, H. Geisler, C. A. Ventrice, Jr., D. A. Hite, P. T. Sprunger, and U. Diebold, *Surface Science* 505, 336 (2002).
4. "Surface resonances and reduced symmetry in the heteroepitaxial Ag/Cu(110) system", D. A. Hite, O. Kizilkaya, P. T. Sprunger, E. Lægsgaard and F. Besenbacher, *Physical Review B* 65, 113411 (2002).
5. "Sulfur on TiO₂(110) studied with resonant photoemission", E. L. D. Hebenstreit, W. Hebenstreit, H. Geisler, S. N. Thornburg, C. A. Ventrice, Jr., D. A. Hite, P. T. Sprunger, and U. Diebold, *Physical Review B* 64, 115418 (2001).
6. "Surface morphology and electronic structure of Ni/Ag(100)", D. A. Hite, O. Kizilkaya, P. T. Sprunger, M. M. Howard, C. A. Ventrice, Jr., H. Geisler, and D. M. Zehner, *Journal of Vacuum Science and Technology A* 18, 1950-1954 (2000).
7. "Growth morphology and electronic structure of ultra-thin TaO_x films on Ag(100)", M. M. Howard, C. A. Ventrice, Jr., H. Geisler, D. A. Hite, and P. T. Sprunger, in "Materials Science of Novel Oxide-based Electronics", edited by D. S. Ginley, D. M. Newns, H. Kawazoe, A. B. Kozyrev, and J. D. Perkins, *Materials Research Society Proceedings*, Vol. 623 (MRS, Pittsburgh, 2000).

In final preparation

8. "Atomic and electronic structure of the surface-alloy phase and de-alloyed overlayer phase in the heteroepitaxial Ag/Ni(110) system", D. A. Hite, P. T. Sprunger, I. Stensgaard and F. Besenbacher, to be submitted to *Physical Review B*.
9. "Dimensionality in the alloy/de-alloy phase transition of Ag/Cu(110)", O. Kizilkaya, D. A. Hite, P. T. Sprunger, J. Choi, E. Lægsgaard and F. Besenbacher, to be submitted to *Physical Review B*.
10. "Surface reconstructions on FeAl(110), (210), and (310) surfaces", O. Kizilkaya, D. A. Hite, P. T. Sprunger, J. F. Wendelken, and D. M. Zehner, in preparation for publication.

E. Personnel Involved with project

Graduate Students involved:

- | | | | |
|-------|---|-------------------|--|
| group | 1) Dustin Hite | Ph.D. August 2001 | Currently postdoc: Nanomagentic
at NIST (D. Pappas) |
| | 2) Shu-Jung Tang | Ph.D. August 2002 | Currently postdoc: U. of Illinois |
| | (Univ. of Tennessee – co-advised with E.W. Plummer) | | (T.C. Chiang) |
| | 3) Orhan Kizilikaya | Ph.D. June 2003 | Currently: Staff Scientist CAMD/LSU |

Number of Undergraduates: 6

During the academic school year, there were 3 Louisiana State University students who worked on various parts of the project. In addition, there were 4 additional summer research students who took part in the project. Two of these students were minority students from HBUC institutions (Grambling State University and Xavier University)