New opportunities in spin-polarized photoemission spectroscopy (invited)

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New opportunities for probing magnetism and magnetic materials are emerging as a result of improved electron-spin detectors, broad advances in materials synthesis and characterization techniques, and refinements in spin-sensitive spectroscopic techniques. A multi-investigator group is currently commissioning a spin-polarized photoemission beamline at the National Synchrotron Light Source that has been designed to synthesize and study magnetic materials. The beamline exploits the significant increase in synchrotron radiation flux that is emitted from a magnetic insertion device. Key issues and new opportunities for advancing the understanding of magnetism and magnetic materials using this facility are addressed.

I. INTRODUCTION

Ferromagnetism has posed fascinating challenges to scientific inquiry for decades. Continued efforts to more fully understand magnetic phenomena are well justified based on scientific issues associated with magnetism as well as the technological importance of magnetic materials. Recent advances in a complementary combination of scientific and technological fields have stimulated new interest in magnetism and magnetic materials, and have resulted in unprecedented new opportunities for scientific work in this important subfield of solid-state physics. Refinements of modern materials synthesis techniques, in particular molecular-beam epitaxy (MBE), and the discovery and development of new structure sensitive techniques for characterizing thin-film structures on an atomic scale have opened up the field of magnetism and magnetic materials to include deliberately modified materials and artificially stabilized structures that do not naturally occur. These novel materials offer important possibilities for new technology as well as opportunities for improving our understanding of the atomic-level factors that govern magnetic behavior.

The present paper considers new scientific opportunities in magnetic materials research which are arising from the advances just cited. In addition to the advances in materials synthesis and characterization, there are other areas in which new discoveries and new technology have combined to yield important new opportunities. These areas include technical advances in the generation and use of synchrotron radiation, advances in spin-sensitive spectroscopic techniques (in particular the development of compact electron-spin detectors), and the continued development (and impressive success) of first-principles electronic structure calculations based on the local density approximation.

These factors constitute the background, and the scientific and technological basis for setting up a new facility at the National Synchrotron Light Source (NSLS) with the capability to perform spin- and angle-resolved photoelectron emission spectroscopy on epitaxial thin magnetic films. The group effort required to accomplish this task is supported by the National Science Foundation under the Materials Research Group Program (MRG) and consists of investigators[1] from national laboratories, government and private sector laboratories, and universities. The present paper outlines selected opportunities and scientific issues associated with this group effort.

II. SCIENTIFIC ISSUES AND NEW OPPORTUNITIES

Ferromagnetism, in transition metals, results when the delicate energy balance involving exchange and correlation between conduction electrons favors a ground state in which more states having one spin are occupied than the opposite spin. Crystal structure, atomic coordination, the size of metallic radii, and various features of the electronic properties all play roles in determining whether magnetic ordering occurs. The same parameters govern the resulting magnetic properties in cases where magnetism exists. Surfaces and thin films provide a rich environment for testing our understanding of magnetic phenomena, as well as for searching for new magnetic phenomena and new magnetic materials. The primary new opportunities for probing magnetism arise from the ability to characterize and deliberately modify the atomic-level structure of thin magnetic films. Examples of properties that can be modified include: atomic coordination, crystal structure, and the electronic properties of the substrate material by selecting different single-crystal growth templates, quality of the surface by preparing stepped or ultrasmooth surfaces, film thickness, and lateral dimensions of film structures by suitable masks.

A broad range of novel magnetic properties has been predicted to arise in epitaxially grown magnetic thin films and superlattices and at surfaces of bulk magnetic materials in the new crystalline phases of matter that can be stabilized by epitaxy. These predictions are based on first-principles calculations which have achieved remarkable success in predicting electronic and magnetic properties of bulk magnetic materials. The predictions of novel magnetic behavior in deliberately modified materials must be taken seriously, based on the well-established predictive capabilities of these *ab initio* calculations. Some of the more striking predictions are considered here as they constitute part of the justification for the spin-polarized photoemission facility described later. Predictions are considered for selected surfaces, thin films, and artificially stabilized bulk materials.

Surfaces of bulk magnetic materials and monolayer epitaxial films exhibit inherently different atomic coordination than found in bulk materials. In addition, local electronic

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effects at surfaces and interfaces can affect magnetic behavior. These factors alone introduce significant modifications in the magnetic behavior of thin films. New physical phenomena that have been predicted to occur in ultrathin epitaxial magnetic films include perpendicular spin anisotropy,[2] enhanced moments,[3] magnetic quenching due to *sp-d* hybridization,[4] and thin-film magnetism in materials that are nonmagnetic in bulk form such as Pd and V.[2,3,5] Layer-dependent magnetic effects involving ferromagnetic and antiferromagnetic interlayer coupling have also been reported.[3] Some of these predicted new phenomena have been confirmed by experiments. For example, there appears to be general agreement based on a variety of experiments[6–10] that $p(1\times1)$ Fe films on Ag(100) exhibit perpendicular spin anisotropy for one and probably two atomic layers. Significant disagreements, however, remain regarding the range of parameters over which the perpendicular spin orientation occurs.[7–10] Enhanced magnetic moments in epitaxial films and superlattice structures continue to be a striking feature of most first-principles calculations,[3] even for the most recent results.[11] However, these effects have been established conclusively in only one case by suitable experiments,[12] and even here, there remains a controversy regarding scaling of the experimental data.[13] There have been some reports of the observation of ferromagnetism in thin films of V and Pd,[14] but other reports contradict these results.[15,16]

Artificially stabilized bulk materials are also of interest. One example is fcc Fe which can be grown on Cu(100). Zero-field magnetic moments of fcc Fe as a function of Wigner–Seitz cell dimension have been investigated by calculating the total energy of nonmagnetic, antiferromagnetic, and ferromagnetic phases.[17,18] These studies indicate that small variations on the Wigner–Seitz cell dimension, around the value established by epitaxy onto Cu(100), can determine whether the material is ferromagnetic or antiferromagnetic. The calculations predict the antiferromagnetic state to have the lowest energy, but experiments disagree on the magnetic properties of thin-film fcc structures. Angle-resolved photoemission,[19] spin-polarized photoemission,[20] and magneto-optical studies[21,22] of fcc Fe on Cu(100) suggest that the system exhibits ferromagnetic behavior whereas conversion-electron Mössbauer spectroscopy[23] suggests that it exhibits antiferromagnetism. The issues surrounding the magnetic behavior of this system are further clouded by questions regarding the film and interface structure.[24–26]

Other examples of a similar nature involve the magnetic properties of V and Pd films. Both Pd and V are paramagnetic in their bulk (equilibrium lattice constant) state and exhibit large paramagnetic susceptibilities. The atomic state of V has a moment of $3\mu_B$, and although atomic Pd has an electronic configuration of $4d^{10}5S^0$ (no magnetic moment) it is isoelectronic with Ni. The belief that both of these metals are nearly magnetic is supported by various first-principles calculations[2,3,5] that predict a rich variety of magnetic behavior in modified structures of both metals including ferromagnetism at expanded lattice constants.

Vanadium surfaces are predicted to be paramagnetic[27] but a V monolayer grown on Ag(100) is predicted to exhibit a large moment ($\sim 2\mu_B$) that is quenched as the film thickness is increased.[3] When spin-orbit effects are included, a free-standing film of V is predicted to have a magnetic moment perpendicular to the film plane.[2] More recent calculations[5] predict that an antiferromagnetic $c(2\times2)$ structure is more stable than a ferromagnetic structure for a V monolayer on Ag(100) and on Pd(100) substrates. The properties of modified Pd lattices are not as well studied theoretically as those of V. However, there are specific predictions of magnetic behavior for expanded bulk lattices.[28]

The experimental situation regarding Pd and V surfaces and epitaxial films is presently very unclear. Electron-capture spectroscopy experiments[14] have been reported which suggest that the (100) surface of bulk V and epitaxial V(100) layers on Ag(100) ranging in thickness from 1–7 atomic layers are ferromagnetic with critical behavior in agreement with the two-dimensional Ising model ($\beta = \frac{1}{8}$). Spin-polarized photoemission experiments[15] and Kerr effect experiments[16] have failed to detect evidence for ferromagnetism in 1–3 layer V films on Ag(100). Some evidence for magnetic ordering has been suggested by inverse photoemission studies of V on Ag(111), but these results are indirect. A few unpublished reports[14] that Pd films are ferromagnetic have appeared, but again preliminary Kerr effect analysis of Pd films on Ag have been inconclusive.

These few examples illustrate some of the new fundamental issues in magnetism and magnetic materials that are arising from the ability to stabilize new bulk phases of matter, and to grow deliberately modified structures. It is clear that the novel materials synthesis techniques combined with the established predictive capabilities of first-principles calculations offer outstanding new opportunities for exploring the fundamental relationships between structure and magnetism.

III. SPIN-POLARIZED PHOTOEMISSION SPECTROSCOPY

Angle-resolved photoemission spectroscopy using synchrotron radiation has now been established as one of the most important probes of the electronic properties of single crystals.[29] Conservation laws (the Einstein formula which governs the photoelectric effect and the conservation of electron wave vector parallel to the surface) permit detailed measurements of the dispersion of electronic states in crystals. The variation of electron escape depth with kinetic energy, and the variation of photoelectron cross section with photon energy offer additional opportunities to exploit tunable synchrotron radiation to discriminate between bulk and surface electronic states, and to obtain atom-specific atomic-level information about electronic states. Polarization dependencies in emission cross sections can be exploited to determine the symmetry of the electronic states involved in the photoemission process. These features render angle-resolved photoemission the preferred experimental method for studying atomic-level electronic properties. The technique is ideal for testing electronic structure calculations because the excitation spectra measured by photoemission contains essentially the same information obtained by the ground-state electronic structure calculations as long as correlation effects are small.

Two factors have hindered taking full advantage of angle-resolved photoemission for the study of magnetic materials.[30] The first is the difficulty of detecting the electron spin. Early electron spin detectors, based on Mott scattering, are large and cumbersome because of the requirements for high-acceleration voltages (~ 100 kV). New spin detectors have been developed[31,32] which achieve detection efficiency comparable to or better than the traditional Mott detectors ($\sim 10^{-4}$), but are much more compact because they require only modest (20 kV) or low (200 V) acceleration voltages. Two new compact spin detectors illustrated schematically in Fig. 1 are compatible with a movable electron analyzer, and permit angle and spin-resolved photoelectron detection. This type of spectroscopy offers the capability to determine the spin-resolved electronic properties of magnetic materials in great detail.

Realizing the angle- and spin-resolved photoemission capability requires dealing with the second factor that has hindered use of the technique. Spin detection is inefficient (factor of 10^4 loss in intensity), and high-resolution angle-resolved photoemission experiments continue to be somewhat limited in sensitivity. Typical counting rates of 10^5 s^{-1} can be achieved in high-resolution (100 meV, $\pm 2°$ angular resolution) experiments under ideal conditions on a high-performance bending magnet beamline at the National Synchrotron Light Source. However, the loss of a factor of 10^4 in intensity required to detect spin reduces this extremely useful technique to a very tedious exercise. In some cases, surface contamination effects render spin-polarization measurements impossible due to the extended integration times required to generate spectra having sufficiently good statistics.

The recent development of insertion devices (refer to Fig. 2) has permitted a sufficient gain in synchrotron radiation flux needed to make routine spin- and angle-resolved photoemission experiments feasible. A state-of-the-art undulator source properly coupled to an efficient monochromator is capable of yielding an increase in usable flux in the neighborhood of a factor of 100 in comparison with a bending magnet source. This increase is enough to enable routine angle-and spin-polarized photoemission experiments of magnetic materials.

IV. PROGRESS AND EXPERIMENTAL DETAILS

Several requirements must be met in order to fully exploit the capabilities of angle-resolved photoemission in studying magnetic materials: efficient spin detection, high flux of monochromatic radiation, and *in situ* capabilities for growing epitaxial magnetic materials and characterizing their structure. More precise capabilities for interpreting experimental data (i.e., capability for calculating spin-polarized angle-dependent photocurrents from ground-state electronic structure models) is an additional desirable capability. The initial phase of the group program of research on magnetic materials adopted these requirements as goals.

All of the spin-polarized photoemission results reported to date have been obtained using first-generation facilities that incorporate an existing undulator (originally designed for free-electron laser studies),[33] a rather primitive $\frac{1}{3}$ meter monochromator, and an endstation featuring a low-energy

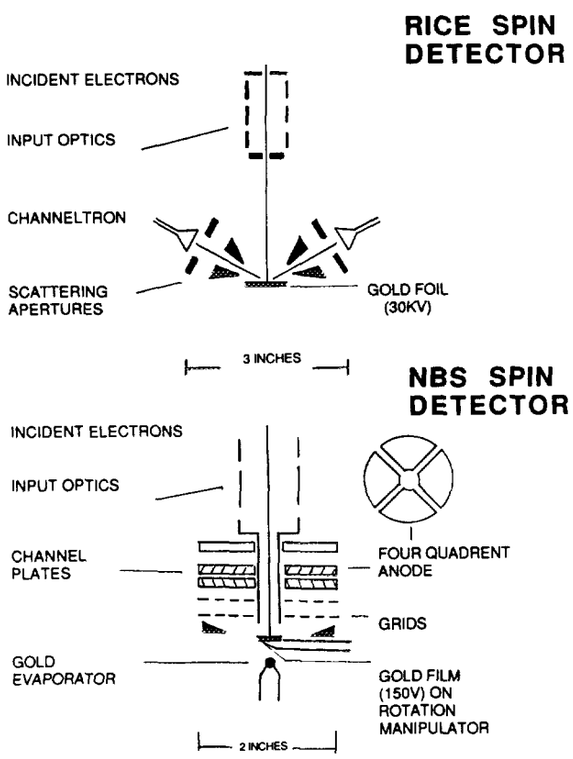

FIG. 1. Schematic representations of two types of compact spin detectors that have been developed by members of the Materials Research Group. Upper panel: mini-Mott detector developed at Rice University by G. K. Walters, F. B. Dunning, and colleagues (Ref. 31). Lower panel: low-energy spin detector developed at the National Bureau of Standards by Pierce and Celotta (see Ref. 32).

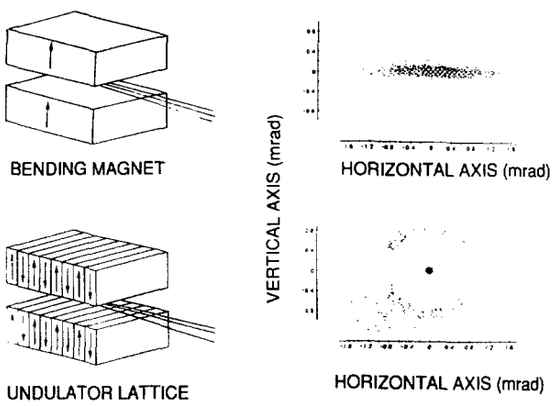

FIG. 2. Schematic representation of a bending magnet source and an undulator source including selected radiation patterns. The undulator source radiation exhibits the intense central spot characteristic of a tuned magnetic lattice source. Proper design of a monochromator required coupling a realistic undulator source generation code (see Ref. 34) with the ray-tracing code SHADOW developed by Cerrina (see Ref. 41).

spin detector (NBS design) coupled to a commercial 50 mm angle-resolving analyzer. All subsystems of the existing facility are now being upgraded. A new variable-gap undulator is being constructed by Spectra-Technology. This new insertion device will permit tuning of the first harmonic from ~20 to 70 eV, and corresponding third harmonic tuning from 60–210 eV. A new 6-m monochromator has been designed[34] and is now under construction which will cover this spectral range yielding high flux and high resolution. Refinements in the spin-detection system have been achieved[35] based on the requirements for stable spin detection in conjunction with synchrotron radiation based excitation. Finally, a comprehensive synthesis and characterization facility is being coupled to the endstation that will permit the growth and structure analysis of samples.

V. INITIAL RESULTS AND FUTURE PLANS

The choice of initial experiments have been subject to experimental constraints imposed by existing instrumentation, primarily the fixed-gap undulator which yields a high photon flux at wavelengths around 52 eV. Two examples from initial experiments are used to illustrate the importance of being able to detect the electron spin in angle-resolved photoemission studies of magnetic materials.

Figure 3 displays $\bar{\Delta}_1$ symmetry surface bands of Fe(100) determined by angle-resolved photoemission plotted on the projected bulk bands (shaded regions of the Fig.). Rectangular points were determined in previous experiments which were unable to distinguish electron spin.[36] Assignment of the photoemission peaks to minority- and majority-spin bands was made based on electronic structure calculations.[37] Triangular points represent new results obtained at the U5 MRG beamline by spin- and angular-resolved photoemission measurement.[38] These data show that the prominent band extending from $\bar{X}$ to $\bar{\Gamma}$ that lies in the

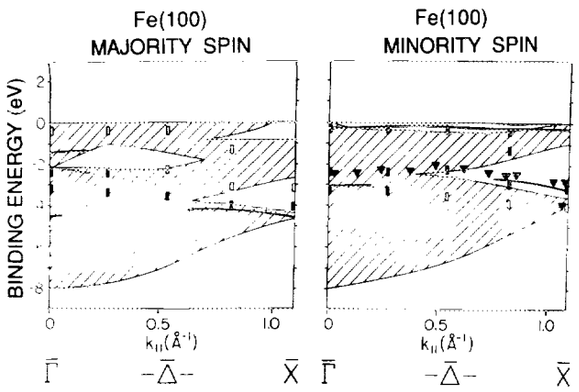

FIG. 3. Projected bulk bands of ferromagnetic Fe (shaded regions) along $\bar{\Gamma}\,\bar{X}$ of the two-dimensional Brillouin zone. Left panel: majority spin $\bar{\Delta}_1$ bands; right panel: minority spin $\bar{\Delta}_1$ bands. Rectangular symbols represent results of nonspin-resolved measurements (Ref. 36); solid points assigned to surface states with spin of that panel; open points assigned to surface states in the other (opposite-spin) panel. Triangular symbols represent results of spin-resolved measurements obtained by Brookes *et al.* (Ref. 38) at the U5 facility.

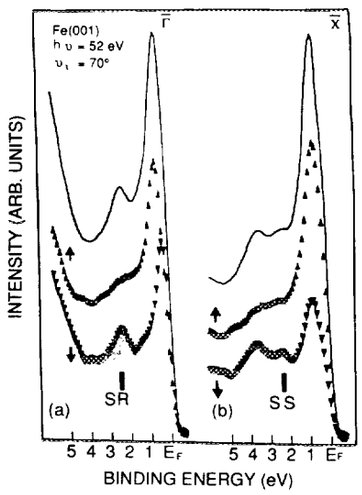

FIG. 4. Spin- and angle-resolved photoemission spectra of Fe(100) at (a) $\bar{\Gamma}$ and (b) $\bar{X}$ of the two-dimensional Brillouin zone [Brookes *et al.* (Ref. 38)]. The experimental data were obtained using even symmetry emission geometry.

$\bar{\Delta}_1\downarrow$ symmetry gap was correctly assigned to a surface state at $\bar{X}$ which becomes a $\bar{\Delta}_1$ symmetry resonance about half the distance to $\bar{\Gamma}$.

Figure 4 displays two spin- and angle-resolved photoemission spectra for Fe(100) at $\bar{\Gamma}$ and $\bar{X}$. The $\bar{\Delta}_1\downarrow$ surface state and resonance peaks are indicated in the spectra. The spectra exhibit a second well-defined structure having minority spin character that suggests that the lowest $\bar{\Delta}_1$ symmetry band is actually a minority-spin resonance at $\bar{X}$ rather than a majority-spin surface state as assigned in the nonspin-polarized measurements. Clearly, detection of spin adds important new constraints to data interpretation!

Figure 5 presents a second example of the utility of spin- and angle-resolved photoemission, in this case applied to an adsorbate system. This figure displays spin-resolved oxygen derived bands of $p(1\times1)$ O on Fe(100) reported by John-

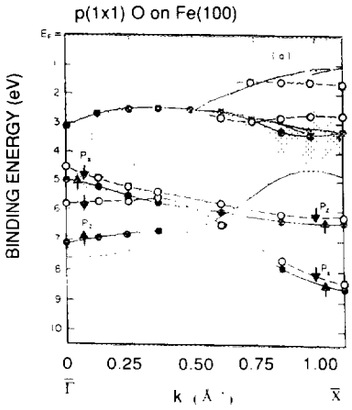

FIG. 5. Spin-resolved dispersion of the orbitals of $p(1\times1)$O on Fe(100) (see Ref. 39). Shaded region, projected bulk bands of Fe along the $\bar{\Gamma}$-$\bar{X}$ direction of the two-dimensional Brillouin zone.

son *et al.*[39] These results establish the existence of exchange coupling between a ferromagnetic substrate and a chemisorbed layer, and illustrate the importance of spin dependencies in the *p*-orbital hybridization of the chemisorbed atom.

VI. FUTURE

The two examples chosen to illustrate the utility of spin detection in angle-resolved photoemission studies provide only a suggestion of the potential of this technique. Limitations of instrumentation in areas of sample synthesis and characterization will soon be eliminated by addition of MBE facilities, and the new monochromator and undulator lattice will improve both resolution and photon flux as well as offer tunability which is extremely important in photoemission experiments. New developments which combine the capability of multiple scattering techniques used in low-energy electron diffraction analysis with first-principles calculations now offer the capability to predict spin-polarized photocurrents. The initial results obtained by Redinger *et al.*[40] for Fe(110) representing the first realistic attempt to calculate spin-polarized photocurrents are quite impressive, and suggest that an important new dimension of data interpretation is now available for analyzing experimental results.

Numerous opportunities for exploiting spin-resolved photoemission will continue to emerge as the experimental capabilities are developed. These include studies of epitaxial films in which the structure can be deliberately modified, as suggested in the Introduction, and spin-polarized Auger and core-level spectroscopy in which spin dependencies in electron correlation and lifetime effects can be studied using excitations which are species specific, and which exhibit energy shifts that are sensitive to surface and bulk local environments. It is clear that a rich variety of important physical phenomena and solid-state systems will be accessible to spin-resolved photoemission spectroscopy.

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