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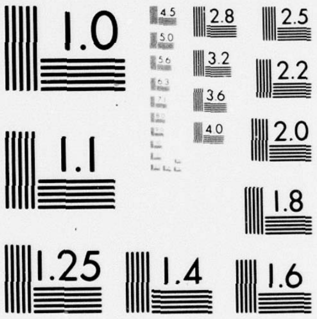
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ELECTRONICALLY INDUCED PHASE TRANSFORMATIONS

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Principal Investigator: Professor A. J. Freeman
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ABSTRACT

The electronic interactions responsible for the observed electronically induced phase transformations in several important classes of materials are being investigated theoretically in close collaboration with experimental programs at other institutions. These include destruction of superconductivity and onset of a normal magnetic state at low temperatures in ternary rare-earth superconducting compounds, charge density waves in layered transition metal dichalcogenides, origin of phonon anomalies in Pd and Pt metals, local density formalism for electronic bands, and metal-insulator phase transition in NbO_2.

PROGRESS ACHIEVED

The high level of scientific progress already made during this last year on the research proposed will become apparent from the accomplishments reported briefly in this section and the list of publications (attached as Appendix), which have resulted from AFOSR support.

A. Destruction of Superconductivity and Onset of a Normal Magnetic State at Low Temperatures in Ternary Rare-Earth Superconducting Compounds

Last year we indicated that the search for materials having higher superconducting transition temperatures and higher critical fields has been extended to the study of ternary compounds. Recently, Matthias and collaborators at La Jolla had found a new group of ternary compounds which show unusual transitions to the superconducting or the ferromagnetic state. Their general formula is MRh_4B_4, where M is either a transition or rare earth (three-or four-valent) element and they are superconducting for M = Y, Nd, Sm, Th, Er, Tm, and Lu and ferromagnetic for M = Gd, Tb, Dy, and Ho. This is only the second true ternary system of high T_c superconductors found thus far. The first was that of the double Mo-sulphides originally reported by Chevrel _et al_. The new system is tetragonal with 18 atoms/unit call.

Matthias _et al_. have reported most unusual behavior for the system $ErRh_4B_4$ at low temperature. As one cools down to 8.9 K, there is a transition from normal metallic conductivity to superconductivity, and as one lowers the temperature, there is _another_ transition at 0.9 K which returns the metal to its normal, but magnetic, state.

Following our proposal last year, we have calculated the electronic band structure of three of these compounds (M = Y, Er, Ho) to determine a possible electronic origin of these transitions using the _self-consistent_ LMTO method of Andersen and the full 18 atoms/unit cell. This is perhaps the only method which can handle such a complex problem with a finite amount of computer time and reasonable accuracy. These calculations have been described as representing a tour de force on what is the most complex band structure problem ever tackled. They yield a good understanding of the origin of the different phase transitions. Briefly, we find that the superconducting transition is governed by the Rh 4d electrons (through the Bardeen-Cooper-Schrieffer interaction) which show a peak in the density of states at the Fermi energy and the competing magnetic/normal state transition is determined by the rare-earth 5d-4f intra-atomic RKKY exchange interaction.

For the alloys from Gd to Ho, the large effective spin moment leads to a magnetic interaction which dominates over the superconducting interaction, and so the magnetic ordering temperature T_m is greater than the superconducting transition temperature T_s. In the Er and Tm alloys, with their smaller spin moments, the "effective" magnetic ordering temperature the system would have in the absence of the onset of the superconducting state is reduced and so $T_s > T_m$. The *observed* value of T_m in Er is smaller than this effective ordering temperature because once the superconducting state has been achieved, the conduction electron susceptibility is zero in principle--at least for the Rh electrons. Hence, for this compound, the magnetic interaction is largely ineffective compared to that in Ho (and earlier elements in the series). However, at lower temperatures the RKKY magnetic interaction is still sufficiently strong to order magnetically the localized Er 4f moments to produce a sufficiently large exchange field to then destroy the superconducting state. This results in the low observed temperature of the re-entrant magnetically ordered state at $T=0.9$ K.

B. Charge Density Waves in Layered Transition Metal Dichalcogenides

The transition metal dichalcogenides, MX_2, where X = S or Se, an important class of materials because of their platelet two-dimensional structure which causes them to exhibit strongly anisotropic and anomalous physical properties, superconductivity, and most recently, the existence of a transition to the charge density wave (CDW) state--a not too well-understood phenomenon.

As indicated last year, we have followed up our successful studies of the origin of the CDW in TaS_2 and $TaSe_2$ with a highly accurate self-consistent study of TiS_2 done with our recently developed numerical basis set self-consistent linear combination of atomic orbitals discrete variational method (SC-LCAO-DVM). Our results showed unambiguously that TiS_2 is an indirect gap (0.25 eV) semiconductor and thus resolved several controversies concerning this important material. Our results showed good agreement with optical properties for energies below 16 eV. Contrary to previous expectations, a <u>small</u> indirect gap (0.2 - 0.3 eV) was found to occur at the points L and M in the Brillouin zone, with a larger direct gap (0.8 eV) at Γ. To our delight, a recent comprehensive analysis of transport, magnetic susceptibility, Hall effect, resistivity, Seebeck, etc., data yielded a gap of 0.2 - 0.5 eV, in agreement with our predictions.

We then called attention to the need for a similarly accurate study of its sister compound, $TiSe_2$. Recent interest in the nature and unusual properties of $TiSe_2$ has centered on the unusual $2a_0$ by $2c_0$ superlattice which forms in $TiSe_2$ at low temperature. Wilson has suggested that this might be an example of the so-called excitonic state rather than a charge density wave state (CDW) such as that found in the Group V layered dichalcogenides. Woo <u>et al</u>. studied the intensity of x-rays diffracted by the superlattice, magnetic susceptibility, resistivity, and far infrared reflectivity, as a function of temperature in nonstoichiometric samples. Their results showed that the transition observed at $T_o = 145 \pm 5K$ is second order, and they concluded that it was apparently a normal-to-commensurate transition driven by the Fermi surface (FS) which has a highly two-dimensional character. Recent neutron studies on stoichiometric samples found $T_o = 202$ K involving transverse atomic displacement with wave vector $\vec{q} = (1/2, 0, 1/2)$; this transition was interpreted as being driven by electron-hole coupling.

Since extrapolation of our results for TiS_2 to the case of $TiSe_2$ is crude at best, and since muffin-tin or semiempirical models are not able to resolve these questions, we undertook an *ab initio* study of the electronic band structure of $TiSe_2$ in order to understand its various measured properties. Of direct interest was to compare with the first angle-resolved photoemission studies of Bachrach, *et al*., which showed conduction band overlap of the valence band along the Γ-M direction by at least 0.5 eV.

The band structure was calculated in the local density-functional (LDF) approach, using our previously published numerical basis set LCAO discrete variational method. We find that $TiSe_2$ is a semimetal with an indirect *negative* gap (0.20 eV) between Γ and L; contrary to some previous expectations, no electron pocket was found at M. The dimensions of the electron pocket at L (0.20 LH, 0.25 LA, and 0.5 LM) indicate the presence of 7-8 x 10^{20} conduction band carriers/cm^3 in the perfect crystal. This is in very good agreement with the most recent independently reported transport and angle-resolved photoemission experiments of DiSalvo and collaborators, and Traum and collaboratores at Bell Laboratories.

What may be said about the origin of the CDW? The several mechanisms proposed involve one or another form of "nesting" of electron-electron or electron-hole Fermi surfaces. This includes the "exciton-insultaor" mechanism which, as emphasized by Wilson and Mahajan, is akin to the large scale "electron hole" nesting present in Cr and responsible for its spin density wave. Because of the degeneracy of the hole bands along Γ-A and their near degeneracy along Γ-M and Γ-K, the volume of the hole pocket is substantially smaller than that of the singly degenerate electron surface and hence direct "nesting" of these surfaces would seem difficult to achieve. It is possible, however, that large peaks in the generalized susceptibility, $\chi(\vec{q})$, arising from characteristic "volume effects" (i.e., two parallel electron-hole bands crossing the Fermi surface) provides the overscreening in these strong electron-phonon coupled systems which drives the observed instability. Plausible candidates in $TiSe_2$ are the very nearly parallel K_3-Γ_3^- and the L_1^+-H_1 bands which are separated by a zone boundary wave vector. Parallel bands, not necessarily crossing E_F, are not peculiar to $TiSe_2$ alone but prevail in many similar compounds such as TiS_2, TaS_2, $TaSe_2$ and VSe_2. Indeed, a major peak in $\chi(\vec{q})$ was found in 1T-TaS_2 and 1T-$TaSe_2$ to be caused almost entirely by "volume" effects. It therefore seems highly likely to us that this same mechanism drives the CDW instability in $TiSe_2$. Expressed in terms of the bonding in the system, such an instability can be described as a partially screened interaction between the electrons at L (with their wave-function amplitudes predominantly on the Ti site) and the holes at Γ (with wave-function amplitudes predominantly on the Se site) with a zone boundary phonon supplying the coupling momentum and carrying out the structural change (e.g., shortening of the Ti-Se bond). Finally, whereas the phenomenological correlation between the observed instability temperature and the c/a ratio (or lattice ionicity) works remarkably well for many layered dichalcogenides, including $TiSe_2$, it predicts an instability temperature in excess fo 100°K for TiS_2. Our analysis also suggests an explanation of the failure to observe such an instability in TiS_2; although both TiS_2 and $TiSe_2$ fulfill the volume effect condition, slight differences in the ionicities between them, which are not reflected in a dramatic change in the c/a ratio, are sufficient to place this "nesting" in a gap region in TiS_2 and in a semimetallic region in $TiSe_2$.

C. Origin of Phonon Anomalies in Pd and Pt Metals

The possible role of electronic structure on observed phonon anomalies in metals remains an important fundamental problem in understanding lattice contributions to phase transitions.

In their classic paper, Miiller and Brockhouse observed an anomaly in the slope of the $(0\xi\xi)$ T_1 branch of the dispersion curves for palladium. The anomaly not only extended over a broad range of wave vector space but also decreased rapidly in amplitude with increasing temperature. Later, Dutton et al. also found a rather similar but not identical anomaly in the T_1 branch of platinum. On the basis of the known Fermi surfaces, these anomalies were suggested as arising from the generalized Kohn effect due to nesting.

We have studied the possible occurrence of generalized Kohn anomalies by direct calculation of the generalized susceptibility, $\chi(\vec{q})$. We find that a peak in $\chi(\vec{q})$ can be directly related to the observed anomaly in the $(0\xi\xi)$ T_1 branch of the dispersion curves of Pt and Pd. We calculated the band structure for Pd using the APW method and the relativistic APW scheme for Pt--both with a warped muffin-tin potential. The band structures were previously found to yield Fermi surface radii, temperature dependencies of the static magnetic susceptibility, $\chi(T)$, resistivity, and a spin lattice relaxation, T_1T, in very good agreement with experiment. In the $\chi(\vec{q})$ calculations, we used 2048 tetrahedra in 1/48'th irreducible

BZ and the energy eigenvalues as fitted to a Fourier series representation. The results of $\chi(\vec{q})$ for q along [010], [110], and [111] directions were calculated for Pd and for Pt for bands 4, 5, and 6 which cross the Fermi energy. The intraband parts of $\chi(\vec{q})$ at $\vec{q} = 0$ for both metals are found to agree with the density of states at the Fermi energy to within 0.5%. Results show that the dominant contribution to X_{intra} arise from the dominant band 5 whose "jungle-gym" FS has strong nesting features; the main peak for Pd occurs at the same q value (=0.65π/a) for $\vec{q}$ along the [oqo], [q,q,o], and [q,q,q] directions. The locus of this main peak is a square in the (0,0,1) plane. The maximum of X_{intra} for q along the [110] and [111] directions are 23% and 13%, respectively, higher than the value of $\chi(\vec{q})$ at $\vec{q} = 0$. For $\vec{q}$ along the [010] direction, the peak is, however, 5.4% lower than the value of X_{intra} at $\vec{q} = 0$. Hence, while phonon anomalies are predicted for the [110] and [111] directions, no anomaly is predicted for the [100] direction. The predicted q value for the [110] anomaly, q = 0.65 π/a is close to the experimental value of ~0.7 π/a. Although there may be a hint of an anomaly at 0.56 [111] in the measurements, a more detailed investigation of this region is called for.

For platinum, X_{intra} for $\vec{q}$ along the [010], [110], and [111] directions has mean peaks which occur at q = o.68 π/a, 0.75 π/a, and 0.85 π/a, respectively. Here too, this main peak comes from the nesting of the jungle-gym Fermi surface which is not, however, as flat as that of palladium. Anomalies are predicted (although weaker than in Pd) along [110] and [111] but not at [100]. The [110] anomaly is close to the measured q value (~0.7-0.8 π/a). Also in agreement with experiment, we predict a weaker [110] anomaly for Pt than for Pd, i.e., the ratio of $[X_{intra}\ (q\ max) - X_{intra}\ (q = o)]$ to $X_{intra}\ (q = o)$ is 23% for Pd versus 12% for Pt. In both Pd and Pt, weaker anomalies are predicted for the [111] direction than for the [110] direction.

We have also calculated $\chi(\vec{q})$ of both Pd and Pt for q along an off-symmetry direction, TW. These results also show peaks from band 5 which arise from nesting FS features but which are lower than $\chi(q = 0)$. These results are consistent with Miiller's observations for the "off-symmetry" direction in the (001) plane making an angle $\theta = 30^\circ$ and is no longer visible at $\theta = 45^\circ$.

D. Local Density Formalism for Electronic Bands

We have continued our development and testing of the local density functional formalism (LDF) approach to the determination of electronic band structures. This is the approach we have already used successfully for the layered dichalcogenides studies described above. We have successfully completed a parallel study of the important semiconductor system, CdS. Long a favorite II-VI compound for study, recent interest in the electronic structure of CdS derives from its use in solar-cells (e.g., in CdS-Cu_2S heterojuctions) and the observation of electron-hole complexes for high excitation densities in this material.

There now exists a vast literature comprising experimental and theoretical investigations of the electronic structure and related properties of the important II-VI compounds. Of obvious importance for understanding and interpreting many of the observed properties of these materials is a detailed knowledge of their underlying electronic band structures. In this regard, recent optical and photoemission experiments have played an important role in elucidating key features of the band structure over an increasingly large range of energies above the fundamental band gap.

On the theoretical side, pioneering ab initio energy band studies were carried out for many of these materials using the non-muffin-tin self-consistent orthogonalized plane wave (SCOPW) method. This technique has been applied in recent years to the study of the electronic structure of a large number of semiconductors and semi-metals, and has resulted in a considerable gain in insight into the systematics of both the III-V and II-VI compounds as well as in a better understanding of the photoemission, high pressure, and optical data for these materials. At that time, the only popular alternative method was the non-self-consistent empirical pseudopotential approach, which avoided completely the specification of the microscopic potential in the solid (i.e., the nature of the Coulomb exchange and correlation fields) by parametrizing empircally the first few Fourier components of an unspecified crystal potential. Although this phenomenological approach has produced a great deal of information on the variation of the gaps in II-VI compounds and the origin of the important band structure critical points in the Brillouin zone, no meaningful comparison of the adequacy of the SCOPW approach, as well as that of the underlying exchange models, could be made.

More recent developments in semi-empirical non-local (non-self-consistent) pseudopotential theory have improved considerably the agreement between the calculated band structure and x-ray and UV photoemission data by introducing a few additional disposable parameters to describe the geometry of the angular momentum dependent model pseudopotential terms. Although a successful parametrization scheme, little could be learned regarding the microscopic nature of the elementary interactions which lead to this success. Further, due to the independence of the parametrized model potential on its associated variational wavefunction, questions such as self-consistency and the nature of the crystal dissociation products (which are well-defined LDF atoms in both LCAO and SCOPW models) have remained large unresolved and have inhibited a meaningful comparison with first-principle models based on well-understood (but less successful) crystal potentials. Subsequent studies on the convergence properties of the OPW model, independent theoretical studies on compounds made of first-row atoms (diamond, boron nitride) and photoemission studies on the core levels of compounds containing the 4d elements, have revealed serious difficulties with this representation. These include: (i) errors of the order of 1-3 eV in the calculated p-like valence and conduction band states of compounds made of first-row atoms due to convergence difficulties in the absence of a pseudopotential cancellation for these $\ell = 1$ states, (ii) spurious shifts of about 12 eV of the core-like 4d levels in the course of the self-consistent treatment, and (iii) errors in excess of 6 eV in the level ordering of the cation 4d and anion s bands relative to recent photoemission data.

We have carried out a self-consistent all-electron first-principles electronic band structure study of cubic CdS carried out within the local density functional (LDF) formalism, using our previously developed linear combination of atomic orbitals (LCAO) technique in a numerical basis set representation.

In the first set of calculations, we employed the same lattice constant, exchange (only) potential and computational parameters as were used by Stukel et al. in their early self-consistent orthogonalized plane wave (SCOPW) investigation so that a direct comparison of results can be made and the validity of the SCOPW approach for covelently bonded 4d systems can be assessed. In the second set of calculations, the Stukel et al. computational restrictions were relaxed, a more accurate lattice parameter was employed and the Kohn-Sham exchange and the Singwi et al. correlation potential used to obtain the local density formalism solutions to the band problem, including variation of the band structure and related properties with pressure (change of lattice constant). Comparison with optical and x-ray and UV photoemission experiments for excitations of both the s-p and metal d bands in the 5-19 eV region indicate very good agreement. The direct gap at Γ was, however, found to be 0.5 eV (25%) too small, a discrepancy similar to that previously found in non-empirical studies for other heteropolar insulators (e.g., Ne and LiF). This is traced to the neglect of the different orbital relaxation at the Γ_{25} and Γ_1 band edges and to the non-cancellation of the self-interaction terms characteristic of the local density potential. Simple atomic total energy models for these effects are shown to bring this gap into good agreement with experiment. From these studies we concluded that a first-principles (parameter-free) exchange and correlation LDF model describes very well the main electronic structure features of the system.

E. Metal-Insulator Phase Transition in NbO_2

Niobium dioxide shows a structural phase transformation (rutile to body centered tetragonal) around 810°C accompanied by rapid changes in resistivity and magnetic susceptibility. The high temperature rutile phase is metallic, while the distorted phase is found to be semiconducting. The transition is less abrupt than in the isoelectronic compound VO_2 and has been characterized as second order by neutron diffraction studies. It is possible to prepare good single crystals of NbO_2 in contrast to the first transition series compounds, so this system provides a good testing ground for comparing theories of electron-phonon interactions and electronically driven transitions with experiment. In addition, pseudobinary compounds such as $Ti_xNb_{1-x}O_2$ are found useful in studying effects of d-electron occupancy on electrical, optical, magnetic and structural properties.

Neutron and x-ray studies have provided accurate values for atomic positions in both phases of NbO_2. The low temperature distorted phase is understood to be essentially equivalent to a dimerization of the metal atom chains found along the rutile c-axis, analogous to the famous Peierls distortion. In the case of VO_2, x-ray diffuse scattering measurements by

Terauchi and Cohen confirm the existence of soft phonon modes centered at the point R = ($\frac{1}{2}$,0,$\frac{1}{2}$) of the Brillouin zone as predicted by a band structure study. However, the mechanism of the phase transition in NbO_2 is less clear and neutron scattering experiments have failed to detect low-frequency soft-mode phonon branches particularly at the wave vector P = ($\frac{1}{4}$,$\frac{1}{4}$,$\frac{1}{2}$) thought to be associated with the static lattice distortion.

We have studied the electronic band structure and the generalized susceptibility, $\chi(\vec{q})$, in order to assess the possible role of electronic instabilities in the observed structural phase transformation. Since, as is well known, first principles calculations on such systems of rather low symmetry are difficult, some calibration against experiment must be made prior to estimating the validity of the theoretically determined electronic response functions. Thus it is especially important for our work that Raccah _et_ _al_. have made extensive optical reflectance measurements on single crystal NbO_2 and $Ti_xNb_{1-x}O_2$ and have derived the associated absorption function $\epsilon_2(\omega)$. These data provide the basis for a detailed comparison between theoretical band structures and experiment.

For the band studies, we used the recently developed linearized-augmented-plane-wave (LAPW) method of Koelling and Arbman, a method proven to provide an efficient and accurate approach for complex structures. Using a rigid band scheme, the results of our calculations are found to describe accurately the optical absorption of the rutile phase of NbO_2 stabilized by 20 at % Ti. Thus encouraged, we determined theoretically $\chi(\vec{q})$ in the constant matrix elements approximation including both Fermi surface "nesting" and so-called "volume" effects. Unlike the case of VO_2, no Fermi surface nesting features are observed and $\chi(\vec{q})$ is not found to have maxima in the region of the point P in the Brillouin zone.

Arthur J. Freeman

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1. "Conduction Electron Polarization, Magnetization Densities and Neutron Magnetic Form Factors in Metals", Physica 91B, 193 (1977)

2. "Electronically Driven Phonon Anomalies and Phase Transformations", Proc. of International Conference on Lattice Dynamics, Paris, France, 1977 (in press)

3. "Re-Entrant Magnetism in Rare-Earth Superconducting Ternary Compounds", J. Mag. & Mag. Mat'ls. 7, 296 (1978) (with T. Jarlborg and T. J. Watson-Yang)

4. "Electronic Structure and Proton Spin-Lattice Relaxation in PdH", Phys. Rev. B (in press) (with M. Gupta)

5. "Theoretical Determinations of Spin Densities", Physica Scripta 15, 80 (1977)

6. "Self-Consistent Numerical Basis Set LCAO Investigation of Electronic and Structural Properties of TiS_2", Phys. Rev. B 16, 906 (1977)(with A. Zunger)

7. "Local Density Formalism Approach to Cohesive Properties of Solids: Diamond, BN, and LiF", Int. J. of Quant. Chem. Symp. 11, 539 (1977) (with A. Zunger)

8. "Defect State Models for Localized Excitations in LiF", Physics Lett. 60, 456 (1977) (with Alex Zunger)

9. "Ground and Excited State Electronic Properties of LiF in the Local Density Formalism", Phys. Rev. B 16, 2901 (1977) (with A. Zunger)

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12. "Calculation of Charge and Spin Densities in Solids", in Mössbauer Isomer Shifts, edited by G. Shenoy and F. Wagner (North-Holland Publishing Company, Amsterdam, 1978).

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14. "Local Density Self-Consistent Energy Band Structure of Cubic CdS", Phys. Rev. B 17, 4850 (1978) (with Alex Zunger)

15. "Generalized Electronic Susceptibility and Charge Density Waves in $1T-TaS_2$ and $1T-TaSe_2$", Phys. Rev. B 15, 885 (1977) (with H. W. Myron and J. Rath)

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16. "Self-Consistent Numerical -Basis-Set Linear-Combination-of-Atomic-Orbitals Model for the Study of Solids in the Local Density Formalism", Phys. Rev. B 15, 4716 (1977) (with Alex Zunger)

17. "Ground-State Electronic Properties of Diamond in the Local-Density Formalism", Phys. Rev. B 15, 5049 (1977) (with A. Zunger)

18. "Band Structure and Lattice Instability of $TiSe_2$", Phys. Rev. B 17, 1839 (1978) (with Alex Zunger)

19. "Electronic Structure of 1T-VSe_2", Phys. Rev. (submitted) (with Alex Zunger)

20. "Structurally Induced Semimetal-to-Semiconductor Transition in 1T-$TiSe_2$", Phys. Rev. Letters 40, 1155 (1978) (with Alex Zunger)

21. "Electronic Band Structure and Properties of α-U", to appear in Proceedings of the 3rd International Conference on the Electronic Structure of the Actinides", Grenoble, France (with D. D. Koelling and T. J. Watson-Yang)