

Chapter 17 Condensed Matter Theory

Reitz, 1954-1965	PTaylor, 1964-	Leff, 1964-1971	Coopersmith, 1964-1969	Silvert, 1966-1969
Segall, 1968-2000	Petschek, 1983-	Lambrecht, 1996-	Mathur 1995-	

Starting in the early 1940's, the experimental study of electrons in metals and their interaction with the atoms of the crystal lattice played a major role in physics research. The goal was to measure the mechanical, thermal, optical, and electrical properties of metals, insulators, and other forms of condensed matter. These measurements would then lead to the development of theoretical models based on the laws of electromagnetism and quantum mechanics. The models in turn would lead to the creation of new materials for applications in electronics, optics and many other areas. We have looked at the *experimental* work of Smith, Gordon, Eck and Schuele in Chapters 7 and 12. Here we shall sample some of the work done by our condensed matter *theorists* in explaining the experimental observations in terms of fundamental physics principles.

John Reitz



Fig. 17-1.
John Reitz.

Les Foldy (Chapter 9) was the first theorist in either the Case or the WRU department. In addition to his papers on atomic and subatomic phenomena, he published work in condensed matter theory, often in areas of interest to his experimentalist colleagues. In 1954 the Case department added a dedicated condensed matter theorist, **John Richard Reitz**. **Fig. 17-1** The 31-year old assistant professor had completed his BS at Case in 1943 and was at the Harvard Underwater Sound Laboratory during the war (another "Dayton Miller acoustics" contribution to the war effort). Reitz' PhD at Chicago in 1949 was based on calculations of atomic electron wave functions. They were performed on the Electronic Numerical Integrator and Calculator (ENIAC) at the US Army's Aberdeen Proving Grounds. "The Effect of Screening on Beta-Ray Spectra and Internal Conversion" *Phys. Rev.* **77** 10 1950. Reitz then spent three years on the staff of the Los Alamos Scientific Laboratory, LASL.

Electrons in materials

One of Reitz's first works at Case was a 95-page "how-to handbook", which he described as an "attempt to consolidate the methods developed during the past fifteen years for calculating electron wave functions and electronic structures in solids." "Methods of the One-Electron Theory of Solids" *Sol. St. Phys.* **I** 1 1955.

He then turned to calculations of properties of materials being measured in Chuck Smith's lab at Case. It seems that Reitz got directly involved with the experiments as well. "Elastic Constants by the Ultrasonic Pulse Echo Method" *J. Appl. Phys.* **29** 683 1958. This was an experimental paper with Stephen Eros, one of C. Smith's students. In a paper with Smith, Reitz looks at the behavior of the shear moduli (e.g. the resistance of the material to being deformed) of dilute alloys as a function of the average number of electrons per atom, which in turn depends on the concentration of foreign atoms. Experimentally observed discontinuities in the moduli at particular values of the electron/atom ratio are successfully reproduced in the model. The model proposed that at certain concentrations, the extra electrons upset the symmetry of the crystal so that it loses some of its stiffness. "Calculation of the Elastic Shear Constants of Magnesium and Magnesium Alloys" *Phys. Rev.* **104** 1253 1956 (with experimentalist Chuck Smith).

Reitz coauthored a largely experimental paper with PhD student W. J. Tomasch in which the output voltage of thermocouples was measured as a function of the composition of the alloys being tested. They observed rather striking variations in the voltage as a function of the percentage of indium. These were ascribed to specific changes in the electronic band structure. "Thermoelectric Power of Dilute Indium-Lead and Indium-Thallium Alloys" *Phys. Rev.* **111** 757 1958. He then joined Bill Gordon and Tom Eck in publishing a paper based on their de Haas-van Alphen measurements (see Chapter 12). "Evidence for Spin-Orbit Splitting in the Band Structure of Zinc and Cadmium" *Phys. Rev. Lett.* **7** 334 1961. In "Peltier Coefficient at High Current Levels" *J. Appl. Phys.* **32** 1623 1961, Reitz discusses the optimum choice of materials for semiconductor junction devices. (*The Peltier effect concerns the transfer of heat from one place to another when current passes through a junction from one metal to another.*)

In an exercise quite different from his electrons-in-matter research, Reitz joined Foldy in tackling a problem in classical electromagnetic hydrodynamics. Starting with Maxwell's equations, they derived expressions for the force and torque acting on a low-conductivity sphere moving in a conducting fluid at right angles to an external magnetic field. "The force on a sphere moving through a conducting fluid in the presence of a magnetic field" *Jour. Flu. Mech.* **11** 133 1961.

While at Case, Reitz maintained his connections with LASL, spending extended periods at the New Mexico lab. He worked there on a variety of theoretical topics. "Thermoelectric Properties of the Plasma Diode" and "Efficiency of the Plasma Thermocouple" *Jour. Appl. Phys.* **30** 1439 1959 and **31** 723 1960. "Elastic Scattering of Slow Electrons by Cesium Atoms" *Phys. Rev.* **131** 2101 1963. "Magnetic Breakdown in Metals" *J. Phys. Chem. Solids* **25** 53 1964.

In 1964, John Reitz accepted a position with the Ford Motor Company in Dearborn MI where he remained until his retirement in 1987. With Case colleague, Fred Milford (Chapter 9), Reitz authored a widely-used undergraduate text which has gone to four editions: *Foundations of Electromagnetic Theory* (Benjamin Cummings 1993).

Phil Taylor

In 1962, a second condensed matter theorist joined the Case department. The 25-year-old London-born post-doc, **Philip L. Taylor**, had done his BSc at London and his PhD at Cambridge. His doctoral research included an analysis of how electrons are scattered by impurities as they bounce around in metals. **Fig. 17-2.**

A condensed matter glossary

*This might be a convenient place to enumerate some of properties of materials which are fair game for experimentalists to discover and theorists to explain. Basically, it's all electromagnetism and quantum mechanics. The ions and electrons have electric charge; the atoms and molecules might have magnetic moments; the molecules might have electric dipole moments (positive at one end, negative at the other), and they all talk to each other through Maxwell's equations. The quantum mechanics comes in because all the pieces are described by wave functions which specify positions, momenta and energies. You might consider the next six paragraphs as a **glossary** which you may come back to later as the terms come up.*



Fig. 17-2. Phil Taylor.

*The **thermal conductivity** is a measure of the rate at which heat flows through a sample when its two ends are held at different temperatures. The **electrical conductivity** determines how much current flows when a voltage is applied to a sample. It depends on how easily the electrons move through the material. The **Hall effect** describes the appearance of a voltage at right angles to a current flowing through a conductor when a transverse external magnetic field is applied. The **thermoelectric power** measures the electric field which appears within the sample when a temperature gradient is applied across the sample. The **dielectric constant** is a measure of how much the electric field inside the sample is reduced when its molecules line up with their own dipole fields opposing the externally applied field.*

***Pyroelectricity** is a rather subtle effect which occurs when a dielectric material is heated. In such a material, all the little electric dipoles line up with an applied electric field, so that surface charges appear on the opposite faces of the sample. If the sample is heated, the dipoles lose some of their alignment and the effective surface charge changes, resulting in a measurable potential difference between the surfaces. These materials can be used as detectors of heat, for example, in infra-red night goggles.*

***Ferroelectrics** are materials which exhibit an electrical polarization even in the absence of an applied electric field. The direction of this polarization can be re-oriented by the application of a strong electric field. The name ferroelectric was chosen in analogy with ferromagnetic because both types of materials display hysteresis behavior on field reversal. Iron has nothing to do with ferroelectrics. The **piezoelectric effect** refers*

to the appearance of a static electric field in certain materials when they are mechanically stressed.

*Now, some magnetic properties: **magnetic permeability** measures the effective strength of the magnetic field within the sample when an external magnetic field is applied. In **diamagnetic** materials, the atoms have no permanent magnetic moment, but the atomic electronic orbits shift a bit so as to slightly reduce the field. **Paramagnetic** materials do have atoms or molecules with small permanent magnetic moments, and these line up to slightly increase the field. **Ferromagnetic** materials have very strong magnetic moments so that the field in the sample might be several thousand times stronger than the applied field. The term **ferrimagnetism** is used for materials in which the reinforcement of the field is lessened because of magnetic interactions internal to the lattice which force some of the dipoles to point the wrong way. This is beginning to sound like a biology textbook – but it's a fact that materials can respond in all these different ways to applied fields.*

*The **speed of light** in the material depends on two of the properties listed above, the dielectric constant and the magnetic permeability. The dielectric constant can depend on the frequency of the applied electric field (e.g. the color of the light), and so therefore does the speed of light. The **index of refraction** of the material is the ratio of the speed of light in vacuum to that in the material. The **optical activity** of a material is a measure of how much the direction of polarization of a beam of light is rotated as it passes through the material.*

*The importance of **band structure** in materials was described in Chapter 12. Recall that this refers to the allowed energy levels for electrons in a material, and how certain bands of energy are not allowed. The existence of these bands is extremely important in determining the electrical and optical properties of the materials. The whole of semiconductor technology depends on band structure. The experimentalists and the theorists of the department have been measuring, calculating, and predicting band structure for the past 50 years.*

In his first paper at Case, Taylor looked at the connection between the electronic band structure of metals and the temperature dependence of the voltage produced when one metal is placed in contact with another metal. This is related to the thermoelectric power studied by his predecessor, John Reitz. (You may have experienced such a voltage when you touched a silver filling in your tooth with a steel fork.) Taylor pointed out that the inclusion in the theory of interactions between the electrons and the phonons leads to a better understanding of the experimental results. "The Thermoelectric Power of Metals" *Phys. Lett.* **3** 245 1963.

One of Taylor's more important contributions to the theory of electrons in solids was a paper entitled "The Boltzmann Equation for Conduction Electrons" The Boltzmann equation describes the probability that an electron will change its momentum from one value to another. In the case where there are no fields or temperature gradients, the equation predicts that the rate at which electrons leave a certain volume in momentum

space equals the rate at which they enter it. That is, not much is happening. Taylor looks at the case where there *are* electric and magnetic fields, as well as a possible temperature gradient, so that there is a lot of direction-dependent rearranging of the electrons and their vector velocities. *Proc. Roy. Soc (London)* **A275** 209 1963.

During his first dozen years at Case, Phil Taylor worked on the theory of electrons in disordered systems. Dilute alloys, in which the uniform crystal structure is disrupted by foreign atoms, and glasses, in which there is no uniform structure at all, are examples of disordered systems. The subsequent decade-and-a-half would be Taylor's "polymer period", and then in the 1990's he would tackle the theory of liquid crystals.

Disordered Systems

The properties of crystals in which small amounts of foreign atoms are introduced provide interesting tests for the theorist. Taylor published two papers showing that there should be band gaps in the allowed energies of electrons in an amorphous semiconductor which has been modified by the introduction of randomly distributed inhomogeneities. "Energy Gaps in Disordered Systems" *Proc. Phys. Soc.* **88** 753 1966 and **90** 233 1967.

In 1973, Taylor and his student James Gubernatis tackled the problem of how the magnetism of amorphous ferromagnetic materials behaves as they are warmed up. Recall that the degree of magnetization depends on the degree of alignment of the electrons' and atoms' magnetic moments, and that these tend to get jostled around as the temperature is raised. If one looks at such a system quantum mechanically, there can be certain wave-like excitations in which the magnetic moments of neighboring atoms change directions smoothly across the lattice, like a line of twirling ballerinas, each one a bit out of phase with her neighbor. These excitations are called spin-waves, and their existence affects the dependence of the magnetization on the temperature. "Spin-wave Spectrum of an Amorphous Ferromagnet" *Phys. Rev.* **B9** 3828 1974.

Thermoelectric effects in dilute alloys would occupy Taylor's interests for the better part of a decade. He points out some of the pitfalls in this endeavor in a whimsical introduction to a review paper. "The theory of thermoelectricity is to be found in a looking-glass land where all our best-loved folk-theorems are cruelly violated. Everyone knows that pseudopotentials are better than Hartree potentials in calculating scattering amplitudes, that higher-order electron-phonon interactions terms are negligibly small, and that the electronic relaxation time for phonon scattering may be approximated by a function that is symmetric about the Fermi energy. And yet Thermoelectricity is a subject whose siren song has lured many an unwary traveler into errors for which history has been brutally unforgiving." *Thermoelectricity in Metallic Conductors* (Plenum Publishing 1978)

Polymers

Starting in the mid-1970's, the experimental and theoretical study of polymers became a major activity in the department. Since that time there have been ongoing col-

laborations with researchers in the materials science and engineering, macromolecular science and engineering, chemical engineering and chemistry departments, as well as extramural collaborations with Kent State University and the University of Akron. The earliest polymer work in the region dating back to the nineteenth century developed in the “Rubber City”, Akron.

Polymers comprise a special class of condensed matter, consisting of chains of repetitive groups of atoms called monomers. Some polymers occur naturally as in tars and fibers and some, like nylon and vinyls, are produced from petrochemicals. Thousands of different structures display a wide variety of mechanical, thermal, electrical and other properties. Phil Taylor became interested in understanding these materials and their properties in terms of the underlying physics.

Taylor, and his collaborator Anton Hopfinger of the CWRU Department of Macromolecular Science, published a series of papers on the problem of crystallization and melting of polymers. By computing the energy of interaction between each monomer and its nearest and next-to-nearest neighbors along the chain, and its nearest neighbors in adjacent chains, they were able to determine the temperature at which “melting is approached through increasing anharmonicity as phonon interactions become dominant and changes in lattice cell dimensions occur.” “Theory of melting in simple polymers. I.” *J. Chem. Phys.* **67** 353 1977.

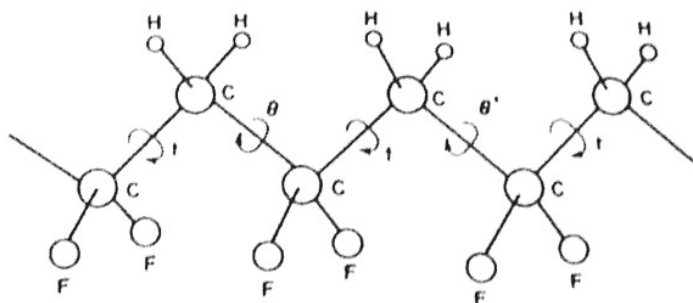


Fig. 17-3. A typical polymer structure.

In the introduction to a 1979 paper, Taylor and his collaborators write, “We believe this to be the first reported work in which such a rich variety of stable and metastable phases of a polymer has resulted from a calculation in which there are no adjustable parameters, and of which the starting point is the calculation of potential energy by means of conformational analysis.” **Fig. 17-3** shows the molecular structure of the “PVF2” polymer. The object of the calculation was to look at the energy of the system as a function of the angles between successive monomers and between adjacent rows of polymers, for varying applied stresses and temperatures. Minima in these energies successfully predict different experimentally observed phases for PVF2. “Theory of Structural Phase Transitions in Poly(Vinylidene Fluoride)” *Phys. Rev. Lett.* **43** 456 1979. (in collaboration with Hopfinger)

When an electric field is applied to certain polymers, there results a degree of alignment of subunits called crystallites. This process of reorientation is called “poling”. Taylor became interested in the process and the way in which a wave of realignment moves through the material. A computer simulation of the motion of a kink moving along the polymer was used to determine the speed of propagation, and this compared

reasonably well with experimental observations. "Kink Propagation as a Model for Poling in PVF2" *Phys. Rev.* **B21** 3700 1980.

The **Hall effect** has been known since 1879, but it was not until about 100 years later that it was discovered that, at low temperatures, when the magnetic field across a two-dimensional (i.e. very thin) sample is raised, the Hall voltage rises not smoothly, but in jerks, like the steps of a staircase. Taylor and his student Olle Heinonen produced a theoretical model of the "quantum Hall effect" based on a thermodynamical equilibrium approach, which correctly described the experimental behavior. In this model, the electrons in the bulk material travel in circles with quantized energies, contributing nothing to the current. At the edges of the conductor, however, the electron orbits are interrupted by the surface, and a net current flows, with negligible dissipation. The following year, a second paper addressed the observation that at a certain critical value of the current density, the resistance to the flow of current rises precipitously. Noting that the breakdown occurred when the drift velocity of the electrons reached the speed of sound in the material, they decided to investigate the role of phonons (i.e., those quanta of vibrational energy in the lattice) in the onset of resistance. It appears that the interaction with phonons disturbed the neatly filled energy levels of the electrons when the electron density gets too high. "Conductance Plateaus in the Quantized Hall Effect" *Phys. Rev.* **B28**, 6119 1983 and "Electron-Phonon Interactions and the Breakdown of the Dissipationless Quantum Hall Effect" *Phys. Rev.* **B30**, 3016 1984.

Experiment had shown that certain membranes made from polymers exhibited markedly different transport properties for positively and negatively charged ionic species. Taylor and colleagues applied their modeling techniques to this phenomenon of "permselectivity". As in all their calculations, energy is the key. This time it is the electrostatic energy between the ions and the membrane and the elastic energy of the polymer. The goal is an understanding of the preferential direction of ionic flow, based on the properties of the surface presented to the bath by the membrane. The application of effects such as these may provide better materials for such technologies as fuel-cells. "Simple Model for Clustering and Ionic Transport in Ionomer Membranes" *Macromolecules* **17**, 1704 1984.

A particular one-page paper stands out as unusual. It was written by Taylor and colleagues, Les Foldy and Rolfe Petschek, and concerns the application of some of these polymer materials to the detection of high energy particles. They point out that incident particles can heat the polymer, destroying its polarization, resulting in a pyroelectric voltage which can be detected. Whether this suggestion was acted upon by particle physics experimentalists is not clear. "Pyroelectric Materials as Electronic Pulse Detectors of Ultraheavy Nuclei" *Phys. Rev. Lett.* **54** 1089 1985.

Everyone knows that when a liquid is cooled it eventually changes phase and becomes a solid. Taylor and his post-doc Vladimir Pines investigated the way in which the transition spreads through the liquid. You may have admired the patterns of ice which grow across a cold window pane, or the fern-like patterns of salts coming out of solution in a petrie dish. At the simplest level, the key parameters are the latent heat and the rate

of heat flow. The speed of the phase boundary depends on how much heat must be removed and how fast can it be moved away. "Stability and Instability in Crystal Growth-I. Symmetric Solutions of the Stefan Problem" *Phys. Rev.* **B32**, 5362 1985.

Most magnetic materials involve metals with unpaired electrons whose magnetic moments can become aligned. Taylor and postdoc Kashi Nath looked into the possibility of building a "ferromagnet" out of carbon, hydrogen, oxygen, and nitrogen – the stuff we are mostly made of. They point out that one way to get the magnetic moments to line up would be to hang the atoms on polymer chains, most probably arranged in parallel helices. They calculated the magnetization and critical temperature for such arrangements for various numbers of unpaired spins per helix loop, and find that "macroscopic ferromagnetism might occur in a bulk sample of these materials." "Electronic Structure and Magnetic Properties of some Possible Organic Ferromagnetic Polymers" *Molecular Crystals and Liquid Crystals* **205** 87 1991.

The interaction between ions in a polymer depends to some extent on the screening of their fields by electrons. "...many-electron theory can be used to derive an approximate expression for the effective Coulomb interaction between pairs of charges in an insulating organic solid". "Dielectric Screening of Coulomb Interactions in Polymers" *Macromolecules*, **25** 1694 1992.

Liquid Crystals

In the early 1990's, Taylor turned his attention to the study of polymer liquid crystals. This work would complement the experimental work on liquid crystals by Chuck Rosenblatt who joined the department in 1987 (Chapter 18). Liquid crystals consist of molecules consisting of a few hundred atoms which are typically longer than they are thick and which tend to line up roughly parallel to one another. There are various ways in which the molecules might align themselves, for example mostly parallel, but with their centers randomly distributed in the crystal (called **nematic** - Greek for thread – or like uncooked spaghetti in the box), or mostly parallel, with centers lying in layered planes normal to the molecules' axes (called **smectic** - Greek for soap – more like uncooked lasagna in the box). The degree of orientation tends to get washed out as the temperature is raised. Liquid crystals are bi-refrigent, that is, their index of refraction depends on the angle between the plane of polarization of the light and the "director" or principal axis of the sample.

It was discovered that these liquid crystal molecules could be attached in an orderly fashion along the length of a polymer. In this way, they could still line up to control the index of refraction, but they are anchored in place and no longer float around in liquid form. It was a natural move for Taylor to apply his polymer expertise to such materials. The theorist's interest would be to determine the degree of the liquid crystal alignment along with the thermal, mechanical, electromagnetic, and optical properties. With the widespread application of liquid crystals to PC monitors, TV screens, and other displays, for example, it is important to know how completely and how quickly one can

change the optical properties of the liquid crystal with the application of external electric fields.

Another thing which might be asked is at what temperature will a solid crystal change into a liquid crystal. Again one must look at the energy associated with the interactions among the molecules and the various degrees of freedom within the molecules. In one paper Taylor determines how the transition temperature decreases as the molecules are elongated by the introduction of monomers which act as spacers. "Theory of the Solid-Nematic Transition in Thermotropic Main-Chain Liquid-Crystalline Polymers" *Phys. Rev.* **A44** 821 1991.

Between 1991 and 2003 Taylor, along with members of his group, published an additional eighty papers on the theoretical modeling of polymers and polymer liquid crystals. Many of these papers were co-authored by his colleague, Chuck Rosenblatt, who leads the department's experimental liquid crystal program.

Phil Taylor authored a widely-used advanced text in 1970: *A Quantum Approach to the Solid State* (Prentice Hall, 1970, 321 pp). Thirty two years later, he and his former student, Olle Heinonen (then at the University of Central Florida), collaborated on a updated version which reflects the enormous advances made in the intervening years: *A Quantum Approach to Condensed Matter Physics* (Cambridge University Press, 2002, 424 pp). He remains active in teaching and research. Taylor has always been a champion of the environment and has regularly taught a popular course in "Environmental Physics". His research has been funded principally by the National Science Foundation, which has made possible the support of a long line of graduate students and post-doctoral collaborators. Taylor has been research advisor to about twenty doctoral students, many of whom returned to campus in 1997 on the occasion of a Festschrift honoring him on his 60th birthday.

Harvey Leff, Michael Coopersmith and William Silvert

Between 1964 and 1966, three new young theorists were hired, two at Case and one at Reserve. Each of them, like Phil Taylor, did "condensed matter theory". New faculty were needed in each department to handle increasing teaching loads. One attraction of hiring theorists is that they require no initial set-up expenditures for labs and equipment. Ultimately, each of these three new theorists would remain six years or less.



Fig. 17-4.
Harvey Leff.

The 27 year-old **Harvey Leff** had completed his doctorate under Max Dresden at the University of Iowa in 1963. **Fig. 17-4.** His principal research interest was statistical mechanics. During the six years he spent at Case and CWRU, Leff published a dozen papers on a variety of problems in statistical mechanics, papers which have been described as significant attempts to explain the complicated mathematics associated with that area of physics theory. In particular, he

sought ways to link the macroscopic variables used in thermodynamics with the descriptions used in statistical mechanics. Among his publications at Case are the following representative papers: "Class of Ensembles in the Statistical Theory of Energy-Level Spectra" *J. Math. Phys.* **5** 763 1964. "Statistical Thermodynamics of Incompletely Specified Systems" *Jour. of Chem. Phys.* **41** 596 1964. "Asymptotic Densities in Statistical Ensembles" *Phys. Rev.* **136** A355 1964. "Difference-Equation Solutions for the Linear Ising Model and Nearest-Neighbor Fluid" *Amer. Jour. Phys.* **36** 591 1968.

Leff's special interest in teaching is illustrated by an article he wrote for the *American Journal of Physics*, a favorite journal of teachers of university physics. The abstract closes with the remark, "The canonical structure, which is demonstrated, is pedagogically useful as (1) a memorization device, (2) an example of the utility of Legendre transformations in statistical mechanics, and (3) an aid in understanding the relationships of the various ensembles to one another." "On the Connections between Thermodynamics and Statistical Mechanics" *Amer. Jour. Phys.* **37** 65 1969.

Leff was promoted to associate professor in 1969 but, as was the case for several others among his colleagues, his 1970 bid for tenure was not successful. Leff was a popular and successful teacher, with 100 of his students signing a petition in his behalf. By the end of the semester, he had accepted a position as chair of the physical sciences department at Chicago State College. In 1979, he joined the Energy Information Systems Program at Oak Ridge National Laboratory.

The second 1964 addition to the department was **Michael H. Coopersmith**. **Fig. 17-5.** The 28-year-old was born in Brooklyn, did his BA at Swarthmore, and his PhD in 1962 at Cornell where he worked with Robert Brout on the theory of phase transitions. His dissertation was on the "Statistical Mechanical Theory of Condensation". *Phys. Rev.* **130** 2539 1963. He was a National Science Foundation Fellow at the École Normale Supérieure and then spent two years as a postdoc at the University of Chicago.



Fig. 17-5.
Michael Coopersmith.

One of the problems Coopersmith tackled, first at Chicago and then at Case, was the behavior of free electrons dancing around in a cold helium vapor. This is quite different from electrons in a crystal lattice, where the forces are long range. Here the helium atoms are hard spheres, and the electrons essentially bounce off them elastically. Experimentally, it had been observed that the mobility of the electrons drops by a factor of a thousand when the pressure of the vapor is raised above a certain critical value. Coopersmith reported that his "bubble model", which looks at the scattering of electrons within a cluster of stationary, hard-core helium atom scatterers, provides an adequate description of the situation. "Multiple Scattering and Many-Body Theory: Free Energy of Electrons in Helium" *Phys Rev.* **139** A1359 1965. "Relaxation-Time Approximation for the Mobility of Electrons in Helium" *Phys. Rev.* **161** 168 1967 (with NASA-Lewis collaborator, Harold Neustadter).

Coopersmith and Leff teamed up to produce two even more mathematical statistical mechanics papers on the distribution of hypothetical hard-core particles in a one-dimensional fluid. "Translational Invariance Properties of a Finite One-dimensional Hard-core Fluid" *J. of Math. Phys.* **8** 306 and 434 1967.

In a series of five single-author papers, Coopersmith looked at the behavior of magnetic or fluid systems undergoing phase transitions near a critical point. The work was summed up in the last paper, whose abstract states that "we have arrived at a picture of a phase transition which is in accord with all currently observed behavior in the neighborhood of a critical point." "Analytic Free Energy: A Basis for Scaling Laws" *Phys. Rev.* **172** 230 1968.

Coopersmith resigned from the CWRU department in the summer of 1969. He took a position on the physics faculty at the University of Virginia where he is currently a member of the emeritus faculty.



Fig. 17-6.
William Silvert.

The third among the new condensed matter theorists was **William L. Silvert**. **Fig. 17-6.** Silvert did his PhD at Brown under future Nobel laureate Leon Cooper. Cooper is the "C" of the BCS theory which is described briefly in Chapter 15. Silvert's research was on the theory of superconductivity. He published a series of papers on surface superconductivity and on non-homogeneous superconductors as a post-doc at Michigan State. In 1966 he was recruited by Chairman Chandrasekhar to a position as assistant professor in the WRU department. Silvert was given a year's leave of absence so that he could participate in a US-USSR Academies of Sciences exchange program. He spent the 66-67 academic year at the Institute of Theoretical Physics in Moscow. His paper on non-homogeneous superconductors was

published soon after his move to Cleveland. The problem which Silvert addressed was the modification of the electron-electron interaction when two different superconducting metals are placed in contact. "Solution of the linearized energy-gap equation in nonhomogeneous superconductors" *Zh. Eksp. Teor. Fiz.* **53** 1693 1967; *Sov. Phys. JETP* **26** 971 1968. Silvert soon moved on to faculty positions at the University of Kansas and at Dalhousie in Halifax.

Segall: band structure in solids

In Chapter 12 we wrote about the experimental work done by Gordon and Eck on the behavior of electrons in a metallic lattice and what one could learn from measuring the magnetization of the material as an applied magnetic field is varied. The looping orbits of the electrons in the material provide information on its band-structure. We discussed there how determination of the Fermi surface and related band-structure fixes the allowed energy levels for electrons which find themselves in the periodic potential of a crystal lattice. It is the *disallowed* energy levels, in the so-called "energy gap", which give the material its interesting properties.

It was clear that the newly merged CWRU department would benefit from the addition of an expert on the theory of electrons in materials. Benjamin Segall joined the department in 1968 and would be productive in this area for the next thirty years. He completed his BS at Brooklyn College in 1948 and his PhD at the University of Illinois Urbana in 1951. **Fig. 17-7.** His dissertation research was in particle theory, under Geoffrey F. Chew. It involved the calculation of the cross section for the photodisintegration of the deuteron ($\gamma d \rightarrow p n$) in the 50 to 100 MeV range. After postdoctoral positions at Illinois and at the Institute for Theoretical Physics in Denmark, Segall decided in 1956 to leave the academic world and join the research department of General Electric Laboratory in Schenectady. He would remain there for thirteen years. Not only did he leave academe, but he also left behind his work in particle and nuclear physics, switching abruptly to condensed matter theory. He would be calculating electronic band structure within the year.

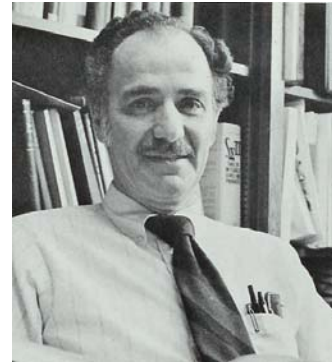


Fig. 17-7. Ben Segall.

Segall's early work at GE was the development of a technique to calculate band structure in a crystal lattice with more than one atom per unit cell. At the end of the 1950's, the first digital computers became available for research laboratories, and Segall had access to state-of-the-art computer power at GE. (typically 16K RAM, punch card or paper tape input, \$50-100K each!)

For a theorist, band structure and Fermi surface calculations begin with an assumed crystal structure and a form for the periodic potential in which the electrons find themselves, and proceed iteratively to find self-consistent wave functions. Most of the technical expertise is in the computational methods used in seeking the solution. Segall worked on the electron structure of such pure metals as copper and aluminum, and on a variety of doped semi-conductors. It gets interesting when impurities are included. The results can be compared with experimental measurements of electron mobility, resistivity, magnetoresistance, the Hall coefficient, and optical properties. Segall published about two dozen papers while at GE, most of them in the *Physical Review*. A significant number were written in collaboration with experimenters, and addressed in-house measurements.

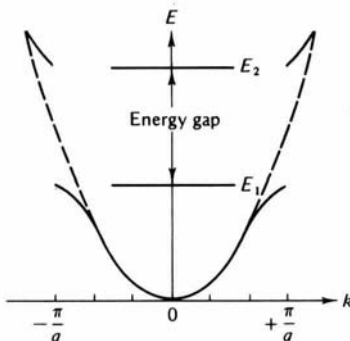


Fig. 17-8. Energy vs. wavenumber in a periodic potential.

An aside on the quantum mechanics “particle-in-a-box” problem and band structure. A particle in a one-dimensional infinite well of width a must have a wavelength so that an integral number of half wavelengths just fits in the well, $a=n\lambda/2$; just like a standing wave on a piano string. The electron's momentum is $p=h/\lambda$, its wave number is $k=2\pi/\lambda$, and its kinetic energy is

$E = p^2/2m$. Therefore, only certain values of λ and k and p and E are allowed. A plot of E vs k for a single particle is a parabola. For a periodic potential such as one would find in a one-dimensional crystal, the allowed values of E spread out into bands of energy. This happens because the E vs k curve takes abrupt jumps at the single particle “square-well” k values. As a result, there are big gaps in the allowed energies. That means, for example, that no electrons have energy between E_1 and E_2 in **Fig 17-8**. It's the size of this band-gap which determines many important properties of the material. Now, all the theorist has to do is find the allowed and forbidden energy values for a three-dimensional periodic potential and predict the material's electrical and optical properties.

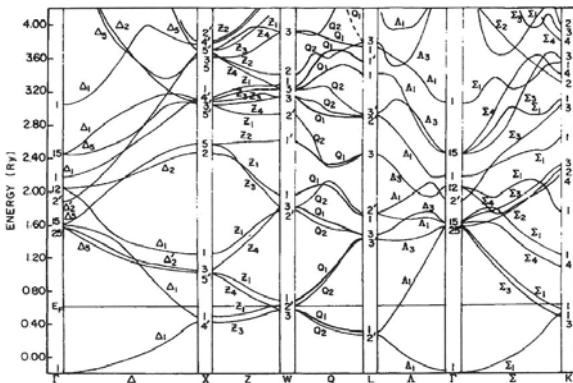


Fig. 17-9. Computed electronic energy levels for a typical crystal..

the potential to some constant level in a sphere around each atom, and zero elsewhere. This potential is then “tuned-up” to match the experimentally observed band-structure. This was one of a series of papers co-authored with post-doc An-Ban Chen. *Phys. Rev.* **B12** 600 1975.

As an example of the electronic energy levels which Segall and his group have calculated, we show in **Fig. 17-9** a rather amazing plot from a paper on the band structure of aluminum. It is a far cry from the little broken parabola in **Fig. 17-8**. The vertical stripes correspond to different directions in the crystal lattice. One can see portions of many parabolae. Perhaps a bit more understandable is the upper curve in **Fig. 17-10** which shows the calculated x-ray spectrum which follows from the electron energies. (The x-rays are emitted when an electron drops from one level to another, so this spectrum corresponds to

A portion of the abstract from a 1974 paper gives an idea of the technique: “A new empirical energy-band parametrization scheme based on the Green's-function method has been developed and was applied to Cu and Ag. The scheme utilizes the logarithmic derivatives associated with an *ab initio* muffin-tin potential $V^{(0)}(r)$. The scheme can be understood in terms of the addition to $V^{(0)}$ of energy and angular momentum dependent square-well potentials, the depths of which are adjusted to yield the correct (empirical) energy bands.” The “muffin tin potential” sets

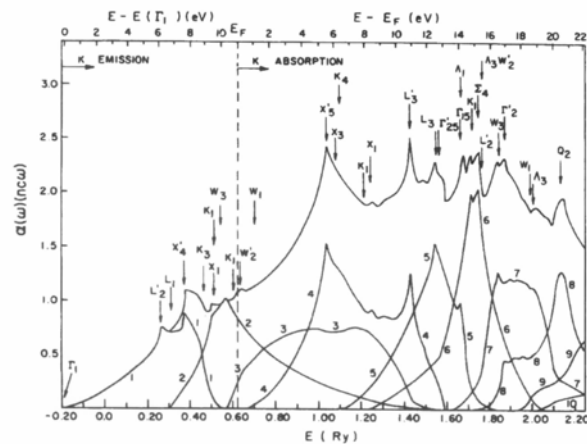


Fig. 17-10. Corresponding computed x-ray spectra for a typical crystal..

energy differences.) Measurements of the x-rays provide a test of the theoretical calculations. This work was done with grad-student Frank Szmulowicz. “K x-ray absorption in aluminum” *Phys.Rev.* **B21** 5628 1980.

Segall was interested in the properties of a great variety of materials, some of which had been measured experimentally, and some of which were hypothetical materials which had not yet been fabricated. In addition to establishing mechanical properties like lattice structure and elasticity, calculations based on first principles, *e.g.* atomic numbers, can predict the dielectric, optical and electrical transport properties crucial to technology. As in the polymer and liquid crystal studies done by Phil Taylor and Rolfe Petschek, the ultimate goal is to design structures with interesting technological potential.

Segall tackled a very different type of calculation when he joined his colleague, the versatile theorist Les Foldy, in a series of papers on the lattice dynamics of certain alkali halide “mirror pairs”. These involved pairs of elements such that one is a positive alkali ion, like potassium, and the other is a negative halide ion, like chlorine, which sits at the opposite end of the line in the periodic table. Another such pair is rubidium and bromine. It was found that materials incorporating such pairs have remarkably similar optical properties, as in the comparison between $\text{RbCl}_x\text{Br}_{1-x}$ and $\text{BrK}_x\text{Rb}_{1-x}$. “Anion-cation mirror symmetry in alkali halide ion dynamics II” *Phys. Rev.* **B29** 2293 1984.

Band-structure calculations can be done not only for bulk materials consisting of a single lattice, but for *heterostructures* (two solids in close contact) or *superlattices* (interleaved layers of two solids). Of special interest to semiconductor technology are interfaces between two different solids, for example, the contact between a semiconductor and a metal. It is important to understand how the electron energy levels behave in the region where the two lattices meet. Another possibility is the study of the interface between two solids of the same material, but with different crystal alignments.

Segall and his colleague **Walter Lambrecht** did extensive calculations on wide band-gap semiconductors such as silicon carbide and aluminum and gallium nitride. These materials have band-gaps well into the ultraviolet (*that is, you need an ultraviolet photon to promote an electron across the gap*) and have robust mechanical and thermal properties, with possible applications to high power electronic applications. Another feature of the nitrides is that they can be used in light emitting diodes (LED's) which produce green and blue light.

To keep this chapter in somewhat chronological order, we'll pick up on Ben Segall's research a bit later when we describe his partnership with Walter Lambrecht. But first, we back up to the 1980's and the arrival of Rolfe Petschek.

The 1980's – New Faculty, New Directions

If one looks at the “time-line” chart in the introductory chapter, it is easy to follow the arrivals and departures of physics faculty members. In the late 1960's, chairman Willard had the unenviable job of slimming down the oversized department. Then in the

1970's, as the newly merged university worked its way through some difficult political and financial challenges, neither chairman Ken Kowalski nor his successor Don Schuele succeeded in adding new faculty. The "intermediate energy" group (Willard, Bevington and Baer) was disbanded and not replaced, and the "high energy" and "cosmic ray" experimental groups were unable to add essential junior members. The situation began to turn around in the early 1980's, with the hiring of Gary Chottiner (Chapter 12) in 1980 and of Rolfe Petschek in 1983. The pendulum was swinging from nuclear/particle/cosmic ray research back to condensed matter research. Thus began two decades, not so much of expansion, but of rejuvenation (literally), as new young faculty were brought in to replace those who decided to retire.

Rolfe G. Petschek

Condensed matter theorist, **Rolfe Petschek**, earned his S.B. degree at MIT and his Ph.D. (1980) under B. I. Halperin at Harvard. Rolfe was born in Los Alamos, New Mexico, where his father worked as a theoretical physicist. **Fig. 17-11.** His doctoral research concerned certain aspects of dynamics near continuous phase transitions, including the

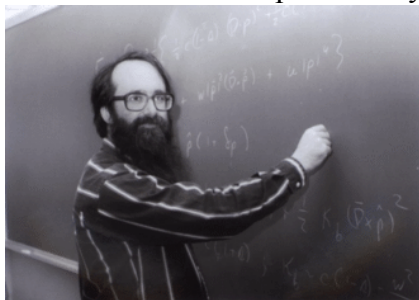


Fig. 17-11. Rolfe Petschek.

rate at which magnetically aligned protons in a crystal of ammonium chloride "relax", i.e. lose their alignment. Each proton in this crystal lattice sits between a nitrogen atom and a chlorine atom. Measurement of the relaxation times as a function of temperature provides information on the interactions between the protons and their neighboring ions, and ultimately on the effect of defects on the dynamics of the phase transition. "Proton-spin-resonance relaxation times near the ordering transition in NH_4Cl " *Phys. Rev.* **B19** 166 1979.

Polymers

Petschek became a graduate research assistant at Los Alamos and later had post-doctoral positions at UC Santa Barbara and UC San Diego. He worked with the eminent physical chemist John C. Wheeler and French physicist Pierre Pfeuty on modeling the conformations of interacting polymers. "Bicriticality in the Polymerization of Chains and Rings (*Phys. Rev. Lett.* 50, 1633 1983)

Petschek joined the CWRU department in 1983. During the following four years he continued the work on polymer growth and phase transitions. In a series of solo papers, he presented mathematical models for the way in which certain polymers undergo phase transitions. Then, along with Wheeler and Pfeuty, he investigated the applicability of a model originally proposed for magnetic systems to analogous behavior in polymers.

A key parameter in the description of these materials is T_c , the *critical temperature*. At such a critical point, the material goes through a phase transition and its properties change abruptly. Petschek described an interesting transition in polymers. When

elemental sulfur is heated, its properties change very rapidly at around 160 C. At this temperature the 8-atom-rings of low temperature sulfur rearrange themselves into polymer chains which have higher entropy than the rings. Such transitions in systems that form polymers have deep connections to magnetic critical phenomena. Theoretical models for polymers attempt to determine how properties change as the critical point is approached, from above or from below. In a paper with Wheeler and Pfeuty, Petschek looked at the critical points of polymers which could contain both rings and long-chain components. The structure and volume fraction of long-chain polymers suggested *bicriticality*, i.e. behaving as one would expect at a point in the phase diagram at which two lines of critical points merge. From the abstract: “*The bicritical nature of the critical point is the result of a competition between a transition to form long-chain polymers and a transition to form an infinite-rings condensate. As a result the fraction of monomers incorporated in chains and in rings varies with temperature according to a different power law than that for the total fraction of polymerized material.*” “Equilibrium polymerization of chains and rings: A bicritical phenomenon” *Phys. Rev.* **A34** 2391 1986.

Liquid Crystals

Petschek soon became interested in the theoretical analysis of liquid crystals (LCs). In 1987, he and grad student Kimberly Wiefeling looked in particular at **ferroelectric** fluids. Recall that ferroelectric materials can have a permanent electric polarization. Here is their abstract: “While there is no fundamental reason that fluids should not be ferroelectric, the only known ferroelectric fluids are chiral smectic-C liquid crystals. In this paper we argue that a variety of nonchiral smectic phases composed of properly designed oligomeric or polymeric molecules will also be ferroelectric. These ferroelectric fluids, and the solids formed by quenching them, should be of fundamental and practical interest. The nature of these phases, the design of the relevant molecules, and the experimental techniques for identifying the phases are discussed qualitatively.”

We introduced some LC jargon earlier in this chapter, e.g. nematic (aligned molecules), smectic (aligned, and in layers). Here is a bit more: If the constituent molecules are **chiral**, i.e. if they look like right-handed or left-handed corkscrews, the LC is called **cholesteric**. Molecules that form liquid crystals can be chemically bonded to each other in various ways. A single chemical unit which forms a liquid crystal is a liquid crystal **monomer**. If a few such monomers are bonded to each other, this is called an **oligomer** (from the Greek “few parts”) – if many are bonded together this is called a **polymer**. The molecules proposed by Petschek and Wiefeling were fraternal twins – two rather different liquid crystal molecules tied to each other.

An aside on the design of ferroelectric liquid crystals: the goal is to have monomers which are electric dipoles (positive on one end, negative on the other) and which can be stuck onto a polymer chain so that their dipole moments line up parallel with one another. The resulting material has enhanced electrical effects, including non-linear optical effects, just what you want in electrically switched liquid crystals. Some chiral smectics and bowl-shaped or disk-shaped LCs show this desired behavior.

The authors stress the potential applications of ferroelectric fluids to liquid crystal technology. From their concluding remarks: “These phases would have practical applications. Solid phases, made by rapid quenching of these ferroelectric liquids, may have desirable mechanical and electrical properties such as plasticity and a well-defined, hard-to-change polarization. For such applications, it may be that long, polymeric molecules are superior. It may be possible to use these fluids in displays or other devices which require rapid change of a liquid crystal’s properties.” Recall that LCs can rotate the direction of polarization of light, so that when they are sandwiched between two polarizers, they can act as electrically activated switches which can turn the transmitted light on and off in microseconds. “Novel Ferroelectric Fluids” *Phys. Rev. Lett.* **59** 343 1987.

Petschek and Dennis Perchak (initially at CWRU, then at Eastman Kodak Research Laboratories) expanded on this work, collaborating on an extensive program of computer simulations of ferroelectric LCs. “Computer simulations of quasi-lattice models for novel ferroelectric liquid crystals” *Phys. Rev.* **A43** 6756 1991.

Petschek, along with new collaborators at the Liquid Crystal Institute at nearby Kent State University, continued the work on ferroelectric LCs. From the abstract of a 1988 paper: “We examine the possibility that molecules with permanent dipole moments can form a ferroelectric nematic phase, the least ordered conceivable ferroelectric phase. We show that reasonable electric dipole interactions between disk-shaped molecules may lead to such a phase, and calculate the phase diagram using mean-field theory.” “Ferroelectric Nematic Liquid Crystals: Realizability and Molecular Constraints” *Phys. Rev. Lett.* **60**. 2303 (1988). These interactions with Kent State, both with its physics department and with the Liquid Crystal Institute, grew over the years, resulting in a large science and technology center called ALCOM (Advanced Liquid Crystalline Optical Materials). With about twenty investigators from CWRU, Kent and the University of Akron ALCOM engaged in important LC research for over a decade.

Post-doc Eugene Terentjev, now at Cambridge, worked with Petschek as part of the ALCOM center. His research was focused on various aspects of liquid crystal molecules which have been linked together. He continued Petschek’s study of ferroelectric liquid crystals, suggesting that liquid crystal mesogens which are connected to each other in a “head-to-tail” fashion may form ferroelectric phases.

Grad student George Hinshaw joined Petschek in studying critical phenomena in systems which they found can be described by a theory related to one which has had great success in particle physics. Surprisingly, this “Yang-Mills” theory had practical applications for liquid crystals. In their abstract: “Possible consequences for designing molecules for chiral smectic-C phases with increased polarizations are discussed.” “Transitions and modulated phases in chiral tilted smectic liquid crystals” *Phys. Rev.* **A39** 5914 1989.

Supporting the experimentalists

In 1989, Petschek began to work extensively with Chuck Rosenblatt and his experimental liquid crystal group. Their goal is to understand, design, fabricate, and test

materials with the most desirable properties, such as transparency, stability, and rapid response time. This work will be briefly described in the “after-1990” Chapter 18. Petschek has played an important role as the “house theorist” for the LC group, collaborating on over a dozen papers in as many years. As an example, an early paper describes an experiment in which a specially designed chiral nematic LC was shown to display an “**electroclinic**” effect, i.e. the angle of tilt of its molecules rotates in an applied electric field. (The samples were typically around 25 microns thick and the rotation was very small: on the order of a tenth of a milliradian for a field gradient of one V/micron.) They studied how this effect changes as the temperature is raised, taking the sample through the smectic-to-nematic transition. “Nematic electroclinic effect” *Phys. Rev.* **A41** 1997 1990. The figure (**Fig. 17-12**) shows the rapid drop in $d\theta/dE$ as the phase transition is approached. The paper concludes with a proposed model for this unexpected behavior.

Between 1990 and the present (2005), Petschek has continued to work with Rosenblatt and the many students who are measuring liquid crystal properties, jointly publishing more than two dozen papers. By the mid-1990’s, Ken Singer had established his experimental program in optical materials, and Petschek soon became a regular collaborator with that group as well. By this time, the Rosenblatt and Singer groups would provide doctoral research projects for about half of the department’s grad students, and Petschek has played an essential role in contributing theoretical support. Moreover, he has continued to produce theoretical work on polymer liquid crystals with graduate students Hinshaw, Richard Sones, and Jonathan Stott and post-doc Terentjev. His statement on the department website summarizes this ongoing work. “*We use analytic and numerical tools of statistical mechanics and quantum mechanics, symmetry analysis, and extensive discussions with near-by experimentalists in order to discover new principles which control the statistical or optical properties of the wide variety of actual or potential structures. ... Our work is simultaneously both applied and basic, with impact on electro-optic and optical technologies, and with impact on the tools with which physicists study the world.*”

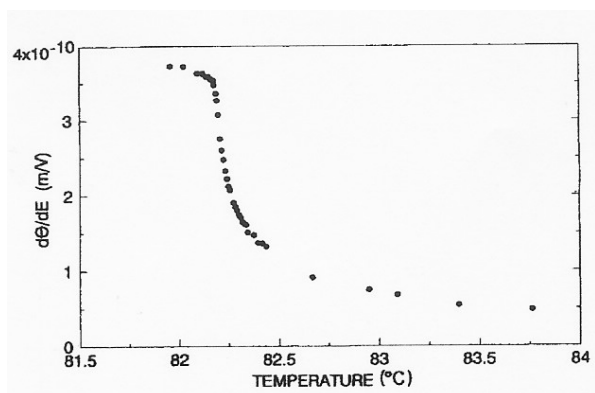


Fig. 17-12. Computed electroclinic effect vs. temperature, through phase transition.



Fig. 17-13. Walter Lambrecht.

Lambrecht, Segall: electronic structure group

In 1987, **Walter R. L. Lambrecht** joined Ben Segall as a senior research associate. Walter had completed his PhD at the University of Ghent in Belgium in 1980. Subsequently he was a visiting professor at the Universidad Nacional del Sur in Bahia

Blanca, Argentina. At the Max-Planck Institute for Solid State Research in Stuttgart, Walter calculated electron energies in diamond-like structures. At CWRU, Walter has worked with Ben Segall on band-structure calculations for over a decade. Their first paper was on heterojunctions, addressing the question of how the energy bands line up at an interface between two semiconductors. They presented a list of their calculated “offsets”, comparing them with measured values for junctions of a series of materials, e.g. silicon in contact with GaP, germanium with AlAs, etc. “Theory of Semiconductor Heterojunction Valence-band Offsets; from Supercell Band-Structure Calculations toward a Simple Model” *Phys. Rev. Lett.* **61**, 1764 1988.

A different type of system was studied by Segall, Lambrecht and visiting Mexican physicist, Carlos Amador. They looked at the phase diagram of an alloy in which there is a large “size mismatch”, in this case nickel-platinum. How do the melting point and the lattice structure change as the percentage of nickel is changed? “Strain Effects on the Phase Diagram of Ni-Pt alloys” *Phys. Rev.* **B47** 15276 1993.

Lambrecht and Segall have regularly interacted closely with experimentalists, both in the analysis of experimental data and by suggesting interesting materials to be explored. One such experimenter is John Angus, professor of chemical engineering, who is CWRU’s “diamond man”. (We met him in Chapter 12 as a collaborator of Gary Chotiner.) For many years, Angus has studied the properties, fabrication and applications of diamond crystals and diamond *thin films*. The diamond structure, a cubic array of carbon atoms, is particularly simple. There is a possibility that diamond can be used as the basis of a new semiconductor technology, with advantages over the silicon-based devices of today. One theoretical question concerned the choice of substrate to be used in growing diamond films. Segall and Lambrecht investigated the feasibility of using boron nitride, whose properties seemed to be an ideal match for diamond. “Electronic structure of diamond/BN interfaces and superlattices” *Phys.Rev.* **B40** 9909 1989. They were later joined by Angus and members of his group in a study reported in *Nature*. “Theory of Diamond Nucleation by Hydrogenation of the Edges of Graphitic Precursors,” *Nature* **364**, 607 1993.

During their fourteen year collaboration, Lambrecht, Segall, and their Electronic Structure Group have published more than fifty papers on electronic structure of materials which are likely to have applications to semi-conductor technology. The emphasis throughout has been on the optical responses such as X-ray, ultraviolet and visible reflectivity and absorption, all deduced from the band-structure. The group has a special interest in wide-band-gap semiconductors such as diamond, silicon carbide and gallium nitride.

The underlying computational technique, the “density functional method”, manages the great complexity of electrons interacting with the crystal lattice in the presence of applied fields. The success of the approach has grown over the years as more powerful computers have become available. It is possible to predict essentially all the properties of a material (e.g. structural, vibrational, mechanical, optical, magnetic, electronic transport) from “first principles” such as the atomic numbers and the crystal structure.

The group's website summarizes: "By calculating the optical response functions from the underlying electronic band structure, and analyzing them, we assist in the interpretation of various types of optical spectroscopy: X-ray, ultraviolet and visible reflectivity and absorption." A recent line of work has been on the integration of *magnetic* materials with semiconductors. These may eventually provide the basis for *spintronics*, a novel form of electronics which uses the spin degree of freedom.

Ben Segall became professor emeritus in 2000. He continues to interact with the department on a regular basis and, with his wife Annette, to promote the goals of a progressive liberal society. Walter Lambrecht, who was promoted to faculty status in 1996, along with his group of post-docs and grad students, continues a vigorous program of materials theory, providing critical support to experimentalist colleagues in the physics department and materials researchers in the college of engineering.

Harsh Mathur

In 1995, two years after Lawrence Krauss (Chapter 18) arrived as chairman, **Harsh Mathur** was appointed to the faculty. Mathur, having done a bachelor of technology degree at the Indian Institute of Technology - Kanpur, had recently completed his PhD at Yale. He came to CWRU after a postdoctoral appointment at Bell Labs and a semester as a general member of the Institute for Theoretical Physics in Santa Barbara.



Fig. 17-14.
Harsh Mathur.

Mathur had already established himself as an extraordinary young theorist, while still a graduate student, with his work on subtle quantum effects of electron spin on electrical conduction in metals at low temperature. This is an area of great interest now, following the birth and explosive growth of the field of *spintronics*. Another significant paper that Mathur wrote while he was at Yale revisited the classic Foldy-Wouthuysen analysis of the Dirac equation (described in Chapter 9 and in Appendix G) and reinterpreted it in terms of a newly identified quantum effect called Berry's phase. "Thomas Precession, Spin-Orbit Interaction, and Berry's Phase," *Phys. Rev. Lett.* **67**, 3325 (1991).

We'll briefly discuss here some representative topics which Harsh has studied while at CWRU. *Briefly*, because my intended soft cut-off was 1990, and *here*, because his work is in condensed matter theory. In Chapter 18, we will offer similarly brief descriptions of the work of the twelve other department members who arrived after 1986.

Mathur's main interest is in quantum effects in condensed matter, particularly effects due to interactions between particles and between particles and impurities. A large part of his work has been concerned with the mobility of electrons in *dirty* conductors. At low temperatures, quantum interference can cause electrons to become *localized* as they scatter from impurities. This leads to a measurable increase in the electrical resis-

tance as the temperature is lowered. Mathur explains: “An important problem in ‘localization physics’, one that is still only partially solved, is to understand *dephasing*. Dephasing refers to processes that suppress quantum effects as the temperature is raised. A broad fundamental problem of physics (sometimes called the decoherence problem) is to understand the processes that allow the classical world to emerge from the underlying laws of quantum mechanics.”

Electrons deposited on the surface of a pool of liquid helium form a flat conducting sheet that is particularly well suited for the study of such localization phenomena. Electrons on helium have been the principal interest of experimentalist Arnie Dahm and his group for many years (as we described in Chapter 15). Thus it was natural for Mathur and his student Damir Herman to collaborate with Dahm and his student Ismail Karakurt in the study of dephasing in this system. The CWRU group found that the electrons are localized by their collisions with helium gas atoms in the vapor above the liquid. The dephasing is caused by the slow thermal motion of the vapor atoms. They developed a theory of such dephasing that proved to agree with their measurements. “Localization scaling relation in two dimensions: Comparison with experiment” *Phys. Rev.* **B56**, 13263 1997. “Damping of quantum interference of electrons on helium” *Phys. Rev.* **B68**, 33402 2003.

Silicon MOSFETs (metal-oxide semiconductor field-effect transistors) are another arena in which localization physics can be studied. They are the building blocks of modern electronics, used, for example, to control high speed switching in integrated circuits. In a MOSFET, a flat conducting sheet of electrons is to be found between a layer of silicon and a layer of silicon oxide. The roughness of the semiconductor-oxide interface determines the electrical properties of the device, including how long it will last. Thus, characterizing and controlling the roughness is a matter of great technological importance and a potential roadblock to further device miniaturization. Mathur and his collaborator Harold Baranger (Duke University) have shown that at low temperature the scattering of electrons from the rough interface can cause localization and that electrical resistance measurements in a magnetic field can be used to measure the roughness of the interface non-destructively. “Random Berry phase magnetoresistance as a probe of interface roughness in Si MOSFET's” *Phys. Rev.* **B64** 235325 2001.

Mathur has extended his study of electrons confined to small regions by tackling the theory of *quantum dots*. He explains: “the ability to fabricate quantum dots is a major development in semiconductor physics. A semiconductor quantum dot is a pool of electrons confined to a small region, often less than 100 nm in size. The number of electrons in the dot can be controlled with exquisite precision and varies from a few electrons in small dots to a few hundred in larger micron sized dots.”

Aside from the possibility that they will play a role in some future nanotechnology, quantum dots can also be of great fundamental interest. Mathur and his collaborators, Ganpathy Murthy (University of Kentucky) and Ramamurti Shankar (physics chairman at Yale) have predicted that, in large quantum dots with low electron density, the electrons will form a *new state of matter* different from the ordinary Fermi liquid state

in which electrons are normally found in semiconductors and metals. Mathur points out that this new state has many remarkable properties - for example the electrons are predicted to carry a persistent current even in the absence of any applied electric fields, even though the new electronic state is not superconducting. "Diamagnetic persistent currents and spontaneous time-reversal symmetry breaking in mesoscopic structures" *Phys. Rev.* **B69** 41301 2004.

Condensed matter theory continues to be an important component of the CWRU physics department and it attracts a significant proportion of its graduate students. They appreciate the opportunities to interact with a variety of physics and materials science experimental groups. Many will go on to careers in which they will apply their calculational and instrumental talents to a rapidly expanding technology.