STRUCTURE AND DYNAMICS IN LOW-DIMENSIONAL GUEST-HOST SYSTEMS DE-FG02-86ER45254

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I. INTRODUCTION

This is the final report of the fourth of four 3-year grants of the same title. The program evolved from an earlier DOE grant on graphite intercalation compounds (GIC). Since its inception 8 years ago, the focus evolved continuously from conjugated polymers to fullerenes, disordered carbons for Li-ion battery applications, and most recently carbon nanotubes, with a side excursion back to GIC's to exploit a recent advance in synthesis of a potentially exciting new phase. The unifying themes are the versatility of carbon in forming novel solids, and the flexibility of intercalation chemistry to provide new materials with potentially useful properties. Results on doped fullerides revealed major gaps in our theoretical understanding of superconductivity and correlation effects in these narrow-band metals. Structural studies of disordered carbons provide clues to explaining their very high Li capacity in secondary batteries. The super-dense metastable graphite compound LiC_2 is stabilized by substitutional boron in the parent graphite, and shows promise for specialty battery applications. An X-ray diffraction study of bulk samples of single-wall nanotubes provided by Prof. Smalley's group confirms the high yield of their laser process and also demonstrates that this material joins diamond, graphite and the solid fullerenes as the fourth crystalline form of pure carbon.

In addition to the research carried out by graduate students supported by the grant, we leveraged our efforts by extensive collaborations with other groups, and by attracting sabbatical and other visitors at little or no cost to the grant. Our long-term connections with labs in France and Russia contributed materially to the success of our program. The total funding for 12 years (1/86 - 12/98) was \$1,725,575, or on average \$144K per annum. This report covers the last 3-year renewal, 7/95 - 12/98, which includes a six month no-cost extension at the end of the grant.

DISCLAIMER

II. HIGHLIGHTS

A. T_c vs Carrier Concentration in Cubic Fulleride Superconductors

X-ray diffraction, Raman scattering, magnetization and ESR were studied in 2 new fulleride families, $Na_2Cs_xC_{60}$ ($0.5 < x < 1$) and $M_{3-y}Ba_yC_{60}$ ($0.3 < y < 2$, M = K, Rb or Cs). These are isostructural with known $Pa\bar{3}$ and $Fm\bar{3}m$ trivalent superconductors respectively, but with variable valence $2.5 < \mathbf{n} < 5$. T_c is strongly peaked at $\mathbf{n} = 3$ and decreases rapidly to < 0.5 K for $\mathbf{n} = 2.5$, 4 and 5, inconsistent with both one-electron band theory and current Coulomb correlation models. These results reveal a fundamental gap in our understanding of fulleride superconductivity.

B. Local Structure and Vibrational Spectroscopy of Disordered Carbons for Li Batteries

Compositions, local atomic structures, porosity and vibrational dynamics of carbons obtained by pyrolyzing epoxy Novolac resins at 650C° and 1000 C° are investigated using several neutron scattering techniques. The ultimate goal is to understand the origin of the very high capacity for Li uptake exhibited by these materials. Neutron radial distribution function analysis and incoherent inelastic scattering show that the structural motif is a planar hexagonal graphene fragment ~ 10 Å on a side, with edge carbons terminated by single hydrogen atoms and random stacking between fragments. Small-angle neutron scattering reveals substantial porosity on a length scale comparable to the size of the graphene fragments. Coupled with computer simulations, these results are consistent with two proposed mechanisms for unusually high Li capacity, one analogous to conventional intercalation but with Li on both sides of isolated graphene fragments, the other involving bonding of Li to H-terminated edge carbons.

C. Superdense LiC_2 as an Intercalation Anode in Li-ion Batteries

LiC_2, the super-dense high pressure phase of lithium intercalated graphite, has been tested as the anode in a two-electrode cell vs. Li with an organic electrolyte. A primary capacity of 910 mAh/g per carbon atom is observed during the first de-intercalation cycle at constant current, almost 3 times greater than the ideal 372 mAh/g value for the normal saturated phase LiC_6. LiC_2 also exhibits the desirable characteristics of low and flat working voltage profile and most of the Li is removed at ~ 18 mV. The first de-interclation cycle also shows weak anomalies which coincide with previously identified phase transitions between high-order Li in-plane superlattices. Repeated cycling yields a reversible capacity close to 372 mAh/g, with Li removed at ~ 100 mV. The high initial capacity and near-ideal reversible secondary capacity suggests that this material could be useful in rechargeable batteries requiring a very large "first - de-intercalation" capacity.

D. X-ray Observation of a 2D Lattice of Single-wall Nanotubes

High-purity samples (10-20 mg.) of single-wall nanotubes (SWT's) have been prepared by laser ablation of graphite rods at 1200°C (catalyzed by Ni/Co/Fe), followed by heat treatment to sublime out the normal fullerenes (Chem. Phys. Lett. **243**, 49 (1995)). X-ray powder diffraction confirms the relative absence of multiwall tubes by a vanishingly small intensity at the graphite (002) position. Instead we observe several reflections which can be indexed on a 2D triangular lattice with $\mathbf{a} \sim 16$ Å, indicating that the SWT's are reasonably uniform in diameter and self-organize into "cables" or "ropes". The optimum conditions for self-organization are studied by variations in powder pattern vs. heat treatment, and attempts to "dope" the "rope" with potassium are described.

E. Metallic Resistivity in Crystalline Ropes of Single-wall Carbon Nanotubes

Laser ablation of (Co,Ni)-doped graphite yields $\sim 70\%$ single-wall nanotubes, predominantly (10,10) armchair tubes which self-organize into crystalline "ropes" > 100 Å in diameter and > 10 μm long. We find $\rho_{\|} = 0.03$ - 0.10 mΩ cm at 300 K, with positive (negative) $d\rho/dT$ above (below) $T^* = 35$ K. Unoriented bulk samples exhibit similar behavior, with higher (directionally-averaged) resitivities and T^*'s. The high-T behavior is consistent with the predicted intrinsic metallic state for this structure.

III. PUBLICATIONS

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5. "Pressure Studies of Alkali, Alkaline Earth and Rare Earth Doped C_{60} Superconductors", J. E. Schirber, W. R. Bayless, A. R. Kortan, E. Ozdas, O. Zhou, D. Murphy and J. E. Fischer, in *Science and Technology of Fullerene Materials*, edited by P. Bernier, T. W. Ebbesen, D. S. Bethune, R. M. Metzger, L. Y. Chiang and J. W. Mintmire (Mater. Res. Soc. Proc. **359**, Pittsburgh PA 1995) p. 289.

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9. "Disorder Effects in Rb_3C_{60}", K.-F. Thier, O. Zimmer, M. Mehring, F. Rachdi and J. E. Fischer, *Physics and Chemistry of Fullerenes and Derivatives*, edited by H. Kuzmany, J. Fink, S. Roth and M. Mehring (World Scientific, Singapore 1995) p. 432.

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20. "No Off-Centering of Cation Positions in Rb_3C_{60}", G. Bendele, P. W. Stephens and J. E. Fischer, in *Fullerenes and Fullerene Nanostructures*, edited by H. Kuzmany, J. Fink, M. Mehring and S. Roth (World Scientific, Hong Kong 1996) p. 142.

21. "^{87}Rb and ^{13}C NMR of Rb_3C_{60} in the Superconducting State", G. Zimmer, M. Mehring, F. Rachdi and J. E. Fischer, in *Fullerenes and Fullerene Nanostructures*, edited by H. Kuzmany, J. Fink, M. Mehring and S. Roth (World Scientific, Hong Kong 1996) p. 147.

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23. "Electronic Properties of Alkali Fullerides: Evidence for Phonon Mediated Resisitivity", P. Petit, J. Robert, T. Yildirim and J. E. Fischer, in *Fullerenes and Fullerene Nanostructures*, edited by H. Kuzmany, J. Fink, M. Mehring and S. Roth (World Scientific, Hong Kong 1996) p. 415.

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25. "On the Pressure-Induced Phase of Na_2CsC_{60}", B. Morosin, J. E. Schirber, J. D. Jorgensen, G. H. Kwei and J. E. Fischer, in *Fullerenes: Chemistry, Physics and New Directions VIII* K. M. Kadish and R. S. Ruoff, editors (Electrochemical Society 1996).

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29. "ESR Evidence for Phonon-mediated Resistivity in Alkali Fullerides", P. Petit, J. Robert, T. Yildirim and J. E. Fischer, Phys. Rev. B **54**, R3764 (1996).

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38. "Temperature Dependent Resistivity of Single Wall Carbon Nanotubes", C. L. Kane, E. J. Mele, R. S. Lee, J. E. Fischer, P. Petit, H. Dai, A. Thess, R. E. Smalley, A. R. M. Verscheueren, S. J. Tans and C. Dekker, Europhys. Lett. **41**, 683-688 (1998).

39. "Metallic Behavior of ABa_2C_{60} ($A = K, Rb, Cs$) Compounds", C. Goze, K.-F. Thier, M. Hehring, F. Rachdi, T. Yildirim and J. E. Fischer, in *Molecular Nanostructures*, edited by H. Kuzmany, J. Fink, M. Mehring and S. Roth (World Scientific, Singapore 1998) p. 266.

40. "NMR Studies of Sodium Fullerides", F. Rachdi, L. Hajji, T. Yildirim, J. E. Fischer, C. Goze and M. Mehring, in *Molecular Nanostructures*, edited by H. Kuzmany, J. Fink, M. Mehring and S. Roth (World Scientific, Singapore 1998) p. 270.

41. "Bundles of Carbon Single-wall Nanotubes: Production by the Arc Discharge Technique and Characterization", C. Journet, W. K. Maser, P. Bernier, A. Loiseau, M. Lamy de la Chapelle, P. Deniard, S. Lefrant, R. S. Lee and J. E. Fischer, in *Molecular Nanostructures*, edited by H. Kuzmany, J. Fink, M. Mehring and S. Roth (World Scientific, Singapore 1998) p. 386.

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44. "Super-dense LiC_2 as a High Capacity Li Intercalation Anode", C. Bindra, V. A. Nalimova, D. E. Sklovsky, Z. Benes and J. E. Fischer, J. Electrochem. Soc. **145**, 2377 (1998).

45. "Statics and Dynamics of Interlayer Interactions in the "Superdense" High Pressure Graphite Compound LiC_2", C. Bindra, V. A. Nalimova, D. E. Sklovsky, W. A. Kamitakahara and J. E. Fischer, Phys. Rev. B **57**, 5182 (1998).

46. "Large Scale Purification of Single Wall Carbon Nanotubes: Process, Product and Characterization", A. G. Rinzler, J. Liu, P. Nikolaev, C. B. Huffman, F. J. Rodriguez-Macias, P. J. Boul, A. H. Lu, D. Heymann, D. T. Colbert, R. S. Lee, J. E. Fischer, A. M. Rao, P. C. Eklund and R. E. Smalley, Applied Physics A **67**, 29 (1998).

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48. "Bulk Properties of Crystalline Single Wall Carbon Nanotubes: Purification, Pressure Effects and Transport", J. E. Fischer, R. S. Lee, H. J. Kim, A. G. Rinzler, R. E. Smalley, S. L. Yagushinski, A. D. Bozhko, D. E. Slovsky and V. A. Nalimova, in *Progress in Molecular Nanostructures*, edited by H. Kuzmany, J. Fink, M. Mehring and S. Roth, AIP Conference Proceedings Vol 442, p. 34 (1998).

49. "In-plane Structure and Thermal Instability of $LiC_{2.18}$ Based on Boron-doped Graphite", C. Bindra, V. A. Nalimova and John E. Fischer, Mol. Cryst. Liq. Cryst. **310**, 19 (1998).

50. "Crystalline Ropes of Single Wall Carbon Nanotubes: Structure, Electronic Transport and Intercalation", J. E. Fischer, R. S. Lee, A. Thess and R. E. Smalley, Mol. Cryst. Liq. Cryst. **310**, 155 (1998).

51. "Layer Disorder in Carbon Anodes", P. Zhou, R. S. Lee, A. Claye and J. E. Fischer, Carbon **36**, 1777 (1998).

52. "Experimental Lattice Dependence of the Density of States in Alkali Fullerides", J. Robert, P. Petit, T. Yildirim and J. E. Fischer, Phys. Rev. B **57**, 1226 (1998).

IV. INVITED LECTURES

1. "Li-Carbon Compounds: Prospects for Next-Generation Secondary Batteries", Colloquium at Hughes Research Center, Malibu CA (July 13, 1995).

2. "Fulleride Polymers", seminar at UC Santa Barbara (July 14, 1995).

3. "Fulleride Superconductors: What We Know and What We Don't Know", Physics Colloquium, Temple University (Oct. 23, 1995).

4. "Synthesis, Structure and Properties of New Cubic Fullerides with Variable Molecular Valence", Euroconference on Unconventional Superconductors, Pisa Italy (Jan. 1996).

5. "Fulleride Intercalation Compounds: Rational Synthesis and Properties", 21st Century Forum, Yokohama Japan (Jan. 1996).

6. "Li-Carbon Compounds: Prospects for Next-Generation Secondary Batteries", Colloquium at Mitsubishi Chemical Corp., Yokohama Japan (Feb. 1996).

7. "New Results on Fullerene-derived Solids", International Winterschool on Electronic Properties of Novel Materials, Kirchberg Austria (March 1996).

8. "Fulleride Solid State Chemistry: Gospel, Heresies and Mysteries", *Fullerenes '96*, Oxford UK (July 1996).

9. "Carbon Materials Science: Sheets, Balls, Tubes and Flakes", Frontiers of Materials Science Lecture, U. Penn (Sept. 20, 1996).

10. "The Fullerenes: From Novel Molecules to Superconductors, Nanotubes and Nano-Engineering", Chemistry seminar, Swarthmore College (Oct. 3, 1996).

11. "Carbon Materials Science: Sheets, Balls, Tubes and Flakes"; Chemistry seminar, University of Southern California (Dec. 10, 1996).

12. "Recent Advances in Novel Carbons for Li-Ion Batteries", Hughes Research Laboratory, Malibu CA (Dec. 11, 1996).

13. "Crystalline Ropes of Carbon Nanotubes: Structure and Properties", International Workshop on Electronic Properties of New Materials, Kirchberg (Tirol) (March 3-7, 1997).

14. "Electronic Transport in Crystalline Ropes of Single Walled Nanotubes", DCMP invited talk at the American Physical Society Meeting, Kansas City (March 17-21, 1997).

15. "Crystalline Ropes of Single-Wall Carbon Nanotubes: Structure, Electronic Transport and Doping", DuPont CR&D, Wilmington DE (May 20, 1997).

16. "Structural Studies of Disordered Carbons for Li- Ion Battery Applications", Universite de Picardie Jules Verne (May 23, 1997).

17. "Intercalation of Single-Wall Carbon Nanotube Lattices", International Symposium on Intercalation Compounds, Bordeaux (May 25-29, 1997).

18. "Crystalline Ropes of Single-Wall Carbon Nanotubes: Structure, Electronic Transport and Doping", ONR-Rice Workshop on *Carbon Nanotubes - Opportunities, Requirements and Challenges*, Rice University (May 30 - June 1 1997).

19. "Enhanced Conductivity in Doped Single-Wall Carbon Nanotubes", *Third International Workshop on Fullerenes and Atomic Clusters*, St. Petersburg (June 29 - July 5, 1997).

20. "Intercalation of Single-Wall Carbon Nanotube Lattices", Workshop on *Science of Carbon Nanotubes*, Lexington KY (July 10-11, 1997).

21. "Self-Organizaton of Single-Wall Carbon Nanotubes: A Novel Intercalation Host Lattice", European Research Conference *Fullerenes in Context*, Espinho Portugal (Sept. 6-11, 1997).

22. "Novel Carbons for Li-Ion Battery Applications", Mitsubishi Research Center, Tsukuba Japan (Jan. 8, 1998).

23. "Bulk Properties of Crystalline Single Wall Carbon Nanotubes: Purification, Pressure Effects and Transport", International Workshop on Electronic Properties of New Materials, Kirchberg (Tirol) (Feb. 28 - March 7, 1998).

24. "Crystalline Ropes of Single Wall Carbon Nanotubes: Structure, Electronic Transport and Doping", U. Paris Sud, Orsay France (March 9, 1998).

25. "Crystalline Ropes of Single Wall Carbon Nanotubes: Structure, Electronic Transport and Doping", ONERA (French Space Agency), Chatillon France (March 10, 1998).

26. "Crystalline Ropes of Single Wall Carbon Nanotubes: Structure, Electronic Transport and Doping", CNRS Orleans France (March 12, 1998).

27. "Carbon Nanotubes: Structure, Properties and Applications", LaserIon© Workshop on Mmicrofabrication, Nanostructured Materials and Biotechnology, Schloss Ringberg/Tegernsee, Germany (June 28 - July 2, 1998).

28. "Materials Science of Carbon: Sheets, Balls, Tubes and Flakes", Eurocarbon Conference, Strasbourg France (July 9-12, 1998). Plenary lecture.

29. "Towards a Science Base for Understanding Disordered Carbon Anodes", Ninth International Meeting on Li-Ion Batteries, Edinburgh Scotland (July 12-17, 1998).

30. "Carbon-derived Synthetic Metals: From Graphite to Nanotubes", International Conference on Synthetic Metals, Montpellier France (July 12-18, 1998). Plenary lecture.

31. "The Physics of Carbon Sheets, Balls, Tubes and Flakes: Challenges and Opportunities", Conference on Physics at the Turn of the 21st Century and 80th Anniversary Symposium of the Ioffe Institute, St. Petersburg Russia (Sept. 28 - Oct. 2, 1998).

V. PHD STUDENTS SUPPORTED BY DOE

Qing Zhu, PhD Materials Science and Engineering (9/95), now employed as superviser of x-ray characterization, Philipps Semiconductor Co., Santa Clara CA

Krysztof Kniaz, PhD Materials Science and Engineering (9/96), employed as computer system analyst at Sapient Corp., New York NY.

Taner Yildirim, PhD Physics (9/96), employed as staff scientist at NIST/U. Maryland (shared support with NSF).

Chetna Bindra, PhD Physics (9/97), now employed as staff scientist, Sarnoff Research Center, Princeton NJ.

Roland Lee, PhD Materials Science and Engineering (expected 1999), working on carbon nanotubes: lattice structure, transport and doping reactions.

Zdenek Benes, PhD Materials Science and Engineering (expected 2000), working on carbon nanotubes: structure and electrical properties of encapsulated C_{60}.

Brian Smith, PhD Materials Science and Engineering (expected 2001), supported summer 1998 by DOE, now on University fellowship. Discovered the existence of "peapods" (encapsulated C_{60} in SWNT) using HRTEM.

VI. OTHER RESEARCH PERSONNEL

Dr. Vera Nalimova, lead researcher, Chemistry Department, Moscow State University. Vera discovered the high-pressure synthesis of LiC_2. With travel support from NATO, several exchange visits took place, including two long visits by my student Chetna Bindra to Moscow.

Prof. H. J. Kim, assistant professor of physics, Hallym University, South Korea. Kim spent a year working with Roland Lee, carrying out measurements of electrical resistivity of pristine and doped nanotubes.

Dr. Marc Monthioux, chargé de recherche, CNRS, Centre d'Elaboration de Matériaux et d'Etudes Structurales, Toulouse, France. Marc spent 8 months at Penn supported by a NATO fellowship. The DOE grant paid for HRTEM facility time which Marc used to participate in the discovery of encapsulated C_{60}.

Dr. Beatrice Burteaux, postdoc from Clermont-Ferrand, France. Beatrice spent 8 months at Penn, supported in part by a French government grant and supplemented by the DOE grant. She carried out preliminary studies of nanotube-polymer composites, including processing, chemical analysis and mechanical testing.

Dr. Ping Zhou, postdoc. Ping was supported by Hughes Research Lab, Malibu CA, to study specific disordered carbons of interest to Hughes. He contributed materially to progress in the DOE-supported task on Li-ion battery materials.

Dr. Peter Papanek, postdoc. Peter is stationed at the NIST reactor, and is jointly supported by NIST and Penn's NSF-MRSEC program. He was intimately involved in our neutron scattering experiments on disordered carbons, fullerides and LiC_2.