

CLOSEOUT SUMMARY, DOE Grant No. DE-FG03-00ER45840
**Investigations of the Electronic Structure and Superconductivity in Newly Predicted
Metallic Crystalline Carbon**

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Among the highlights of our accomplishments are; 1) development of two laboratories with several *state-of-the-art* equipments for Raman spectroscopy with diamond anvil cell, photoemission spectroscopy, low-temperature electrical conductivity measurements, high-vacuum thin film deposition, 2) publications of new important results, 3) education of several graduate/undergraduate students, and postdoctoral research associate, 4) completion of three PhD Dissertations, and 5) presentations by students and PI at national, international and regional scientific meetings and institutional colloquia.

MAJOR NEW RESULTS

- Identification of the crystal structure of C₆₀ under 31.1 GPa; mixture of body-centered orthorhombic and rhombohedral phases
- Observation of several phase transitions of C₆₀ between ambient and 31.1 GPa; possibly new effects between 4 and 8 GPa; even the possibility of a different approach for the synthesis of a recently discovered phase of C₆₀ with magnetic properties
- Photoemission determination of the valence band structures of thin film C₆₀ and La_{0.1}C₆₀ supporting density functional theory
- Observation of interface effects in C₆₀/Cu-oxide/Cu structures
- Synthesis of highly conducting (mΩ-cm) thin films; new effects of uv-irradiation on the microstructure and low temperature conductivity of these films; crossover between the Variable-Range-Hopping and Activation Energy mechanisms of conductivity at low temperatures
- Observation of significant effects of stress on the valence band structures
- Adsorption of water molecules inside single-walled carbon nanotubes

PUBLICATIONS

1. S. C. Sharma, D. Singh, and Y. Li, "Raman scattering study of adsorption/desorption of water from single-walled carbon nanotubes", *J. Raman Spectroscopy*, **36**, 755 (2005)
2. D. Singh, Y. Li, and S. C. Sharma, "Effect of pressure on the Raman spectra of methanol-ethanol-water mixture at room temperature", *J. Raman Spectroscopy*, **36**, 24 (2005)
3. S. C. Sharma, D. Singh, and Y. Li, "New features in the pressure dependence of photoluminescence spectra of C-60 at room temperature", *Solid State Commun.* **133**, 797 (2005)
4. S. C. Sharma, "Results from our study on compressed C-60 and water adsorption into single-walled carbon nanotubes", Invited Paper, Proceedings of the Department of Atomic Energy, India, Solid State Symposium, **49**, 17 (2004)
5. J. H. Rhee, D. Singh, Y. Li, and S. C. Sharma, "Crystal structure of C₆₀ following compression under 31.1 GPa in diamond anvil cell at room temperature", *Solid State Communications*, **127**, 295 (2003)
6. Y. Li, J. H. Rhee, D. Singh, and S. C. Sharma, "Raman spectroscopy and x-ray diffraction measurements on C₆₀ compressed in diamond anvil cell", *Physical Review B*, **68**, 024106 (2003)
7. B. Ha, J. H. Rhee, Y. Li, D. Singh, and S. C. Sharma, "Photoelectron spectroscopy measurements of the valence band structures of polymerized thin films of C₆₀ and La_{0.1}C₆₀", *Surface Science* **520**, 186 -192 (2002)

8. Y. Li, J. H. Rhee, D. Singh, and S. C. Sharma, "Raman spectroscopy measurements of interface effects in C₆₀/CuO/Copper", *Mat. Res. Soc. Symp. Proc.* **734**, 291-296, (2003)
9. B. Ha, J. H. Rhee, Y. Li, D. Singh, and S. C. Sharma, "Photoelectron spectroscopy measurements of the valence band structures of C₆₀ thin films on single crystal silicon and polycrystalline copper", *Mat. Res. Soc. Symp. Proc.* **734**, 279-284, (2003)
10. R. Govinthasamy, J. H. Rhee, and S. C. Sharma, "Temperature dependence of the electrical conductivity of C₆₀ thin films", *Mat. Res. Soc. Symp. Proc.* **734**, 285-290, (2003)
11. S. C. Sharma, B. Ha, J. H. Rhee, and Y. Li, "Effects of pressure on the vibrational, structural, and electronic properties of C₆₀ powder and thin films", *Mat. Res. Soc. Symp. Proc.* **695**, 97-101 (2002)
12. S. C. Sharma, B. Ha, J. H. Rhee, and Y. Li, "Raman scattering, x-ray diffraction, and photoemission measurements on C₆₀ and La-doped C₆₀ thin films", Invited Paper presented at NATO Advanced Research Workshop, and published in "Frontiers of High Pressure Research II: Applications of High Pressure to Low-Dimensional Novel Electronic Materials", Kluwer Academic Publishers, Netherlands (2001), pp. 493-505

ABSTRACTS OF PRESENTATIONS BY STUDENTS

1. Y. Li, D. Singh, and S. C. Sharma, "Raman spectroscopy measurements of the vibrational properties of uv-polymerized C₆₀ thin films and C₆₀ powder compressed in a diamond anvil cell", *Bull. Am. Phys. Soc.* **47**, 4 (2002).
2. B. Ha, J. H. Rhee, D. Singh. and S. C. Sharma, "Photoemission and x-ray diffraction measurements to study the effects of pressure on the valence band structures of copper and silver", *Bull. Am. Phys. Soc.* **47**, 5 (2002).
3. D. Singh and S. C. Sharma, "Theoretical investigation of the effect of pressure on the valence band structures of copper and silver by using the tight-binding linear muffin-tin orbital method", *Bull. Am. Phys. Soc.* **47**, 4 (2002).
4. J. H. Rhee, Y. Li, D. Singh, and S. C. Sharma, "Growth of thin films of C₆₀ and single-walled carbon nanotubes and their characterization by x-ray diffraction, scanning electron microscopy, and Raman spectroscopy", *Bull. Am. Phys. Soc.* **47**, 4 (2002).
5. R. Govinthasamy and S. C. Sharma, "Design of an experiment to study the temperature and pressure dependence of the electrical conductivity of C₆₀-based materials", *Bull. Am. Phys. Soc.* **47**, 7 (2002).
6. B. Ha, D. Singh, J. H. Rhee, and S. C. Sharma, "Electronic valence band structure of copper compressed under 377 MPa: comparison between photoemission spectroscopy measurements and band structure calculations", Department of Atomic Energy Symp., Dec. 2002, India.
7. D. Singh, Y. Li, J. H. Rhee, S. C. Sharma, "New features in the vibrational modes and crystal structure of C₆₀ compressed under 31.1 GPa", Department of Atomic Energy Symp., Dec. 2002, India.
8. B. Ha, J. H. Rhee, and S. C. Sharma, "Design and preliminary results from Raman, xrd, and photoemission measurements on C₆₀ under pressure", *Bull. Am. Phys. Soc.* **46**, 92 (2001).

PhD DISSERTATION COMPLETED

1. "Photoelectron spectroscopy measurements of the electronic structure of C₆₀ and other carbon-based materialsthin films", B. Ha, completed, December, 2002
2. "Growth and characterization of C-60 thin films", J. H. Rhee, December, 2004
3. "Raman spectroscopy measurements on C-60 compressed under high pressures", Y. Li, May, 2005

MS THESIS COMPLETED

“Temperature dependence of the electrical resistivity of C-60 thin films”, R. Govinthasamy, August, 2003

STUDENTS SUPPORTED

Graduate Students: 1) B. Ha, 2) J. H. Rhee, 3) Y. Li, 4) R. Govinthasamy

Undergraduate: Michael Cramer

Postdoc: Dr. D. Singh

INVITED COLLOQUIA

1. “Electronic, structural, and vibrational properties of C₆₀-based fullerenes”, University of Texas at Dallas, Richardson, Texas, April 2, 2003.
2. “Effects of high pressure on the electronic, structural, and vibrational properties of C₆₀-based fullerenes”, University of Texas at Arlington, February, 2002.

VISUAL TOUR OF THE LABORATORIES

Raman Spectroscopy Lab., CVD thin film growth, Photoemission spectroscopy, lattice defects characterization, and work at the national synchrotron radiation facility

