

identified<sup>1</sup>. The X-point maxima can be considered as precursor effects of the low temperature Pa  $\bar{3}$  phase, while the other diffuse scatterings may reveal the existence of competing phases. By comparing the observed intensity distribution to that calculated using a microscopic mean-field theory (with the formalism of the symmetry adapted functions, up to the  $l=12$  terms) we evaluate different models of intermolecular potential. Van der Waals-type intermolecular interactions are found to account for the main features of the observed diffuse scattering<sup>2</sup>. Elaborate models of intermolecular potential are being tested.

Below  $T_0$ , the remaining X-ray diffuse scattering is analyzed to clarify the orientational order of the nearly degenerate configurations of the  $C_{60}$  molecules ("penta" and "hexa") which coexist in the Pa  $\bar{3}$  phase.

<sup>1</sup> P. Launois, S. Ravy and R. Moret, Phys. Rev. B52, 5414 (1995).

<sup>2</sup> S. Ravy, P. Launois and R. Moret, submitted.

**MS10.11.03 GEOMETRY AND STABILITY OF GRAPHITIC ONION-LIKE STRUCTURES.** Terrones, H., Instituto de Fisica UNAM, Apartado, Postal 20-364, C.P. 01000, Mexico, D.F. and Terrones M., School of Chemistry and Molecular Sciences, University of Sussex, Brighton BN1 9QJ, U.K

Using energy minimization with heptagonal and pentagonal rings of carbon in a graphite hexagonal mesh, we have produced quasi-spherical giant fullerenes which are suitable for forming stable bucky onions. A formation mechanism which explains the transformation, during high electron irradiation, of polyhedral graphite particles into graphitic onions is proposed. According to our mechanism, the most strained parts of the polyhedral particles (pentagonal rings and adjacent atoms) are destroyed during the irradiation generating flexible holey structures which can be moulded by energy minimization to obtain quasi-spherical giant fullerenes with holes. The holes are filled with heptagonal and pentagonal rings preserving the sphericity and avoiding the faceting characteristic of giant fullerenes with just 12 pentagonal rings. We also show that bucky-onions can be ordered (symmetric) or amorphous (non-symmetric) on the surface of a sphere. In general, the role of defects such as pentagons, heptagons and octagons in fullerenes, nanotubes and negatively curved graphite is analyzed. All these new structures open the field of a generalized crystallography in which atoms rest on surfaces with different curvatures: zero Gaussian curvature for nanotubes, positive curvature for fullerenes and negative curvature for cork-screw nanotubes and other hypothetical arrangements waiting to be discovered.

**MS10.11.04 NEW STRUCTURAL STUDIES OF CHEMICALLY MODIFIED FULLERENES.** Alan L. Balch, Marilyn M. Olmstead, David A. Costa, Arwa Ginwalla, David Lane, Department of Chemistry, University of California, Davis, CA 95616.

Recent results of structural work on chemically modified fullerenes that bear organometallic or organic functionalities covalently bonded to the fullerene surface will be described. Emphasis will be placed on the characterization of fullerene oxides and oxidation products (i.e.  $C_{70}O$ ) and on addition products where Vaska's Compound,  $Ir(CO)Cl(PR_3)_2$ , is used to prepare suitable crystalline samples.

**MS10.11.05 MOMENTUM DENSITY OF  $K_xC_{60}$ .** G. Loupías, Ch. Bellin, M. Marangolo, J. Moscovici, S. Erwin, S. Rabii, C. Hérold, J.F. Maréché, P. Lagrange. Université Pierre et Marie Curie (Paris 6), 4, place Jussieu 75252 Paris Cedex 05.

Compton scattering measurements have been demonstrated to provide an accurate check of valence electron densities of solids, in the electronic ground-state. Since the scattering is incoherent, this technique, which is a bulk probe, is insensitive to crystal defects.

Compton profiles, i.e. energy-loss spectra of scattered photons were measured on powder samples, using 16keV monochromatic beam provided by the french synchrotron facility. All the  $K_xC_{60}$  samples ( $x=3,4$ , and 6) were intercalated by C. Hérold *et al.* and kept under vacuum. For comparison,  $C_{60}$  powder was measured in same experimental conditions. Average calculated Compton profiles are simulated by S. Rabii from the *ab initio* and all-electron SCF energy band structure calculated by S. Erwin within the local-density approximation (LDA).

In order to describe the electronic structures, differences between  $K_xC_{60}$  and  $C_{60}$  measured Compton profiles are compared with theoretical profile differences. Since Compton scattering is particularly sensitive to the hybridization between carbon and alkali orbitals as it was demonstrated in the case of graphite intercalation compounds, the distortion of  $C_{60}$  molecule is discussed as a function of  $x$ . In addition, "charge transfer" between the intercalate and the  $C_{60}$  molecules as well as magnitude of e-e- correlations (essential to understand the superconductivity) are studied in this set of materials.

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**MS10.11.06 PHASES IN THE  $A_1C_{60}$  SYSTEM (A=K, Rb, Cs).** G. Faigel, G. Bortel, L. Gránásky, G. Oszlányi, S. Pekker, T. Pusztai, M. Tegze, Research Institute for Solid State Physics, H-1525 Budapest, POB. 49., Hungary; L. Forró, IGA, Ecole Polytechnique Federale de Lausanne, 1015 Lausanne, Switzerland; P.W. Stephens, G. Bendele, Department of Physics, SUNY, Stony Brook, NY 11794, USA.

The crystalline structure of the various phases of  $A_1C_{60}$  type salts (A=K, Rb, Cs) were determined from x-ray powder diffraction.

In the short time since the discovery of  $C_{60}$ , an amazing variety of compounds have been found. In most of them the intermolecular separation is mainly determined by van der Waals interactions. Recently some exceptions have been found, in which  $C_{60}$  molecules are linked by covalent bonds. Among them the orthorhombic phase of  $A_1C_{60}$  was the first for which x-ray diffraction clearly proved the existence of linear polymer chains. In all cases the basic mechanism of polymerization is [2+2] cycloaddition which involves hexagon-hexagon bonds of neighbouring  $C_{60}$  molecules.

Polymer formation in  $A_1C_{60}$  can be prevented by fast cooling from high temperature. In this case covalent  $(C_{60})_2$  dimers are formed through a single C-C bond which differs from the bonding configuration of the polymer.

The sequence of phase transitions between the various phases was successfully modelled by a parameter free Monte Carlo type calculation giving a microscopic picture of these processes.

An inhomogeneous structural phase specific to  $K_1C_{60}$  appears at 400 K. In this "intermediate state" the K ions are distributed in such a way that small  $K_3C_{60}$  and K free  $C_{60}$  regions are formed while the  $C_{60}$  sublattice remains continuous. The structure has important consequences on the physical properties.