**ORIENTATIONAL FLUCTUATIONS, DIFFUSE SCATTERING AND ORIENTATIONAL ORDER IN SOLID C60**

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Starting from a microscopic model of interactions between C60 molecules on a fcc lattice, we formulate the orientational interaction potential in terms of symmetry adapted rotor functions. All irreducible representations of the cubic group up to the third order are formulated in terms of these normal coordinates. We calculate the diffuse scattering law throughout the Brillouin zone. The theory describes in a very satisfactory way recent X-ray and neutron scattering experiments. We study the orientational order parameter taking into account all T2g and T1g representations up to the first order of the phase transition.

**RARE-GAS INTERCALATED C60**


The intercalation of the rare gases into interstices of C60 at 0-6 kbar pressures has been studied by neutron diffraction using a gas pressure cell at the Intense Pulsed Neutron Source (Special Environment Powder Diffractometer). He intercalates easily while Ar does not: for Ne, intercalation kinetics may be monitored using lattice parameter changes as a function of time following sudden pressure release, diffusion out of the C60 occurs at rates too fast to measure by this technique (i.e., a few minutes).

The fcc-sc (Fm3m to P43) orientational ordering transition occurs at a pressure which is higher for He, intermediate for Ne and smallest for Ar, the latter with a value in agreement with literature values for several nonpenetrating media. For each intercalated compound in either the fcc or sc phases, these data yield the room-temperature compressibilities. Rietveld refinement of the time of flight data for the more extensive room temperature Ne data sets show that only the octahedral interstices are occupied with Ne, that there is a pressure dependence on the octahedral site occupancy, and that the cubic lattice parameter increases linearly with the amount of intercalated Ne. The observed lattice parameter behavior is similar to the problem of packing of hard spheres with large size dissimilarity, previously addressed with molecular dynamics calculations. We believe that this is the first observation of this effect in a realistic physical system.


PS10.11.13 CRYSTAL STRUCTURE AND PHASE TRANSITION OF FULLERENE C70


High-resolution synchrotron x-ray powder diffraction experiments of a fullerene C70 crystal have elucidated its structure and successive phase transitions. Two types of crystal lattices, fcc and hcp, coexist with different stacking sequences as conventionally denoted by ABAB(hcp) and ABCABC(fcc). Lattice constants at room temperature are obtained as a=15.42Å (fcc) and a=10.93Å, c=17.72Å (hcp). A precise measurement of these reveals the following phase transition sequence with respect to molecular rotation:

<table>
<thead>
<tr>
<th>Phase</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(T&lt;140K)</td>
<td>orientationally disordered glass state</td>
</tr>
<tr>
<td>(140K&lt;T)</td>
<td>free rotation state.</td>
</tr>
<tr>
<td>(T&lt;420K)</td>
<td>c/a = 1.60, orientationally ordered.</td>
</tr>
<tr>
<td>(420K&lt;T)</td>
<td>c/a continuously varied.</td>
</tr>
<tr>
<td>(T&lt;600K)</td>
<td>free rotation state.</td>
</tr>
</tbody>
</table>

Calculations of intensity by an ellipsoid-shaped molecular model suggest that in Phase I the long rotational axis of molecules aligns in the stacking direction. In Phase II a molecular rotation about its long axis whose direction fluctuates. By applying pressure we have also studied phase boundary between I and II of the hcp structure. The present experimental results qualitatively agree to the recent NMR studies. We also discuss the lattice stability conditions by combining our previous works on C60.

1. Y. Maniwa et al., to be published.

**CRYSTAL STRUCTURE AND LUMINESCENCE PROPERTIES OF THE MOLECULAR COMPLEXES C60 AND C70 WITH 9,9’-trans-bis (TELLURAXANTENYL)**


The structures of molecular complexes C60 and C70 with 9,9’-trans-bis(telluraxanteny) were determined by X-ray analysis. The molecular complexes C60 and C70 with 9,9’-trans-bis(telluraxanteny) were investigated and compared with the corresponding properties of the initial C60 and C70.

X-ray experimental data for the single crystals of a molecular complex C60 with tetraphenylidipyridyliden were obtained: a=13.199(3), b=15.592(2), c=22.199(3) Å, α=102.87(1)°, V=4453.8 Å³, Sp.gr. I2/m, 1806 refls. (MoKα). Its crystal structure is in progress.