Bonding nature and structural phase transition in rare earth doped fullerides

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Synthesis, structure, transport, and magnetic properties are reported on rare earth doped fullerides. The structural analysis of Sm intercalated C_{70} revealed that the bonding nature between C and rare earth metals in these compounds considerably differs from that in alkali metals doped fullerides: The covalency is much stronger than the alkali metal intercalated counterparts, causing a significantly different structural properties.

The electron density distribution for nominal Sm_3C_{70}, calculated by a maximum entropy method (MEM) based on the Rietveld analysis of synchrotron X-ray diffraction pattern, unambiguously demonstrated a covalent Sm-C bond, which produces a C_{70}-Sm-C_{70} dimer structure as shown in Fig. 1 [1]. The formation of dimer seems to be common for RE_3C_{70} (RE = Sm, Eu, Yb), due to the similarity in x-ray diffraction pattern of these compounds.

High-temperature x-ray diffraction experiments for RE_3C_{70} (RE = Sm, Eu) showed that the diffraction pattern is unchanged up to 500ºC, following by a structural phase transition, indicating that the dimer structure is maintained to 500ºC. This amazing stability of the dimer concomitantly implies that the Sm-C bond is much stronger than the conventional interfullerene bonds [2].

On the other hand, high-pressure powder x-ray diffractions revealed that RE_3C_{70} (RE = Sm, Eu) undergo a reversible first-order structural phase transition at 1.5 GPa, associated with reduction of the unit cell volume [3]. Structural analyses showed that C_{70} molecules are realigned at high pressure, and the derived charge density map indicates that the transition is regarded as a structural change from dimers to three dimensional polymers of fullerenes. These features are ascribed to the unique bonding nature in rare earth C_{70} compounds.

[1] H. C. Dam et al., Chem. Phys. Lett. **359**, 177 (2002)
[2] H. C. Dam et al., IWEPNM2002, AIP Conf. Proc. **633**, 51-54 (2002).
[3] H. C. Dam et al., preprint.

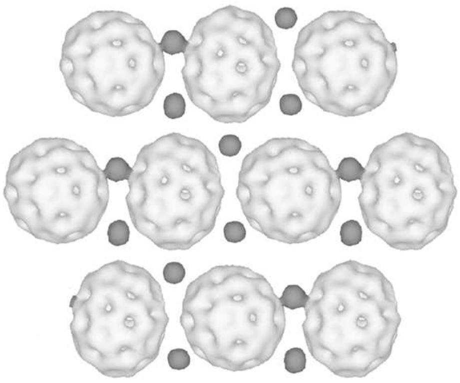

Figure 1. Dimer structure in Sm_3C_{70}.