<일반연제 2-3>

The Ambiguity in the Crystal Structure of C_{60} Thin Crystal

S. A. Song

Samsung Advanced Institute of Technology, 440-600 Suwon, Korea

INTRODUCTION

The Buckminsterfullerene C_{60} molecule has generated great interest because of its unique molecular structure [1, 2, 3] and of superconductivity exhibited in its akali-doped solids [4]. There have been a number of reports on the crystal structure of its thin films and powders. Early papers reported that C_{60} thin crystals have close-packed hexagonal (hcp) structure [2], but recent ones report they have face-centred cubic (fcc) [5, 6] or both of them [1, 7]. At the present the structure genenrally accepted seems to be fcc rather than hcp. However if we think about its molecular stacking influenced only by van der Waals force and gravity, there is no reason that the crystal structure should essentially be fcc for the isotopically rotating molecule at ambient temperature. In this report, the molecular stacking and crystal structure (at ~RT) of C_{60} thin crystals formed on amorphous carbon film are reported.

MATERIAL AND METHODS

The C_{60} powder was prepared by the method of Krätschmer et al.[2]. The C_{60} powder which was chromatographically purified was dissolved in benzene and then a drop of the solution was spread onto a carbon film covered grid and dried [8]. There were many thin crystals formed and these were observed with a 300kV transmission electrone microscope (Hitachi H9000). Electron diffraction analysis

and direct imaging of its molecular stacking were carried out.

RESULTS AND DISCUSSION

Usually the C_{60} molecules of 10.0Å diameter (regarding the buckyball as a hard sphere) were arrayed hexagonally on the substrate surface, and the 8.7Å lattice planes were quite open found in several types of ED patterns, which can never be explained with a fcc model. Therefore the structure of the C_{60} thin crystals must be hcp. However there still exists ambiguity in the structure because variation of electron diffraction intensities among hexagonally arrayed patterns has not been well understood. Meanwhile the [0001] hcp pattern of Krätschmer et al. could be interpreted as [111] fcc with some planar defect of hcp stacking in a crystal. Although there are reports [9] on the phase transition from "fcc" to simple cubic at ca. -30℃ by freezing the isotropic rotation of C_{60} molecules at the crystal site, such transition could not be detected by electron diffraction analysis from in-situ temperature-controlled experiment. TEM approach seems to be by far less sensitive in probing the "orientational ordering of C_{60}" than the X-ray method [10, 11, 12].

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