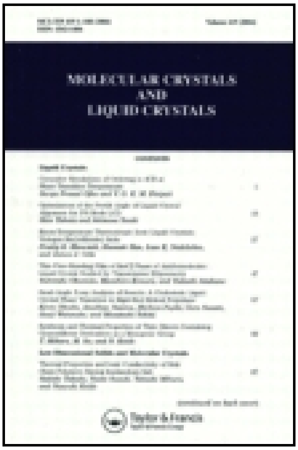


Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:
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# Investigation of the Interaction between $C_{60}$ and Si Atoms

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Version of record first published: 24 Sep 2006

*Mol. Cryst. and Liq. Cryst.*, 2000, Vol. 340, pp. 701-705
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# Investigation of the Interaction between $C_{60}$ and Si Atoms

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*(Received May 30, 1999; In final form July 8, 1999)*

The interaction between $C_{60}$ and Si atoms was investigated using X-ray photoelectron spectroscopy (XPS) for the photo-irradiated Si-deposited $C_{60}$ film in order to establish a method of a synthesis for the Si-coated $C_{60}$. It was found that the C1s spectrum of the photo-irradiated film contains a peak due to C-Si bonding, while no peak due to C-Si bonding was observed for the film before photo-irradiation. This indicates that Si atoms stick to $C_{60}$ when using the present method.

*Keywords:* Si-coated $C_{60}$; XPS; photo-induced reaction

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## INTRODUCTION

Si-coated $C_{60}$ is a fascinating material because it can be treated as a kind of single-shaped Si cluster [1,2]. In fact, Osawa and his co-workers theoretically predicted that $C_{60}Si_{60}$ is more stable than the isolated $C_{60}$ and $Si_{60}$, and that its energy levels of the frontier orbitals are similar to those of $Si_{60}$. This molecule is expected to be used as a functional nano-device when a method of its synthesis is established. Many attempts to produce the Si-coated $C_{60}$ have been tried until now: the laser-ablation technique to a silicon carbide substrate and fullerene-deposition onto a Si surface[3-8]. However, the formation of the stable $C_{60}Si_{60}$ has not yet been achieved. This reason may be attributed to the presence of a bottleneck in the formation process of the $C_{60}Si_{60}$[9]. In this regard, it is important to investigate the interaction between $C_{60}$ and Si atoms as the starting point for the $C_{60}Si_{60}$ synthesis. In the present study, the authors discuss the chemical bond formation between $C_{60}$ and Si atoms by analysis of the X-ray photoelectron spectra of a photo-irradiated Si-deposited $C_{60}$ film prepared in an ultrahigh vacuum chamber.

## EXPERIMENT

A brief description of the experimental setup used in this study is given, since detailed descriptions have been reported elsewhere[10,11]. A CsI substrate of 20 mm diameter was heated to 100 °C for more than 1 hour in an ultrahigh vacuum chamber (less than $1\times10^{-9}$ Torr) in order to evaporate water molecules adsorbed on the substrate. The $C_{60}$ molecules evaporated from a quartz crucible containing $C_{60}$ powder were then deposited on the substrate at 100 °C. The thickness of the

$C_{60}$ film thus formed was estimated to be about 50 nm. After the substrate temperature was cooled and maintained at 0 °C, the $C_{60}$ film was exposed to a Si-atom beam effusing from a silicon rod heated by high-energy electrons. The average thickness of the deposited Si layer was about 2 nm. Afterwards, the Si-deposited $C_{60}$ film was irradiated with UV-visible light of 1 $W \cdot cm^{-2}$ for 10 hours at 100 °C. After the sample was taken out of the vacuum chamber, it was introduced into a box filled with helium gas and was carried to another facility for the XPS measurements within 1 hour. The sample was introduced into a load-lock prechamber in the facility in order to be degassed under low pressure ($10^{-3}$ Torr) for 30 minutes. The sample was then transferred into the XPS-measurement chamber (less than $1 \times 10^{-9}$ Torr) and the XPS (MgK$\alpha$) spectra were obtained.

## RESULTS AND DISCUSSION

Figure 1 (a) shows the XPS spectrum of the C1s photoelectrons in the binding-energy range of 279 – 291 eV for the pristine Si-deposited $C_{60}$ film. The solid curve is an experimental spectrum. The dashed curve is the calculated spectrum originating from the chemical bonding labeled in the figure and is obtained using a Gaussian-type function. The binding energy of the peaks was defined using the O1s (533 eV) peak as a reference. The spectrum is composed of the dominant peak (285 eV) originating from the carbon atoms consisting of the $C_{60}$ and the minor peak (286.5 eV) due to the C-O bonding originating from air-contaminated layer, while no peak due to the C-Si bonding is observed. These features imply that the $C_{60}$ itself does not react with the Si atoms in the film.

On the other hand, Fig. 1 (b) shows an XPS spectrum of the C1s photoelectrons for the Si-deposited $C_{60}$ film after photo-irradiation. The new peak (283.5 eV) appears in the photo-irradiated film. It is considered that this peak is due to the C-Si bonding formed between the $C_{60}$ and the Si atoms because of the following reasons: (1) the chemical shift of the peak corresponds to that for the C-Si bonding[12], and (2) it is insufficient to decompose the $C_{60}$ by photo-irradiation in this photon-energy range[13] that Si atoms are considered to react with the $C_{60}$. This C-Si bond formation was also confirmed in the Si2p spectrum. The present work may provide a way to synthesize the $C_{60}Si_{60}$.



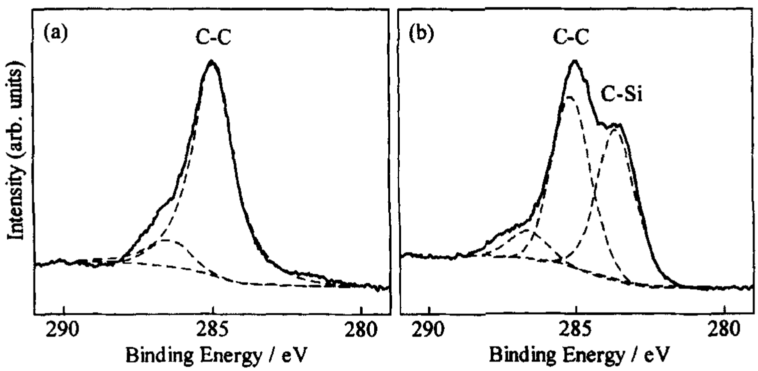


FIGURE 1 The XPS spectra of the C1s in the binding-energy range of 279 – 291 eV for the Si-deposited $C_{60}$ film (a) before and (b) after photo-irradiation. The solid curve is an experimental spectrum and the dashed curve is a spectrum calculated using a Gaussian-type function based on the assumption of the chemical bonding labeled in the figure.

**Acknowledgments**

The present work was supported in part by a Grant-in-Aid for scientific research by both the Science and Technology Agency of Japan and the Ministry of Education, Science and Culture of Japan.

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