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Growth of crystalline C₆₀ by evaporation

T. Moorsom

This application note describes the growth of crystalline thin films of C₆₀.

1 Introduction

C₆₀, also known as Buckminsterfullerene, is the most common and stable of the fullerenes, comprising a near spherical cage of sixty carbon atoms. C₆₀ has a wide range of applications in molecular electronics and spintronics, solar cells and molecular magnetism. [1–3] The growth of high quality, crystalline C₆₀ films is vital for the production of hybrid meta-materials and devices. In this note, we outline the optimal growth parameters for the evaporation of highly crystalline C₆₀ films from an effusion cell onto Pt substrates.

2 Growth

C₆₀ can be grown easily on various metallic and semi-conducting substrates. C₆₀ grows poorly on oxides due to high surface tension, causing large clusters to form. [4] Epitaxial platinum with a (111) texture is an ideal metallic substrate for C₆₀ growth. Pt (111) films were grown on Al₂O₃ substrates (see application note for e-beam Pt growth). The substrate temperature was maintained at 20° C. C₆₀ was evaporated from a graphite crucible in a single filament effusion cell. The effusion cell temperature was increased from standby at a rate of 10 °C per minute to 430 °C. The deposition rate was measured to be 0.5 Å/s using a quartz balance. The rate varies during growth, reaching a maximum value of 0.74 Å/s. The substrate was rotated at 90°/s during deposition. the background pressure was 8×10^{-10} mbar. After growth, the film was capped with a 15 nm thick film of Nb to protect it from oxidation.

3 Properties

Structural characterisation was obtained using X-ray reflectivity (XRR) and TEM. Figure 1 shows the XRR data taken of the bilayer film. C₆₀ has a very low density of 1.65 g/cc. However, a structural peak is observable at 11°. Because of the low scattering length of C₆₀, this peak is only visible in samples with extremely high crystallinity. A GenX reflectivity fit was performed for this data. The low angle fit does not

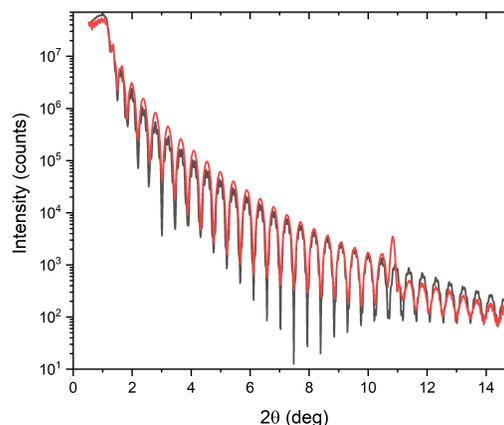


Figure 1: X-ray reflectivity data of a platinum C₆₀ bilayer (red) and GenX fit (black). The structural C₆₀ peak at 11° is not captured by the low angle fit.

capture the structural peak as this method does not simulate crystal structure.

A lamella, 80 ± 10 Å thick, was cut from the sample using a Dual-Beam Ga Ion FIB. This lamella was then measured using a Titan FEI TEM at 100 kV. The van der Waals lattice of the C₆₀ is clearly visible with (111) vertical orientation. The interface between the Pt and C₆₀ is atomically sharp. The lattice spacing of the C₆₀ film is 1.05 ± 0.03 nm.

The vibrational spectrum of C₆₀ films was recorded

GenX fitting parameter	Value
Thickness - C ₆₀ (Å)	975±0.7
Density - C ₆₀ (% of bulk)	100±0.01
RMS Roughness - C ₆₀ (Å)	1.8±0.9
Thickness - Pt (Å)	191±0.2
Density - Pt (% of bulk)	100±0.01
RMS Roughness - Pt (Å)	1.7±0.1

Table 1: Structural parameters obtained through the fitting of XRR data with GenX

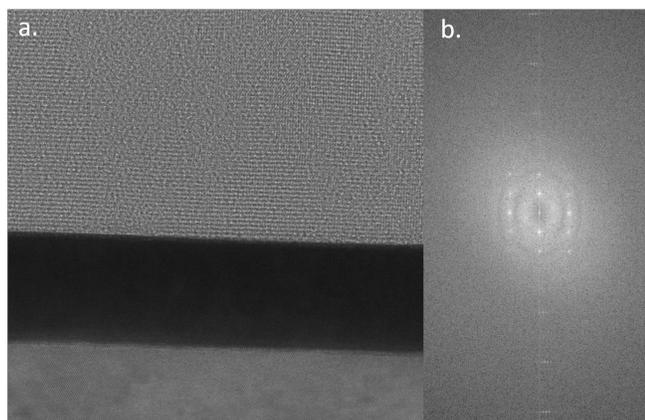


Figure 2: a. TEM obtained from the Pt/C₆₀ bilayer lamella, showing clear molecular layers and an atomically sharp interface. b. FFT of the C₆₀ layer, showing 3D crystal structure.

Mode	Raman Shift
Ag(2) - Δcm^{-1}	1470 \pm 2
Hg(7) - Δcm^{-1}	1434 \pm 5
Hg(8) - Δcm^{-1}	1575 \pm 5

Table 2: Positions of the major Raman active modes of C₆₀.

using a Horiba Raman Microscope with a 471 nm diode laser, Figure 3. The three highest intensity Raman active modes: Ag(2), Hg(7) and Hg(8) are used to determine the quality of the film. [5]

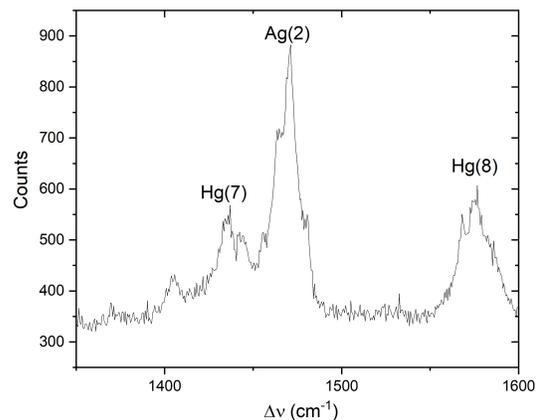


Figure 3: Raman spectrum of C₆₀ film. The three major Raman active modes are present and the characteristic mode of graphite at 1600 cm^{-1} is absent. The splitting of the Ag(2) peak is characteristic of electron transfer across a metallic interface.

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