The Dynamical World of Carbon Nanostructures

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SYMMETRY AND ANGULAR MOMENTUM IN COLLISIONS WITH LASER-EXCITED POLARIZED ATOMS

1985/1986

UV laser pulse

polyimide

Advance in Chemical Physics, Volume LXXII
Edited by I. Prigogine, Stuart A. Rice
Copyright © 1988 by John Wiley & Sons, Inc.
Curl, Kroto and Smalley’s discovery, 1985

Nobel Prize in Chemistry
1996

$C_{60}$  $C_{70}$

Suggestion of hollow cage structure to explain magic numbers in mass spectra: the fullerenes
Serendipity on a materials science detour

UV laser ablation of polyimide was a very topical subject in the mid-eighties.

We had to do "something relevant" and decided to look at the masses of the ablation products.
Solid $C_{60}$: a new form of carbon

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Solar cells

![Graph showing the number of papers related to solar cells from 1985 to 2005.](Image)
Fullerenes: Model systems for learning about the dynamical behaviour of complex molecules.

- High vib. excitation
- ns laser + Collisions
- Black body radiation
- + e delayed ionisation
- Metastable fragmentation
Dynamics of Fullerene Collisions

Fusion

C$_{120}$

Fragmentation

Intra-cluster molecular fusion
Capturing Atoms

$C_{60}^+ \rightarrow \text{He} \rightarrow \text{Mass Spectrometer} \rightarrow \text{Det.}$

Two mechanisms for capture:

1. $6 \text{ eV}$
   $R_{12} < 1 \text{ Å}$

2. $17 \text{ eV}$
   $R_{12} \approx 3 \text{ Å}$

Endohedral Fullerene

\[ \sigma = \pi R_{12}^2 \left[ 1 - \frac{V_B}{E_{CM}} \right] \]
1992 Adlershof
There were times when it didn’t seem such a good idea......

Pictures taken 2 weeks before the planned lab move from Freiburg
But soon we were ready to celebrate the official opening of the Max Born Institute
How do highly excited fullerenes behave?

When does statistical behaviour appear?

MBI

Ultrashort Pulses (< 50 fs)

Strong field - multiple ionisation

Coherent control

Gothenburg

Longer pulses, lower intensities

Statistical modelling

Ionisation mechanism
PES & MS same fluence, different pulse duration

Electrons

ca. 3.5 J/cm²

Ions

MPI
(t < 50 fs)

hot electrons

cold "lattice"
(50 fs < t < 500 fs)

statistical energy
distribution, strong
vibrational excitation
(t > 500 fs)

Use VMI to study the energy and angular distribution of the emitted electrons

Tunable <100 fs and ps light
Temperature controlled beam source
UHV conditions
Coincidence measurements
The thermal delayed ionisation (thermionic emission) seen with ns excitation is homogeneous, as expected (C. Bordas)
3 x $10^{12}$ W/cm²

130 fs, 800 nm, linear

STS of single C$_{60}$ on substrate

Atomlike hollow core-bound MO of C$_{60}$

Feng et al., Science, 320 (2008) 359
Clusters fragment by evaporating fullerene monomers


Heden et al., EPJD 43 (2007) 255

<table>
<thead>
<tr>
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<th>$C_{60}$</th>
<th>$C_{70}$</th>
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<tr>
<td>Fusion Threshold (eV)</td>
<td>$85 \pm 5$</td>
<td>$100 \pm 10$</td>
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<tr>
<td>Largest Detected Dimer Fragment</td>
<td>$C_{116}^+$</td>
<td>$C_{130}^+$</td>
</tr>
<tr>
<td>Expected Max Fragment Ion Range</td>
<td>108-118</td>
<td>126-138</td>
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Low mass cut-off determined by competition with double ionisation

$C_{106}^+$ corresponds to initial internal energy of ca. 125 eV. For this energy, double ionisation of $(C_{60})_2$ occurs with a rate of ca. $6 \times 10^{13}$ s$^{-1}$. 
Competition between fusion and multiple ionisation

Calculated dimer fragment distributions from different neutral precursor clusters

Narrower than observed experimentally - real cluster IP’s not properly accounted for

Size and mobility of excitons in (6, 5) carbon nanotubes
Nature Physics 5 (2009) 54

T. Hertel
Advantages of Carbon Nanotubes for NEMS

- Low Mass
- High Young’s modulus (E)
- High integration density??

Continuum beam mechanics can be used to model behaviour

- **Pull-in voltage**: Want low mass, low E and long tube (L) to minimise pull-in voltage

\[
V_{PI} \propto \sqrt{\frac{Em}{L}}
\]

- **Frequency**: Want high E and short tube (L) for high frequency

\[
f \propto \frac{1}{L^2} \sqrt{\frac{E}{\rho}}
\]
Contact Mode Nanotube Nanorelay


$V_{sd} = 0.5 \text{ V}$
High Frequency Properties

Contact  Non-contact

The resonance frequency can be tuned by several GHz by tuning the gate voltage.

\[ V_g = V_{g0} + \delta V \sin \left[ 2\pi f_{\text{mod}} (t - \tau) \right] \Theta(t - \tau), \]

Apply a DC bias between source and drain. CNT becomes charged and a capacitive coupling is induced.

If the CNT is at mechanical resonance, the electric field will vary harmonically, thus inducing an ac current at the drain that can be measured.

Modeling: J. Kinaret, A. Isacsson, CTH

Anders Eriksson et al., Nano Lett. 8 (2008) 1224
MEMS/NEMS from arrays of vertically aligned multiwalled nanotubes

No voltage applied

Voltage applied between tubes
Want thin, tall walls to minimise voltage needed to actuate the varactor.
CNT grown on 200nm thick Mo electrodes using 1nm Fe/Alumina, acetylene growth
Looking down on Varactor with Optical Microscope

Top focus

Catalyst separation: 20 µm
Thickness: 6 µm
Height: 70 µm
Effective Young’s Modulus 4 MPa
(cf 300 GPa - TPa)

MEMS modelling T. Idda, LAAS
N. Olofsson et al., Nanotechnology 20 (2009) 385710
The Team

Nanotubes

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Theory Collaborations

Fullerenes/fs laser int.

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Cluster Deposition

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