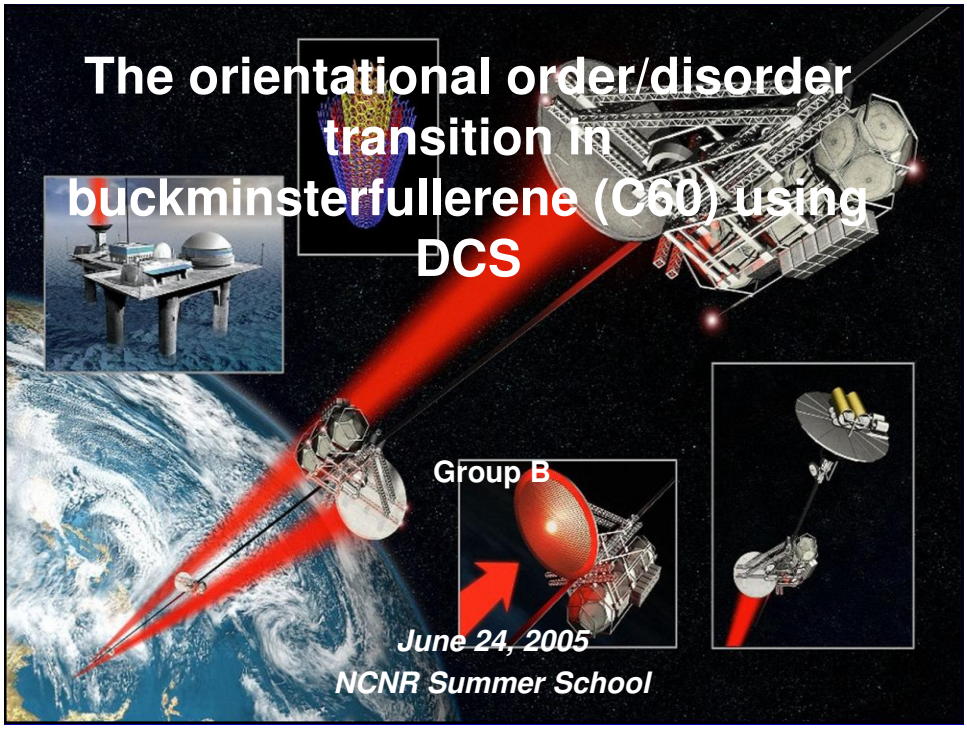
The orientational order/disorder transition in buckminsterfullerene (C60) using DCS



Group B

June 24, 2005

NCNR Summer School

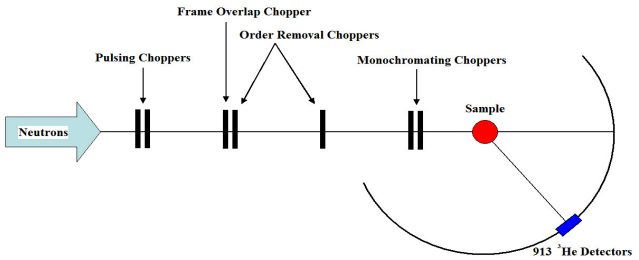
The Disk Chopper Spectrometer (DCS)

(1) The neutron guide

(2) The choppers

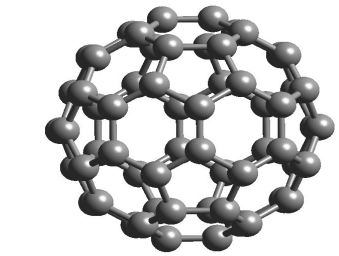
(3) The sample area

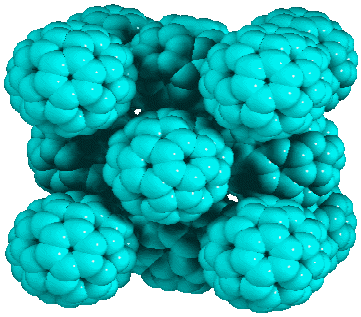
(4) The flight chamber and the detectors



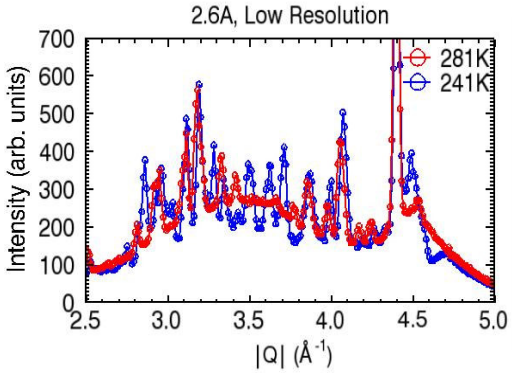
Buckminsterfullerene (C_{60})

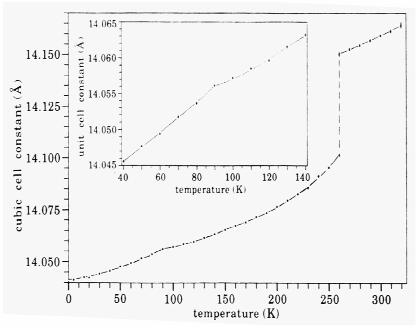
- 60 equivalent C atoms on the vertices of a truncated icosahedron (i.e. soccer ball)
- 2 characteristic bond lengths:
  - single bonds, d_1=1.45Å
  - double bonds, d_2=1.40Å
- Molecular radius≈3.55Å





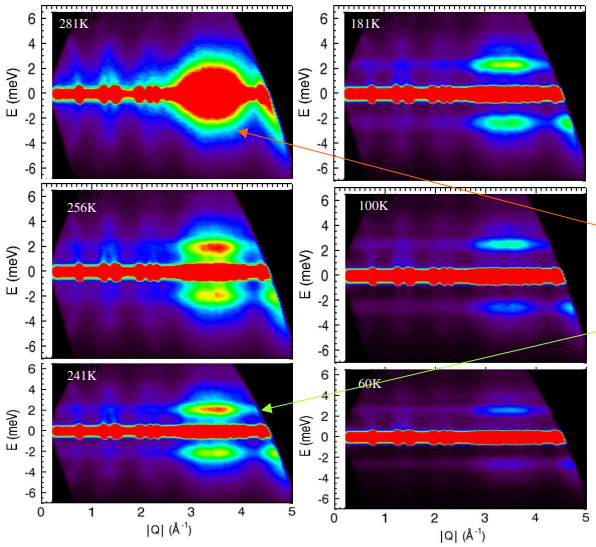
The Orientational Phase Transition of C_{60}





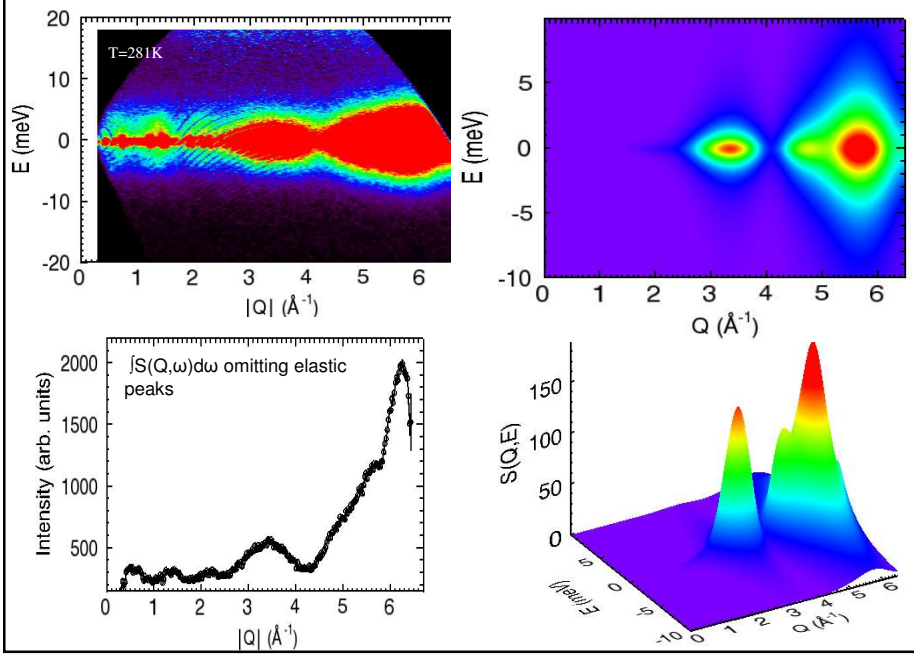
- 1st order phase transition at Tc=260K
- T>Tc: C_{60}s FCC symmetry, a_0≈14.15Å, rotational motion
- T<Tc: C_{60}s SC symmetry, a_0≈14.09Å, librational motion

Temperature evolution of S(Q,ω)

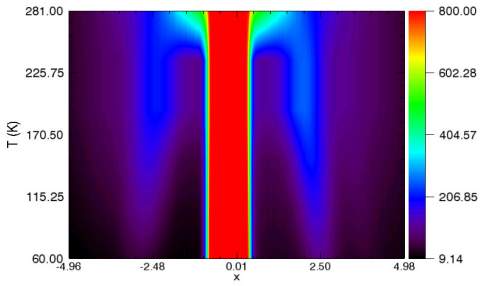


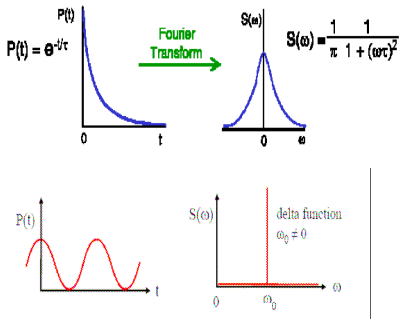
As T is lowered below T_c, quasielastic peaks evolve into inelastic peaks.

Comparison to Theoretical Models

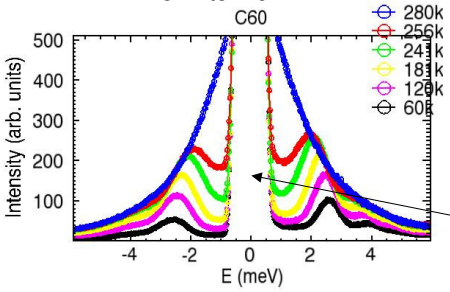


Temperature dependence of librations



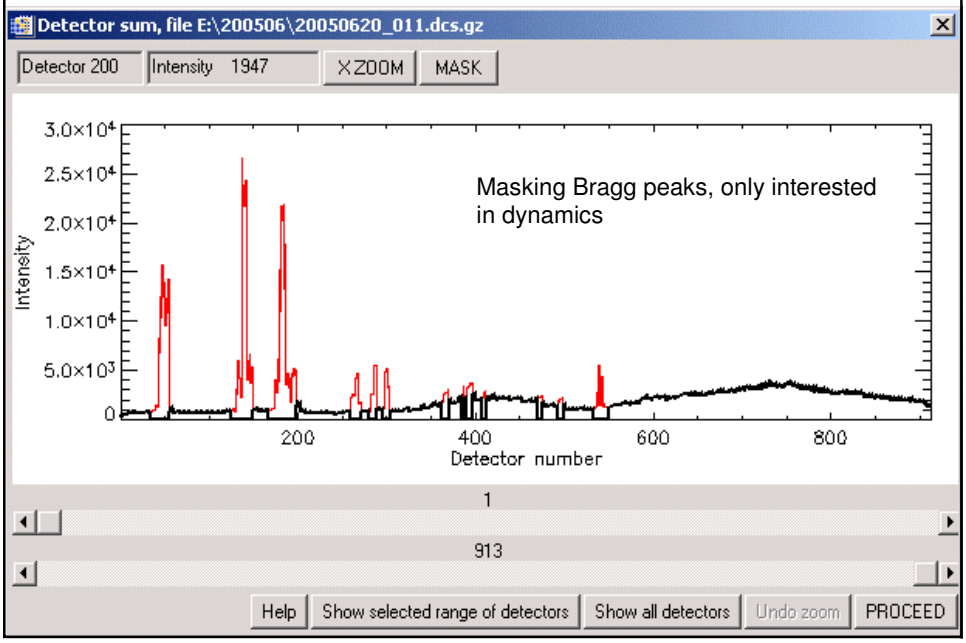


Q-Integrated between 2.5A^{-1} to 4.6A^{-1}.

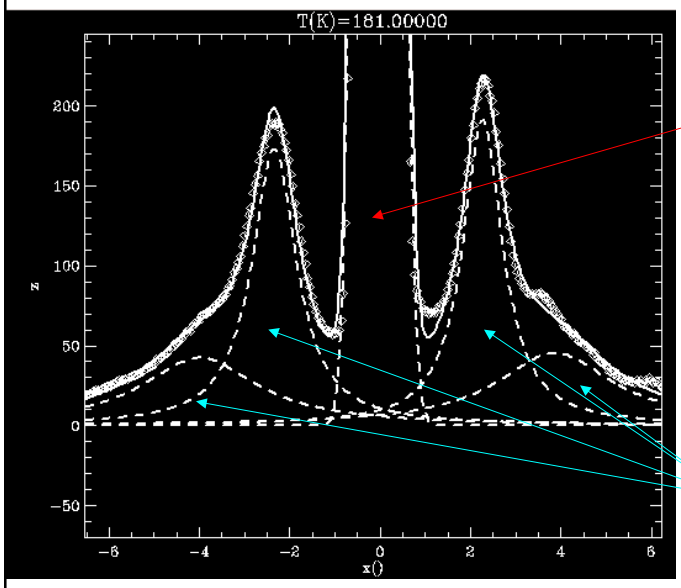


Asymmetry reflects detailed balance factor.

Data Reduction



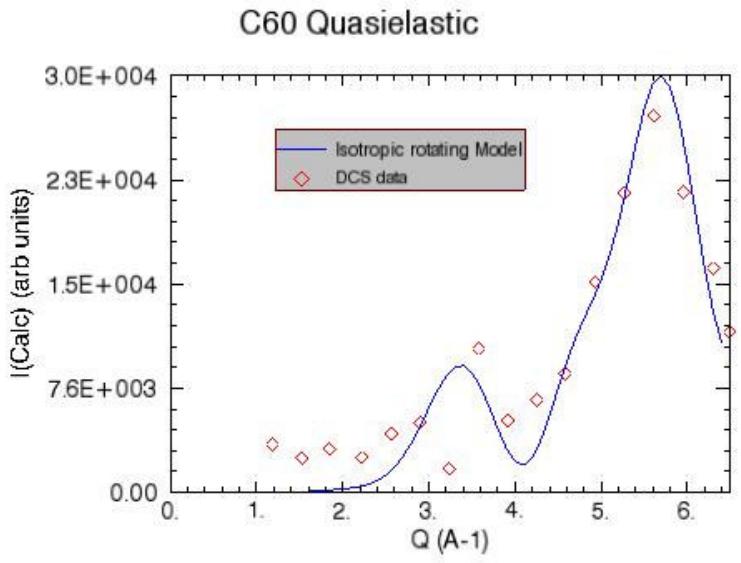
Data Reduction



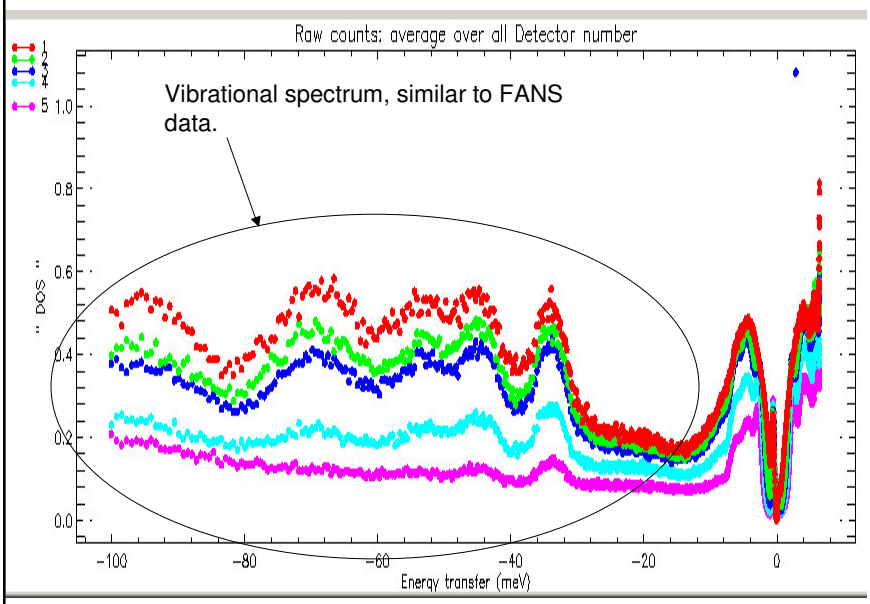
Fit elastic peak with Gaussian

Fit 4 inelastic features with Lorentzians

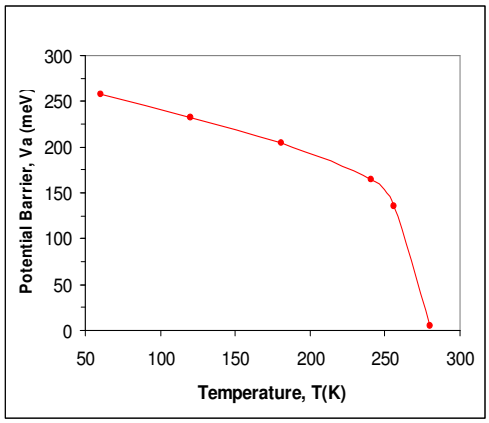
Comparison to Theoretical Model



Vibrational density of states



Potential Barrier as a Function of Temperature



- V_a: potential barrier/ activation energy for C_{60} rotational jumps
- Defined by:

$$\hbar\omega = (2\pi/\theta_{hop})\sqrt{BV_A}$$

- θ_{hop}=angle between minima of orientational potential
- $B = \frac{\hbar^2}{2I}$= rotational constant

•Accepted value: Va= 220-290 meV

Acknowledgements

Thanks to DCS instrument scientists: ☺□♒■ 👍□□●♏♲, Craig Brown, **Yiming Qiu**.

Thanks to everyone at NIST for planning and funding the summer school.

Thanks to Julie Keyser for travel and hotel arrangements

Thanks to group B members: David Hsieh, Susan Fullerton, Ashley Stowe, Patrick Clancy, Ted Lee, Andrei Savici, Christopher Shogbon, Jiying Li.