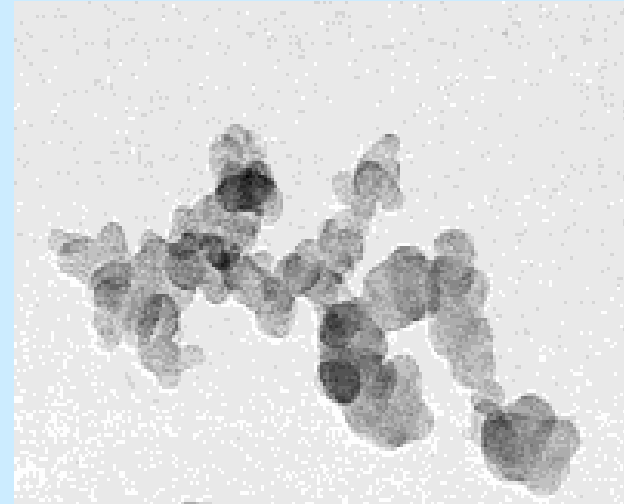
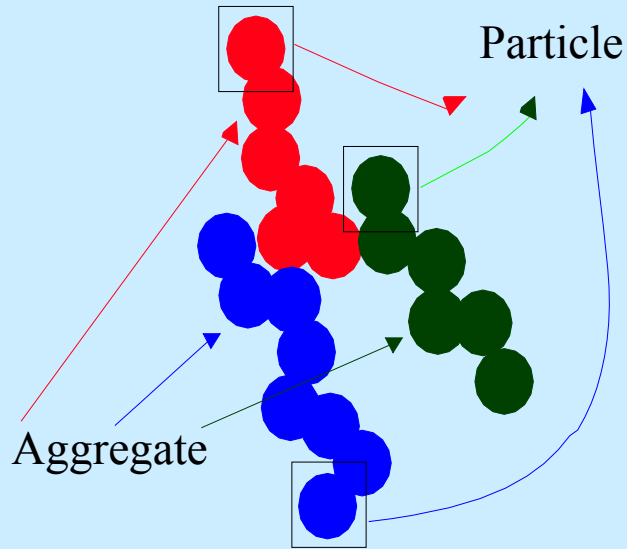


Furnace Black Characterization

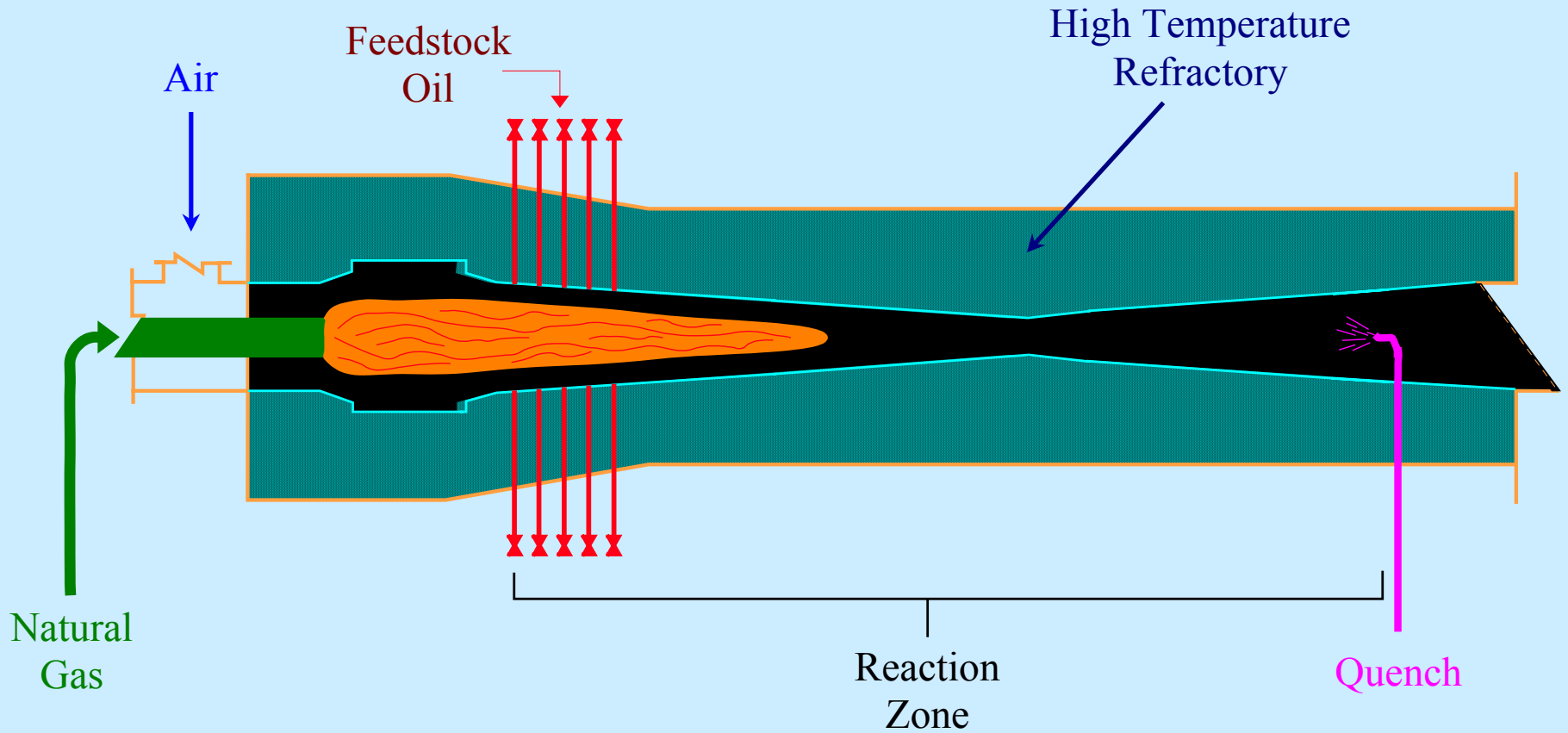
Definitions



Particle (?) = 20nm to 100nm "Diameter"
Aggregate = 200nm to 1,000nm "Length"
Agglomerate = Set of Percolated Aggregates

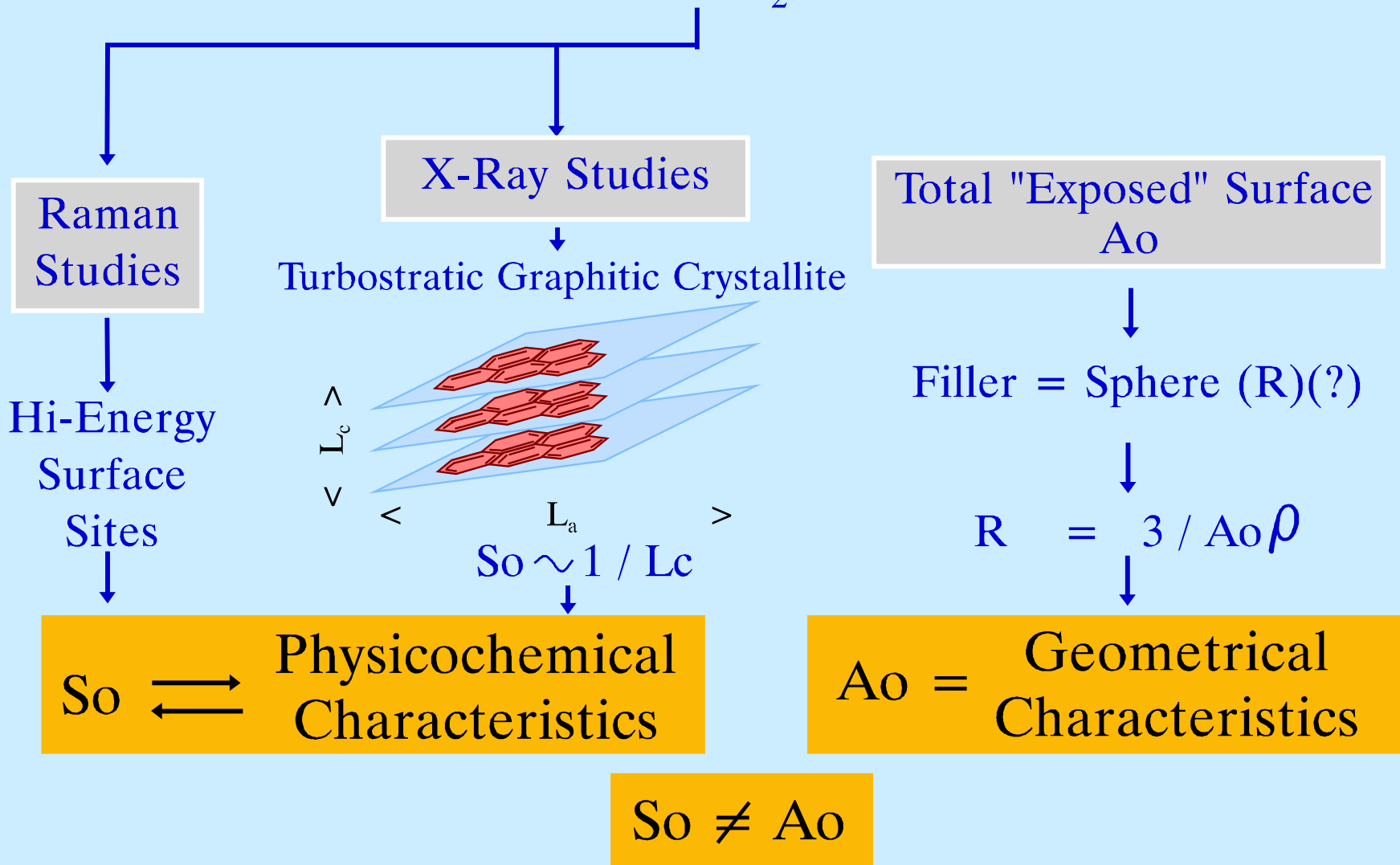
Constituents Size = Tech/Scientific Challenge

Furnace Process

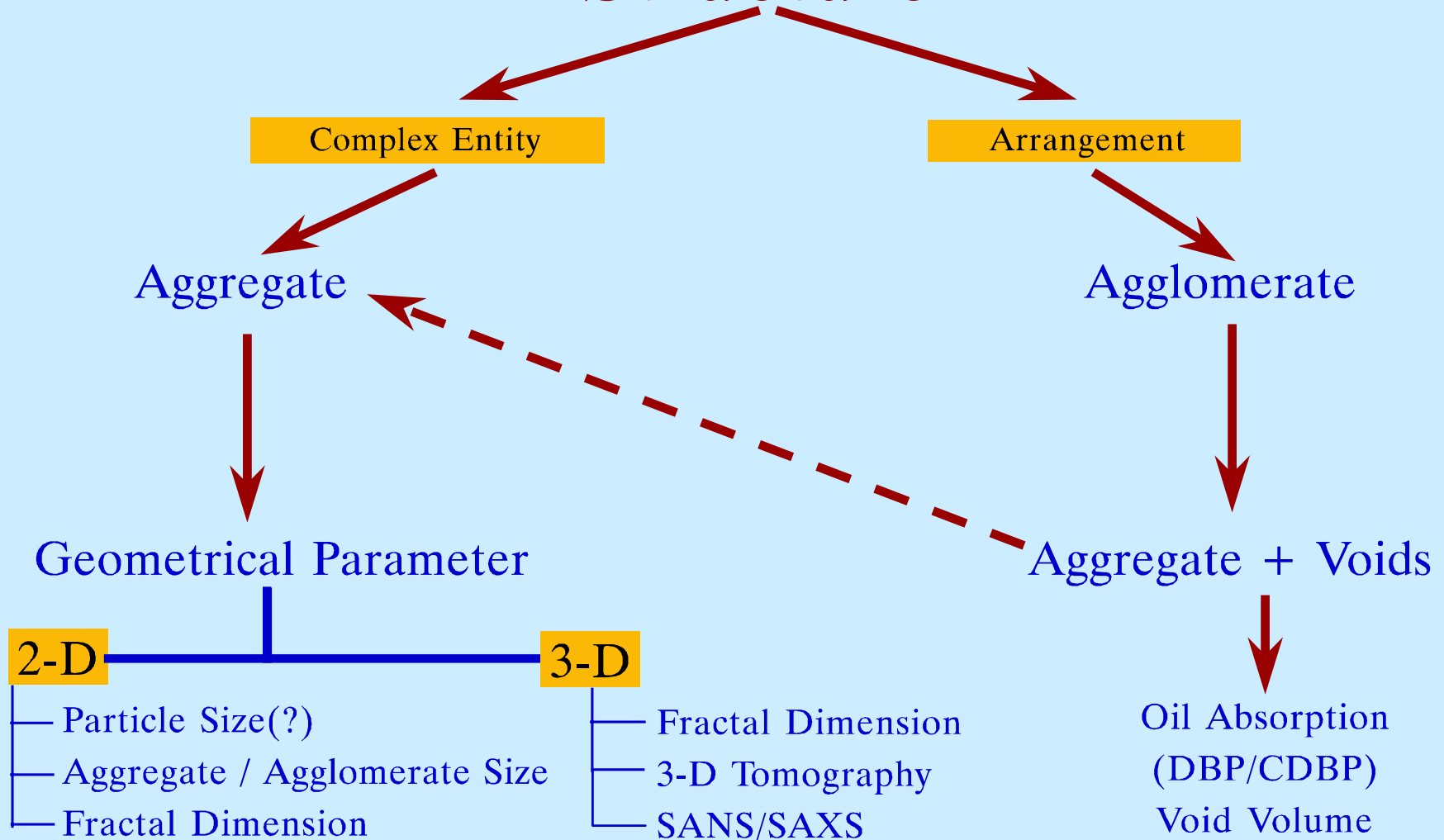


Specific Surface Area

BET - N₂SA



Structure



3-D Morphology Key Characteristic

Summary
of
Crystallographic Studies

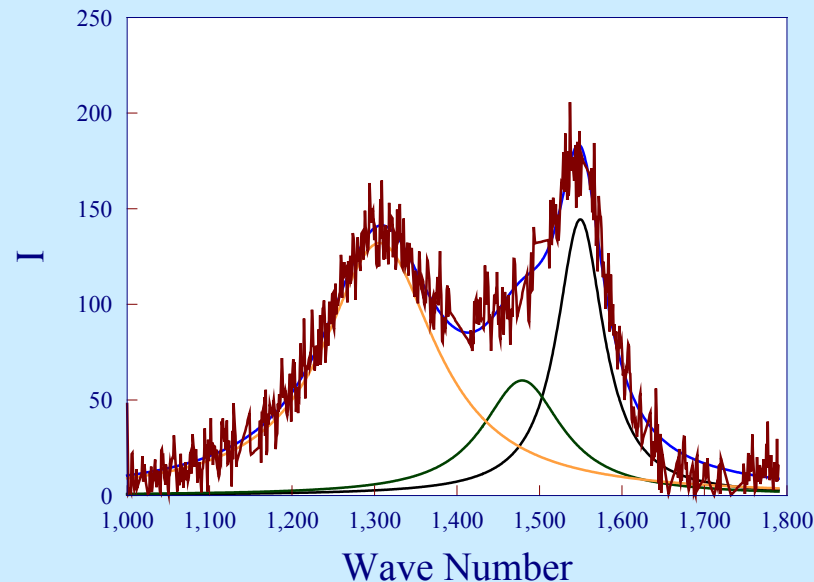
Summary

- For all furnace carbon black
- Crystallite $\left\{ \begin{array}{l} 12\text{\AA} < L_C < 17\text{\AA} \\ L_a \approx 25\text{\AA} \end{array} \right.$
- Amorphous Carbon
- No micropores
- Very few surface groups (hetero atoms)

Effect of Heat Treatment on Amorphous Carbon

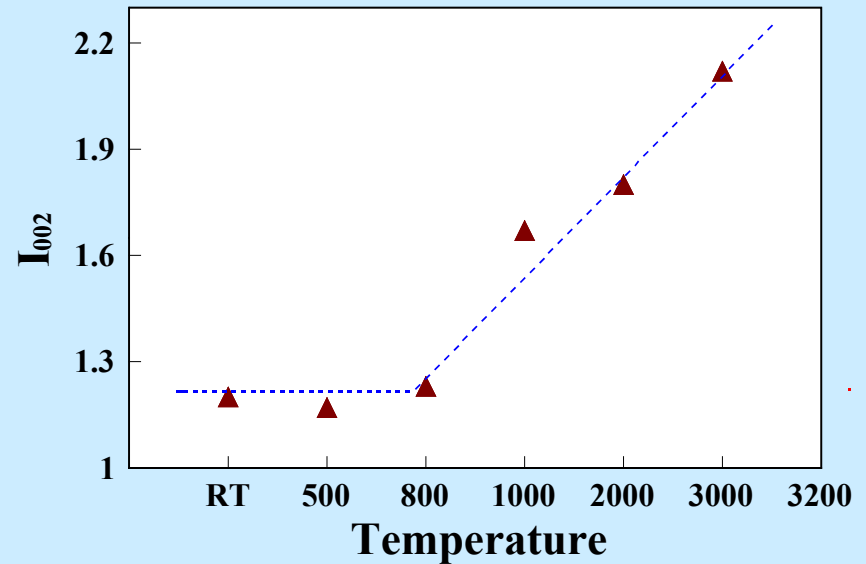
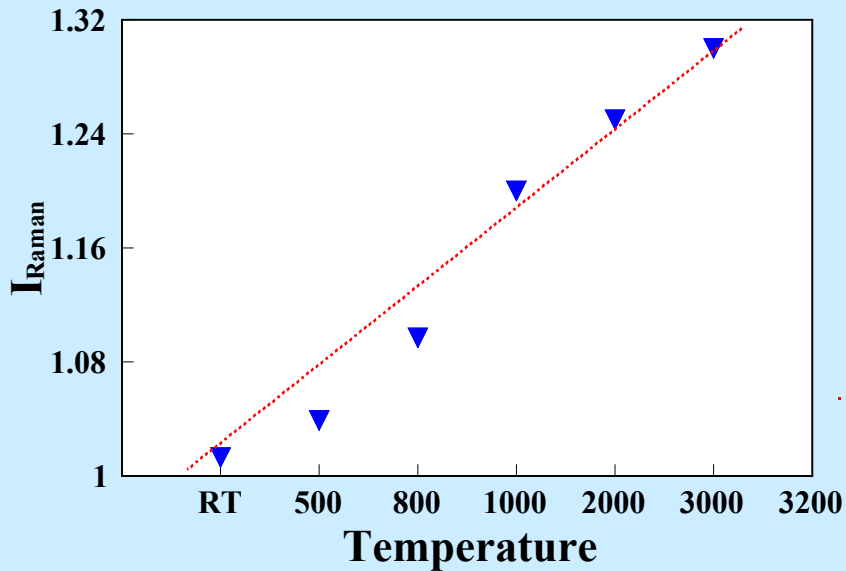
Raman Study and Hydrogen Content

· Raman Spectrum of N299



<u>Heat Treatment Temperature</u>	<u>Amorphous Area / Total Area</u>	<u>Hydrogen Content, (ppm)</u>
Untreated	0.348	2407
500°C	0.152	2502
800°C	0.114	2393
1000°C	0.038	2325
2000°C	0.029	10

Results (Cont'd)



$T < 1000^{\circ}\text{C} \rightarrow$ “Reorganization” of graphitic planes on the surface
 $T > 1000^{\circ}\text{C} \rightarrow$ Formation of microcrystallites

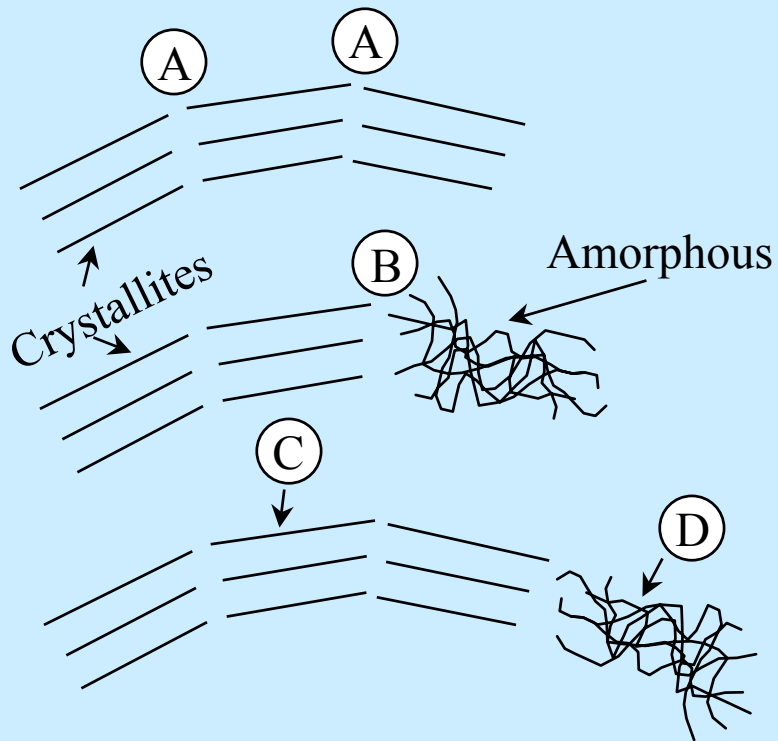
Surface Unorganized Carbon Identified

SRCC's Model



Carbon Black Surface Activity

- Edges of crystallites → High concentrations of π electrons



Active Site

- Energy Scale
 $E_A > E_B > E_C$
- E_D ? → Role of hydrogen atoms?

Important Surface Energy Density

Energetic Surface Structure of Carbon Black (Summary)

A. Schroeder | R. Schuster

DIK

Polymer - Filler “Bonding”

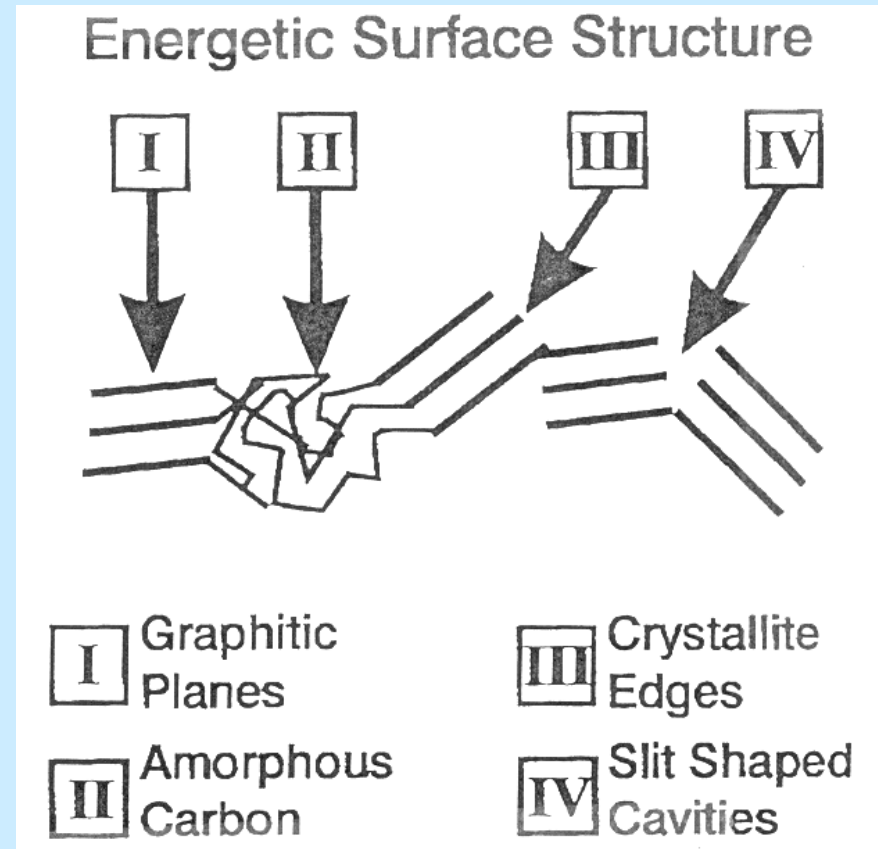
$$\Delta G_{ads} = \Delta H_{ads} - T\Delta S$$

ΔH_{ads} = *Enthalpy of Adsorption*



Adsorption Isotherm

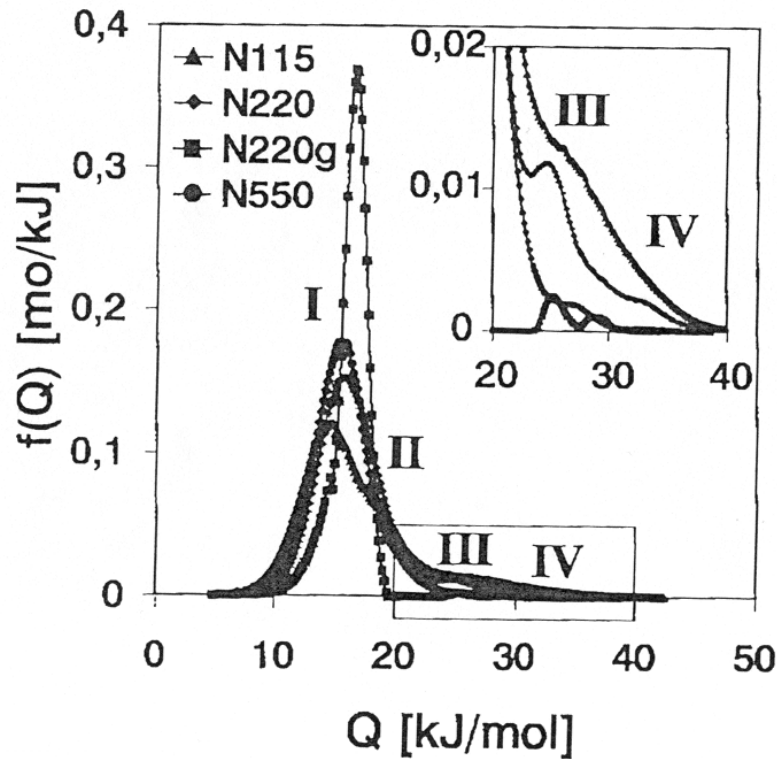
$$\Theta(\rho, T) = \int_0^{\infty} \theta(\rho, T, Q) f(Q) dQ$$



$f(Q)$ = *Distribution of Energetic Sites*

Energetic Surface Structure of Carbon Black

Energy Site Distribution $f(Q)$
 C_2H_4 on N115, N220, N220g and N550



Fraction [%]

	I	II	III	IV
N115	69	13	15	3
N220	84	7	7	2
N220g	99	-	< 1	< 1
N550	93	6	1	< 1

Energy [kJ/mol]

	I	II	III	IV
N115	15	19	24	31
N220	16	19	24	32
N220g	17	-	25	29
N550	15	21	26	32

Role of Active Sites

Active sites → High density of π electrons

A Sites for Van der Waals bonding with neighbor aggregates → carbon black network

B Sites for weak (Van der Waals ...) bonding with polymer chains

Carbon Black Surface Groups

* As per Professor Bertrand (Belgium) ACS Rubber Division, Spring 1998

- Heterogroup → Very few
- Hydrogen atoms → Significant amount

Hydrogen Most Relevant Surface Group

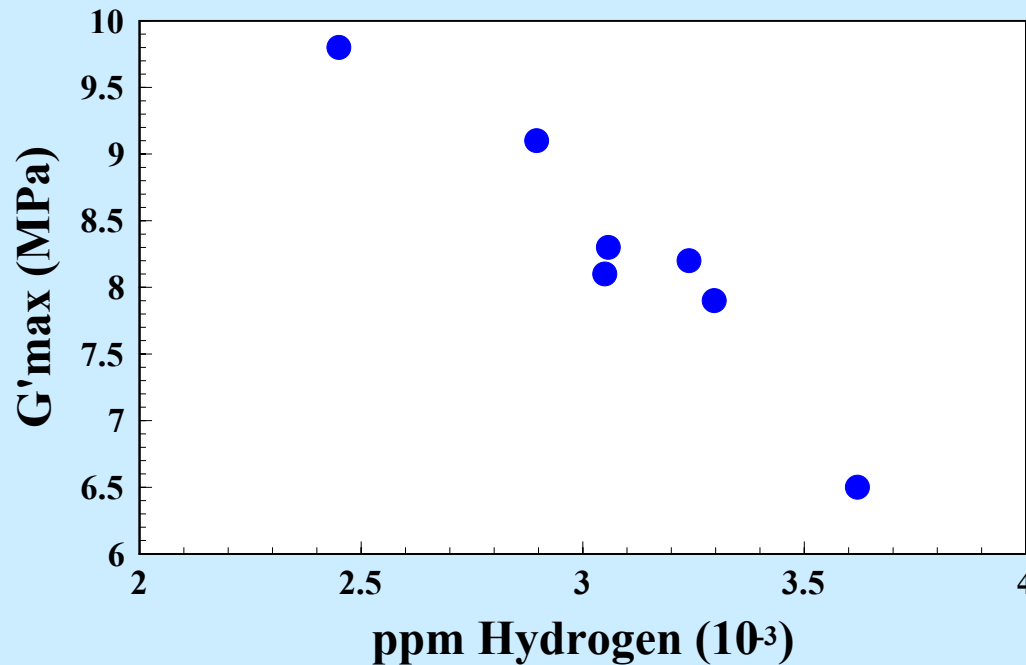
Surface Hydrogen Group

- Study to be started with Professor Bertrand (Belgium)
 - SIMS T.O.F.
 - E.S.C.A. / Auger
- Surface hydrogen proportional to total hydrogen
Total Hydrogen → Leco Technique

Amorphous Carbon \propto Hydrogen Content

Hydrogen Content of Amorphous Carbon

- Carbon black of
 - same “particle” diameter (TEM)
 - different Nitrogen adsorption
- Special process to increase the amorphous carbon



Hydrogen Directly Linked to Amorphous Carbon