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Graphitization of disordered carbons for batteries - structure determination by neutrons

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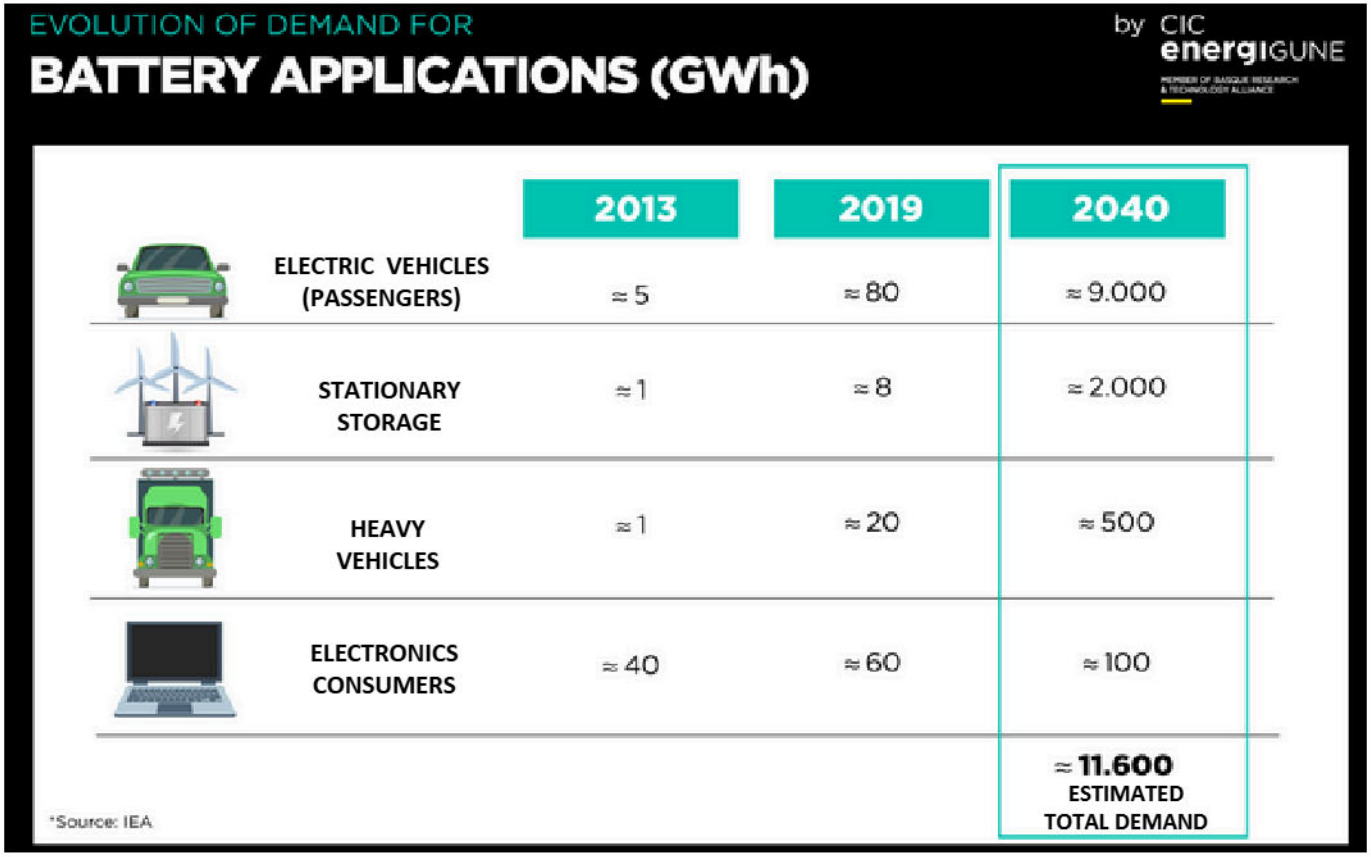
1st Workshop on Research & Innovation in Poland dedicated to present and future Polish Contribution to the European Spallation Source ERIC in Lund, Sweden

2nd December 2025, Kraków, IFJ PAN

High demand for energy storge systems



International Energy Agency predictions

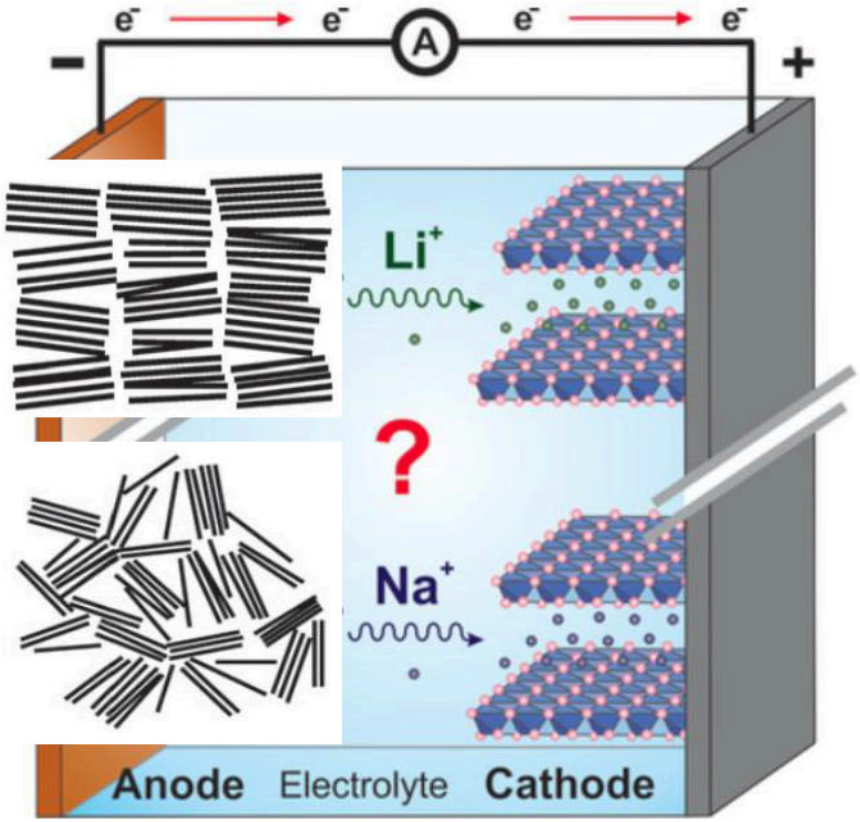
source: https://cicenergigune.com

Solution: lithium- and sodium-ion technologies as partners to lead

key active anode materials:

graphite

disordered
(hard – non-graphitizing)
carbons

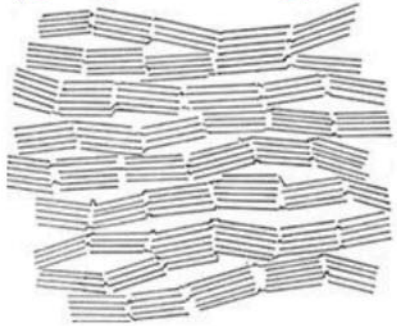


LIB

SIB

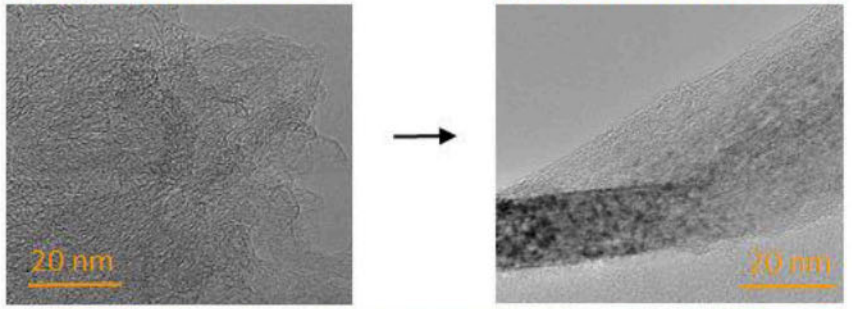
Transformation of the structure of carbon precursors in the heat-treatment process

soft (graphitizing) carbons



Franklin, R. E. Proc. R. Soc. London, Ser. A 1951, 209 (1097) 196– 218

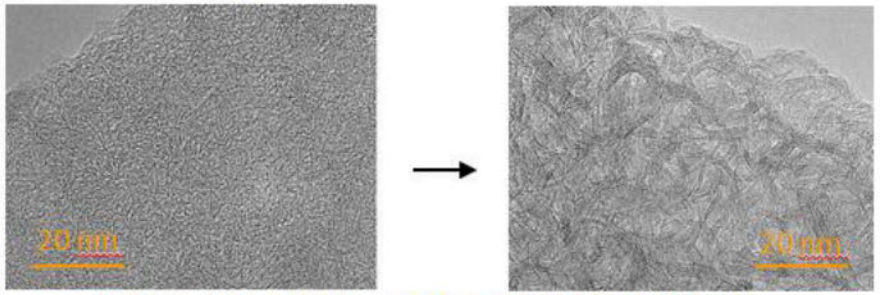
graphitizing coke → graphite structure



1000 °C → 2500-3000 °C

hard (non-graphitizing) carbons

non-graphitizing glassy carbon → disordered structure



Jurkiewicz, K., Pawlyta, M. et al. (2018). *Journal of Materials Science*, *53*(5), 3509-3523.

Characterization of the structure of disordered carbons by wide-angle neutron diffraction data

D4 neutron diffractometer
ILL, France

$\lambda = 0.4989$ Å, $Q_{max} = 23.5$ Å^{-1}

Q-space

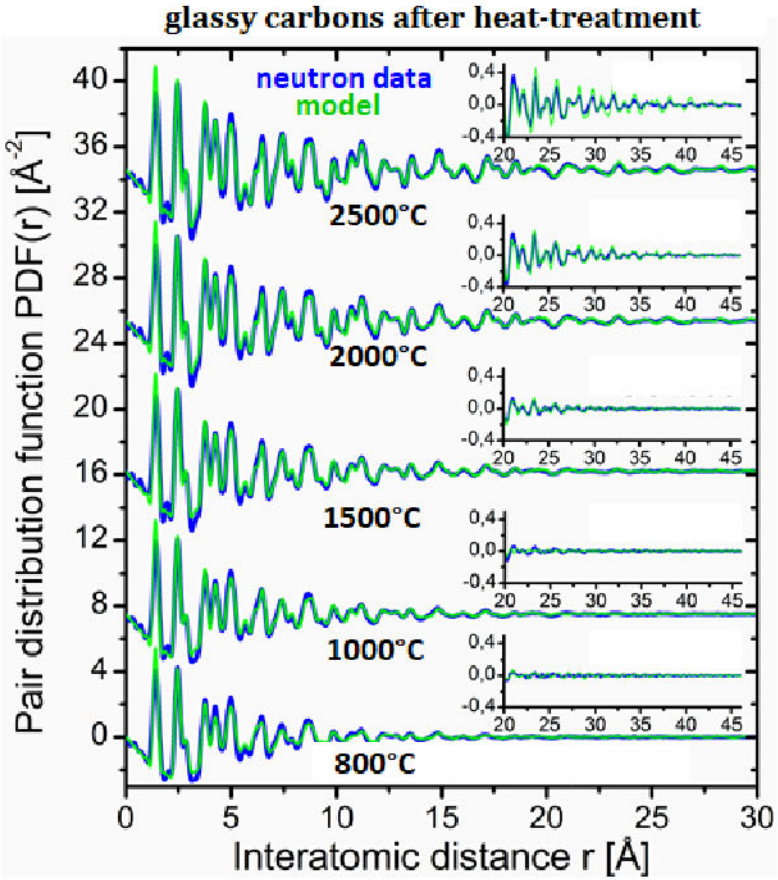
$$S(Q) = 1 + \frac{I(Q) - \overline{b^2}}{\overline{b}^2} \qquad Q = 4\pi \sin\Theta/\lambda$$

r-space ↕ Fourier transform

$$\mathrm{PDF} = 4\pi r[\rho(r) - \rho_o]$$

$$= \frac{2}{\pi} \int_0^{Q_{max}} Q[S(Q) - 1] \sin(Qr) \frac{\sin(\pi Q/Q_{max})}{\pi Q/Q_{max}} \, dQ$$

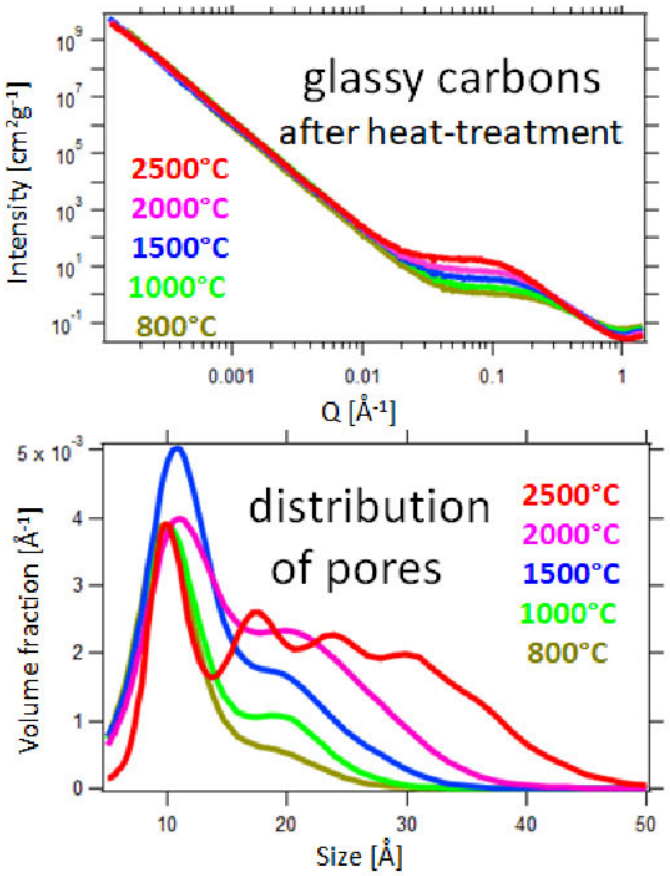
Verification of structural models of disordered carbons by wide-angle neutron diffraction data



optimized structural models from molecular dynamics simulations

Jurkiewicz, et al. (2017)
***J. Appl. Cryst.*, *50*(1), 36-48**

Verification of structural models of disordered carbons by small-angle scattering data (X-rays or neutrons)



R_G - radius of gyration for sphere

V_f - volume fraction

glassy carbon	R_G [Å]	V_f [%]
3000°C	15.2	25
2500°C	13.4	24
2000°C	10.2	20
1500°C	8.5	17
1000°C	7.6	12
800°C	6.5	10

optimized structural models from molecular dynamics simulations

Novel methods of tuning the graphitic order and porosity of disordered carbons towards battery applications

CATALYTIC GRAPHITIZATION

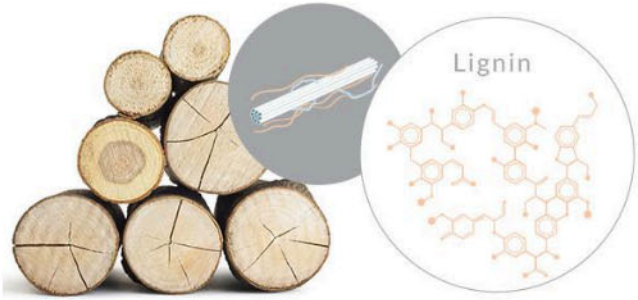
Some metals and semimetals may induce formation of graphitic order by dissolution precipitation and carbide formation-decomposition mechanisms.

Tang, L., et al. (2022). Catalytic graphitization in anthracite by reduced iron particles and investigating the mechanism of catalytic transformation via molecular dynamics. *Carbon*, *188*, 336-348.

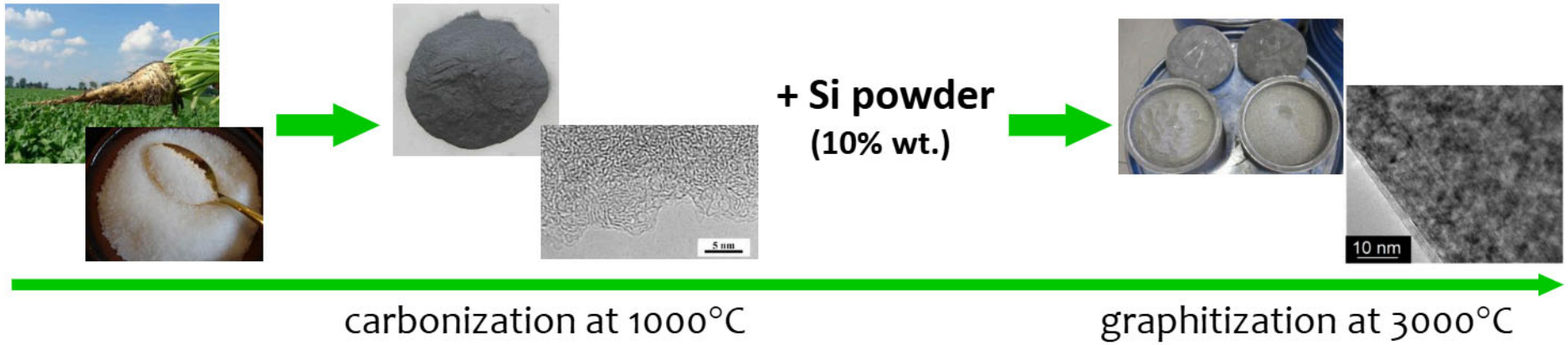
Novel methods of tuning the graphitic order and porosity of disordered carbons towards battery applications

CATALYTIC GRAPHITIZATION

This effect is currently intensively investigated to tune the structure of various bio-derived precursors towards anode materials for SIBs and formation of graphite for LIBs.



Production of graphite from sucrose



Research Article

ADVANCED FUNCTIONAL MATERIALS

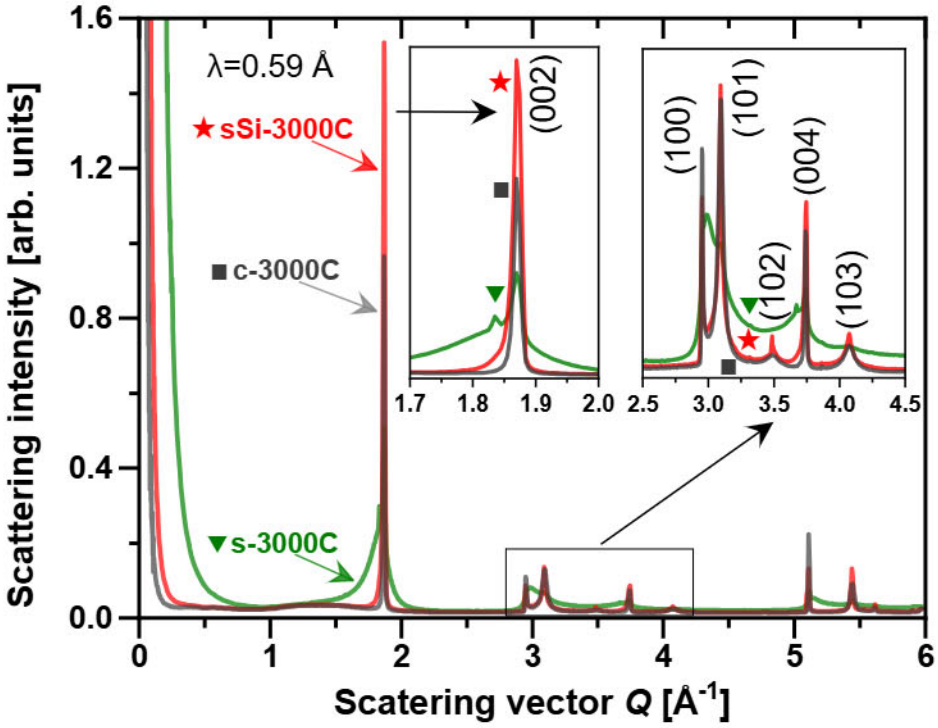
Sucrose-Based Dense, Pure, and Highly-Crystalline Graphitic Materials for Lithium-Ion Batteries

Karolina Jurkiewicz, Barbara Liszka, Paweł Gancarz, Szymon Smykała, Dorota Zygadło, Patryk Nokielski, Taoufik Lamrani, Ewa Talik, Roman Wrzalik, Mariusz Walkowiak, Jan Ilavsky

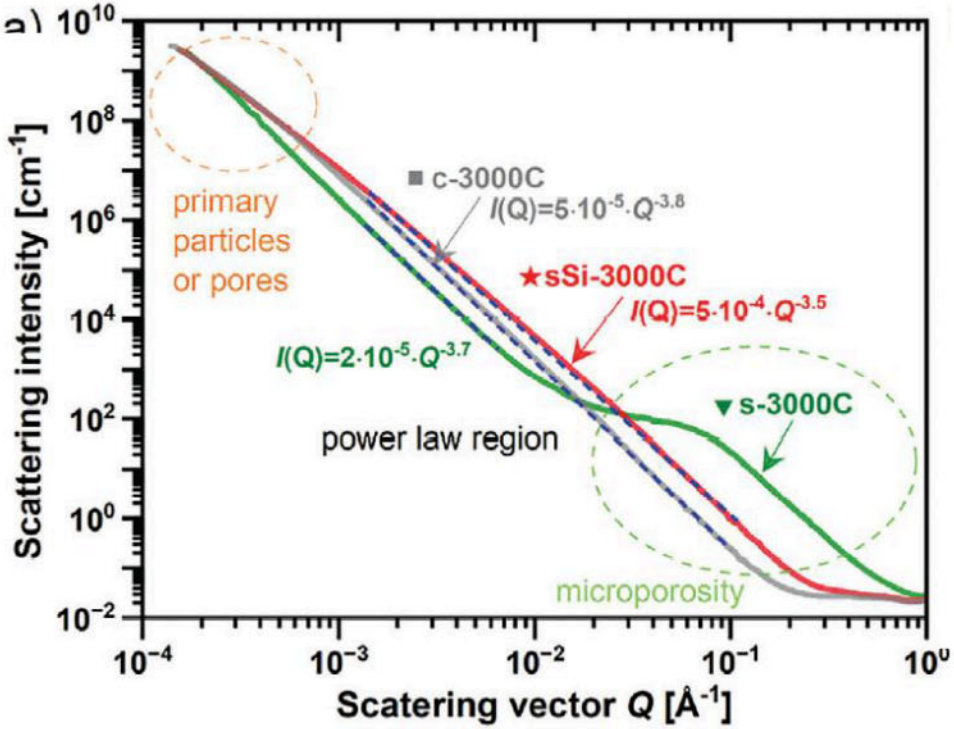
First published: 31 July 2024 | https://doi.org/10.1002/adfm.202410409 | Citations: 8

Production of graphite from sucrose

synchrotron X-ray diffraction:



synchrotron small-angle X-ray scattering:



c-3000C, s-3000C, sSi-3000C – pure coke, pure cellulose, cellulose+Si, all heat-treated at 3000°C

Current research directions of catalytic graphitization

and how neutron research at the ESS can help us

Challenges

- decreasing the graphitization degree < 2000°C
- replacing transition metal catalysts by lighter metals
- in-situ studies of the graphitization catalysts' phases during the heat-treatment to explain the mechanism
- in-situ studies of the transformation of both the atomic scale order and porosity to find heat-treatment conditions feasible to the desired structue

EUROPEAN SPALLATION SOURCE

HEIMDAL

Hybrid Diffractometer

Opportunities at the ESS

Multi-length-scale neutron scattering instrument designed for studying advanced functional materials.

The instrument **combines high resolution or high speed thermal powder diffraction with Small-Angle Neutron Scattering (SANS).**

- Q-range coverage of up to 25 $Å^{-1}$ allowing PDF analysis of the carbon materials
- SANS coverage a broad length scale allowing muliscale porosity studies
- sample enviroment system in the temperature range up to 2000 K allowing *in-situ* investigations during the graphitization process
- neutrons more sensitive than X-rays to detect light elements, which will be studies as potential graphitization catalysts