Why some carbons may or may not graphitize? Interpreting graphitization data with a phenomenological model inspired from thermodynamics.

Ouzilleau, Philippe[1], Gheribi, Aïmen E.[1], Chartrand, Patrice[1], Gervais, Soucy[2], Monthioux, Marc[3]

Presenting author's e-mail: philippe.ouzilleau@polymtl.ca

[1] *Polytechnique Montreal, Canada*
[2]*Université de Sherbrooke, Canada*
[3]*Université de Toulouse, France*

ABSTRACT TEXT

Not all carbons graphitize in equal measure. Some develop (following heat treatment) a structure which approaches the one of perfect graphite (graphitizable carbons), while others will do not (non-graphitizable carbons). The present work develops a phenomenological model for the conceptual understanding of graphitizability (capacity to graphitize). To support this model, a mathematical formalism, partially inspired from thermodynamics, is proposed to calculate the Ultimate Graphitizability (ηg) of some graphitizable and non-graphitizable carbon materials. ηg is the average interlayer spacing (d_{002}) of a graphenic carbon following graphitization at ~3400 K. η_g can be estimated assuming a topological graphitization mechanism operating between ~1700 K and ~3400 K. Two independent variables define η_g: $d_{002}(T_\alpha)$ and $d_{002}(T_\beta)$. T_α and T_β are arbitrarily selected temperatures between 1700K and 2550 K (the graphitization threshold). In order to better understand the parameters affecting $d_{002}(T_\alpha)$ and $d_{002}(T_\beta)$, new carbonization/graphitization experimental results are presented. These suggest that $d_{002}(T_\alpha)$ and $d_{002}(T_\beta)$ are correlated to the oxygen/hydrogen composition ratio and the relative mesoscale crystallite orientation of some graphitizable carbons following the end of primary carbonization.