o.m7.p3 **Structural studies of non-graphitized cokes (experiment and modelization)**. I. Rannou, *Centre de Recherche sur la Matière Divisée ; UMR Université d'Orléans-CNRS ; 1B rue de la Férollerie, 45071 Orléans Cedex 02, France.*
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This study will take place in a general comparison of structural informations obtained by different techniques about structure and microtexture of a serie of non graphitized microporous cokes. Raman spectroscopy and transmission electron microscopy have been or will be performed as described for amorphous-like carbons[1].

Structural study by X-ray diffraction is presented here. Patterns have been recorded for seven samples ; three saccharose cokes heat treated at 400, 1000 and 2800°C ; two reticulated vitreous carbons heat treated at 2200 and 2800°C and two laser pyrolysis based carbon (from pyrolysis of ethylene – M.Cauchetier and N.Herlin, CEA, Saclay, France) raw and heat treated at 2800°C. All of these samples are non graphitized even treated at high temperature.

The experimental device is a curved position sensitive detector. Patterns are registered with the $Mo_{K\alpha 1}$ (λ= 0.70926 Å) from s= 0.001 $Å^{-1}$ to 1.400 $Å^{-1}$ and corrected from capillary contribution and Compton diffusion.

First attempts of modelisation of 00l reflections are presented here. Modelisation is an ab-initio calculation and calculated patterns are compared to experimental ones. Model described elsewhere[2] take into account the mean interlayer spacing d_{002} (from one to three of them with statistical parameters permitting to describe interstratification phenomenon), the mean square deviation of the distances, the stacked graphene layers mean number and a statistical distribution around this mean size. We decided to modelize the vitreous carbons at first, as it is known to have no graphitized part even at 2800°C, unlike saccharose cokes. Calculations showed a displacement of the maximum of the 002 reflection as a function of the mean layer number, as well as the mean square deviation of the distances. This could explain the discrepancy between mean d_{002} obtained by X-ray and image processing on TEM photographs. For 2200°C glassy carbon, interstratification model permitted to describe the 00l row by contribution of graphene layer stackings with d_{002} = 3.42 Å and defects, which could be described as ultramicroporosity visible on TEM photographs, constituted by two layers separated by a 5 Å mean distance with a large mean square deviation. The mean layer number is 6.5. Others modelisations, as well as hk bands calculation, are in progress.

[1] J.N.Rouzaud, C.Clinard, A.Galvez and J.M .Bény : « Structural study of amorphous-like carbons », Extended Astracts Eurocarbon ; 1998, pp.763-764.
[2] V.A.Drits and C.Tchoubar: X-Ray Diffraction by Disordered Lamellar Structures, Springer-Verlag (Berlin Heidelberg 1990)