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DISTINCTION OF POLISHED AND UNPOLISHED SP^2 CARBONS VIA PRINCIPAL COMPONENT ANALYSIS

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We have earlier shown [1] that mechanical polishing of graphite-like structures leads to the unpredictable increase in the defect-conducted (D) band (~1350 cm^{-1}) in their Raman spectra, whereas the G band (~1580 cm^{-1}) interpreted as an intrinsic characteristic of these materials remains visually unchanged. In this respect, special attention is paid to the characterization of polished carbon materials via Raman mapping that enables one to scan the area of interest within the sample surface and to evaluate the effect of polishing at the structural level. Data collected during the mapping can be processed via a simple analysis of spectroscopic parameters (intensity, width, and peak position) or through the multivariative statistical methods (principal component analysis). According to various studies [2-4], the latter has been widely used in the last years due to its simplicity and the possibility to substantially reduce the processing time, which is especially convenient when working with huge-volume data composed of thousands of spectra.

In this work the principal component analysis (PCA) was applied to distinguish polished and unpolished sp^2 carbons by the example of anthracene-based cokes. For this purpose the Raman spectra were acquired on samples pyrolized at temperatures of 1600, 2000 and 2900ºC and exposed to polishing. According to the preliminary results, the difference between polished and unpolished specimens becomes more obvious as the temperature of pyrolysis increases (above 2000ºC), leading to a pronounced distinction at a temperature of 2900ºC. Thus, the method allows one to distinguish the specimens whose structural differences are due to pyrolysis or polishing.

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