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X-Ray diffraction analysis of coal and related materials

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Coal is a fossil fuel and is the altered remains of prehistoric vegetation that originally accumulated in swamps and peat blogs. The energy that we get from coal today is the energy that plants absorbed from the sun millions of years ago. Coal is still one of the major energy sources. It is used as a reducing agent in the metallurgical industry, in the cement industry coal is a source of energy and it is still used in power generation.
X-ray diffraction (XRD) studies can confirm the presence of mineral constituents as indicated by microscopic investigations within raw coal and an approximation of the amount of carbonateous matter can be made. In addition X-ray diffraction can also be used to characterize the crystal structure of graphitic carbons. During the graphitization process (heat treatment) the degree of ordering within the crystal structure increases. This is reflected in changes within the crystal structure and influences the performance characteristics i.e. electrical resistivity and conduction, coefficient of thermal expansion.
Graphitic carbons can be characterized in 3 dimensions. The interplanar spacing d002 between individual graphene layers (3.345Å for pure graphite), can be used as an indicator of the degree of graphitization, which is a function of heat treatment. The intensity and sharpness of the peaks give an indication of the degree of order compared to that of a pure graphite crystal, reflected by the crystallite size. This can be calculated using the crystallite size function as part of Rietveld analysis.
The graphene layer stacking height, Lc, (determined from the FWHM of the 00l diffraction lines) as well as the lateral diameter (crystallite width), La; determined by hk0 diffraction lines, can be calculated using the Scherrer equation.

Preliminary results of X-Ray diffraction and Computed Tomography studies on Coal, Char and Coke using PANalytical Empyrean X-Ray Diffraction equipment will be presented.