The significance of some structural parameters obtained by X-ray methods for graphitic and non-graphitic carbons.

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This paper is a critical review of the significance of the terms "non-organized carbon", "single layers", "disoriented layers" and related parameters.

It is shown that the interpretation of an excess of the overall diffuse scattering in terms of domains of carbon atoms with a gas-like distribution ("non-organized carbon", Franklin, 1950) cannot be justified. The diffuse scattering is more likely to be due to imperfections, especially vacancies, in the structure of the graphitic layers and in some cases to the presence of "foreign" atoms. No convincing evidence has been found so far for the existence of other types of structure than the hexagonal layer structure.

The evaluation of the excess of diffuse scattering concentrated on the (00)-rod in terms of "single layers" (Franklin, 1950) cannot be considered as the only possible. A similar effect is produced by an imperfect stacking of layers as well as by a variation of size and perfection of the layers in a given stack. The interpretation of this effect should thus be considered with care.

The model of a random sequence of "disoriented layers" and "oriented layers" proposed for the structure of graphitic carbons (Franklin 1951) is inconsistent with the observed variation of the interlayer spacing with the amount of "disoriented layers" p. If the sequence is random, the relation between p and the interlayer spacing should be linear. The model proposed by Méring and Maire (1957, 1960) avoids this difficulty by assuming that the mutual orientation of adjacent layers is hindered by the presence of interstitial atoms linked very closely to the surface of a layer. This model is fairly consistent with the observed data as far as the relation between the disorientation of the layers and the average interlayer spacing is concerned; it is, however, somewhat difficult to accept the hypothesis of the peculiar kind of interstitial atoms necessary to explain the relation observed.

An alternative model has been proposed recently (Ruland, 1965) in which the assumption is made that the imperfect stacking of the layers is predominantly due to translational deviations from the ideal positions. An interpretation of the X-ray data in terms of such a model has revealed a linear relation between the mean-square values of the translational deviations parallel to the layer planes and the average interlayer spacing. The existence of this relation seems to indicate that the distances of closest approach between layers which are shifted parallel to each other form a paraboloid of rotation with the ideal position as the apex. With this assumption, which appears to be reasonable for small deviations from the ideal position, it can be shown that the linear relation between the mean-square shift and the average interlayer spacing will be produced by any type of shift distribution, i.e. this relation is independent of the actual form of the shift distribution.

It seems to be very likely that the translational deviations are due to a non-planarity of the layers caused by small interstitial layers, vacancies and dislocations. A small bend in a stack of layers can produce an appreciable shift between adjacent layers over a considerable part of the layer planes. This can also account for the difference between the measured La and the actual extent of the layer surface. Considering all the implications of the proposed model one finds that it provides a more acceptable explanation of the structural changes occurring during graphitization than the models favored up to now.

References :

R.E. Franklin (1950), Acta Cryst. 3, 107.
R.E. Franklin (1951), Acta Cryst. 4, 253.
J. Maire and J. Méring (1958), Industrial Carbon and Graphite Society of Chemical Industry London, p. 204.
J. Méring and J. Maire (1960), J. Chim. Phys. 57, 803.