

Acta Cryst. (1965). 18, 578

A model for the structure of 'glassy carbon'. By J. KAKINOKI, *Department of Physics, Faculty of Science, Osaka City University, Sugimoto-cho, Sumiyoshi-ku, Osaka, Japan*

(Received 11 August 1964 and in revised form 7 September 1964)

So-called 'glassy carbon' is characterized by the following physical properties: its hardness is very high; it stands high temperature heat treatments and cannot easily be graphitized by usual heat treatments; it shows, however, a good electrical conductivity although the conductivity is less than that of graphite.

Noda & Inagaki (1964) and Furukawa (1964) suggested that the three-dimensional network of carbon atoms in glassy carbon is composed of tetrahedral parts (*T*-parts) and graphitic parts (*G*-parts) as shown schematically in Fig. 1. The first neighbour distance in

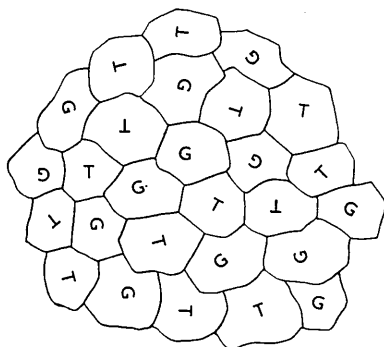


Fig. 1. The structural model for glassy carbon proposed by Noda & Inagaki (1964) and Furukawa (1964). *T* means a tetrahedral part in which the first neighbour distance is 1.55 Å and *G* a graphitic part in which the first neighbour distance is 1.42 Å.

T-parts is 1.55 Å corresponding to a normal covalent single bond found around the tetrahedral carbon, while that in *G*-parts is 1.42 Å as found in graphite. They came to these conclusions from the analysis of the first peak in the radial distribution curve obtained from X-ray intensity data.

Such a model for glassy carbon, however, is quite similar to, or, rather the same as, that proposed by Kakinoki, Katada, Hanawa & Ino (1960) on thin films of evaporated carbon for which the size of individual parts was estimated to be 10–20 Å. These films were found to be graphitized gradually by usual heat treatments at temperatures lower than 1100–1200 °C (Kakinoki, Katada & Hanawa, 1960), in contrast to glassy carbon which can be graphitized only by heat treatments at temperatures as high as 2500–3000 °C (Noda & Inagaki, 1964). Therefore, the model for either of the two substances should be modified in order to explain their difference in graphitization.

One of the possibilities for modifying the model for the glassy carbon is to put oxygen atoms between *T*- and *T*-, *T*- and *G*-, and *G*- and *G*-parts along their boundaries as shown in Fig. 2. The assumption of oxygen

bridges seems to be in accord with the result of Yamada (1964) that the oxygen content in the glassy carbon is about 5–6 wt%. One may conceive that such oxygen bridges hinder the glassy carbon from graphitization on usual heat treatments at temperatures lower than 1100–1200 °C but are destroyed by the heat treatments at temperatures as high as 2500–3000 °C.

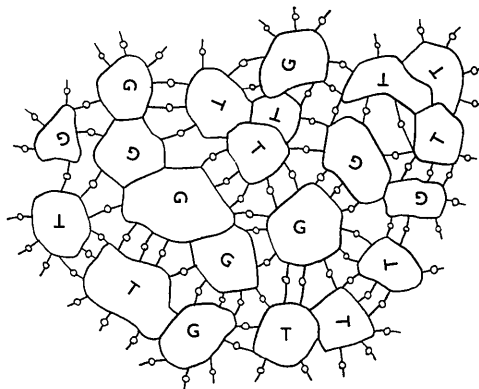


Fig. 2. A proposed model for the structure of glassy carbon. *T* tetrahedral part; *G* graphite part; —o— oxygen bridge.

Shimada & Kikuchi (1964) reported that some samples of glassy carbon showed a slight increase in electrical conductivity at an early stage of bombardment by neutrons. Such a fact may be understood by the new model if we assume that the oxygen bridges are partly destroyed by the bombardment. The removal of oxygen bridges will make it possible for graphitization to proceed, and will lead to the increase in electrical conductivity.

Although, in the new model, oxygen atoms are put between individual parts, some of them may also be present inside the *T*-parts.

References

- FURUKAWA, K. (1964). *Nihon Kessho Gakkaishi*, **6**, 101 (in Japanese).
 KAKINOKI, J., KATADA, K. & HANAWA, T. (1960). *Acta Cryst.* **13**, 448.
 KAKINOKI, J., KATADA, K., HANAWA, T. & INO, T. (1960). *Acta Cryst.* **13**, 171.
 NODA, T. & INAGAKI, M. (1964). Unpublished. Reported at the Symposium on Carbon, Tokyo, July, 1964.
 SHIMADA, T. & KIKUCHI, T. (1964). Unpublished. Reported at the Symposium on Carbon, Tokyo, July, 1964.
 YAMADA, S. (1964). Unpublished. Reported at an informal meeting in the Symposium on Carbon, Tokyo, July, 1964.