AGGLOMERATION MODEL OF CARBON NANOSTRUCTURES[*)]

R. Kerner

Laboratoire de Physique Théorique de la Matière Condensée, Université Pierre et Marie Curie (Paris-VI), Paris, France.

We present a model of agglomeration of carbon clusters from small molecular fragments torn out from graphite at high temperature. The bond-bending energies of such clusters, especially those containing pentagonal and hexagonal rings, are taken into account and used in the Boltzmann factors corresponding to each step of agglomeration. Probabilities of clusters with growing number of carbon atoms are calculated. The principles of self-similarity and least free energy can be then applied. The self-similarity requirement means that the growing clusters tend to conserve their local curvature; the least free energy means minimizing the bond-bending contributions.

These two hypotheses provide a good insight into the statistics of various types of clusters depending also on the temperature. The relative yield of various fullerenes and graphene fragments can be then estimated.

[*)] This work develops the ideas exposed in my recent book R.Kerner, "Models of Agglomeration and Glass Transition", Imperial College Press 2007