

Spatial atomic and electronic structures of graphene, diamond, graphite and fullerene

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When the spatial atomic and electronic structures of graphene, diamond, graphite and fullerene were formed with using the mechanism of pairwise interpenetration of atoms [1], ideas about hibredization of s and p electrons, covalent and σ and π bonds, about potentials and other did not used absolutely.

The atom model with well-defined sizes of inner electrons area and external electrons shell [2, 3] correspond to quantum rules according to which the electronic structure of atom is shaped.

When atoms approach their shells can interpenetrate, but in according Pauli's exclusion principle only pairwise.

Values of interatomic forces which form the spatial atomic structures were calculated without fitting and utilize potentials.

The sizes of interpenetrated carbon atoms were calculated from the condition of balance of interatomic forces in diamond and graphene.

It is shown that the distance between basic planes of graphite (between graphenes) which is calculated with using of mechanism pair interpenetrating and presence of carbon atoms between graphenes (0.3357nm) is very close to those known from experiments (0.3354nm).

The schemes of self-organization of atoms of carbon into pentagons necessary for forming fullerenes are shown.

The spatial electronic structures are shaped with areas of a pairwise interpenetration.

Each atom in graphene has only three areas of pair interpenetrating. Electronic density of them may be two times more than in shell of the free atoms and four times more than in univalent metals. The centers of them form triangle with equal sides.

Each atom in diamond has four atoms in the first coordination sphere. Accordingly each atom in diamond has four areas of pair interpenetrating. They less than at graphene and the distance between them and nucleuses more than in graphene; their centers form right tetrahedron.

Thus the spatial electronic structures explain why graphene is more stable than metals and diamond and helps to analyse properties of materials.

- [1] Titorov D.B Sixth international conference «Single crystal growth and heat & mass transfer». Proceedings 3, 646 (2005), Obninsk, Russia (in Russian).
- [2] Titorov D.B. *Kristallografiya* **1**, 25 (2001). [*Crystallography Reports* **1**, 19 (2001)].
- [3] D.B. Titorov, *Poverkhnost'*. **6**, 100 (2003).