

# ENERGY OF DIAMOND AND GRAPHITE NANOPARTICLES

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## Introduction

The determination of diamond and graphite crystal energy in wide range of particle sizes is necessary to solve the problem of nucleation, growth and phase transition of these phases. The low pressure diamond synthesis by CVD [1] and by decomposition by laser of ethylene [2] and a founding of diamond particles in meteorites [3] indicates the homogeneous nucleation. But it is a question whether diamond nanoparticles are stable in comparison with graphite ones since the low pressure diamond formation occurs in metastable for the diamond bulk crystal pressure - temperature range. We can suppose a size-related stabilization of diamond. The effect of stabilization of a phase that is unstable in the bulk crystal state has been established experimentally for many substances and explained by the energy advantage caused by small particle sizes [4,5]. The aim of the present work is to create models and methods to compute the energy for various particle sizes and answer the question about the possibility of stabilization of diamond at low pressure caused by small particle sizes.

## Models

The models of crystal charge lattices have been determined to compute the lattice energy

by summation of pair potentials acting between elements (ions, electrons) of the lattices. The diamond lattice is presented by excess negative bond charges and positive ions. Beside of this traditional model we also consider a model that does not contain of atoms located at crystal apices and edges. The non-traditional model is more favorable energetically because of the larger value of bonds per atom in this model. Graphite charge lattice consists of ion-electron hexagonal nets and conduction electrons located between the nets. Conduction electrons in the graphite model provide the stable structure since the attraction between the conduction electrons and hexagonal nets compensates the repulsive forces acting between the nets.

Models of octagonal clusters of carbon atoms have been created to consider a mechanism of nucleation of diamond. The ten atomic octagonal carbon cluster can be transformed to the ten atomic diamond cluster forming the diamond crystal structure (Figure 1) by turn of quartets of atoms (designated by dashed triangles) relatively to sides of the square so that the each of atoms 3 becomes the common of two opposite quartets and is bonded with two atoms of type 1. This transition is favorable

energetically because of two additional covalent bonds in diamond cluster in comparison with the octagonal one.

The octagonal clusters consist of the same fragments of atoms as graphite hexagonal nets. But the difference is that diamond crystals are generated from octagons of atoms and graphite ones are formed from hexagons.

Results

Intersection of free energy dependences on particle sizes of diamond and graphite shows that diamond nanoparticles are more stable than graphite ones until point of intersection  $L_0$ . So the size  $L_0$  is the boundary of stability regions of diamond and graphite which depends on temperature. The established

values of  $L_0$  are: 10 nm at room temperature, 6 nm at 525°C, 4.8 nm at 800°C, 4.3 nm at 1100°C.

The computation results show that the diamond model that does not contain one-bonded atoms is energetically more favorable than the traditional diamond model.

References

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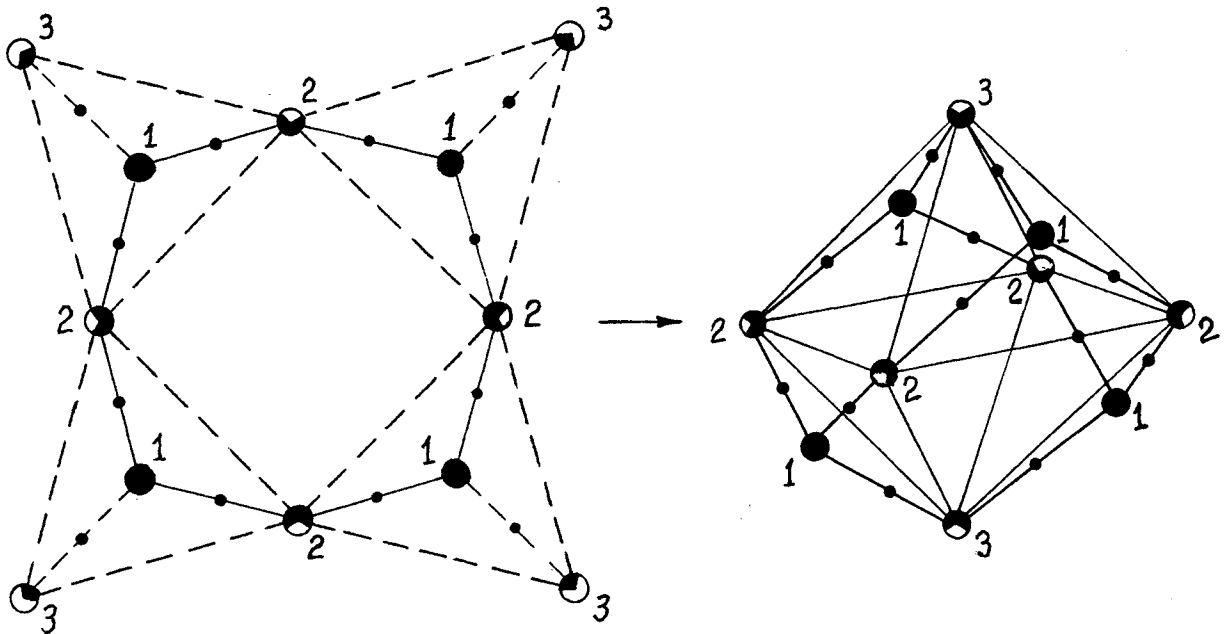


Figure 1 - Mechanism of nucleation of diamond: transformation of the octagonal carbon cluster (left) to the ten atomic diamond cluster (right); small black circles are the covalent bond charges