

Nanocomposites and nanomaterials

Ab-initio investigation of Fe₃AlC nanolayers as substrate for diamond growth

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Fe₃AlC compound (K-phase) is a diamond formation catalyst [1, 2, 3]. Since the difference of unit cell parameters of K-phase and diamond is about 5%, it can act as a substrate for epitaxial growth of diamond.

To confirm this hypothesis calculations of electronic structure of supercells consisting of several nanolayers of ordinary stoichiometric and of modified K-phase cells, on which epitaxial growth is actually happening, were carried out.

Minimal necessary thickness of substrate was found to be 4 layers of unit cells of K-phase. Substrate with smaller number of unit cells needed inflow of heat for its formation and was unstable because its Fermi level fell on anti-bonding area of density of states graph.

Densities of states of carbon in modified K-phase and in diamond had similar features, namely: overlapping of maximums of p-electron's densities; width of gap (in diamond) and pseudogap (in K-phase). At the same time because of influence of iron carbon in modified K-phase lacked any s-p hybridization and s-states were shifted towards higher energies. In calculations with additional layer of diamond s-p hybridization emerged, but s-states were still shifted.

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2. *Putyatin A., Davydov V., Nesterenko S.* High temperature interactions in the Fe-Al-C system at 6 GPa pressure // *J of Alloys & Comp.*-1992.-**179**, N 1-2.-P.165-175.
3. *Andrushenko V. et al.* // K-phase and diamond // *Met. Phys. Adv. Tech.*-2009.-**31**, N 9.-P.1257-1269.