Nanostructured surfaces

Substantiation of epitaxial growth of diamond crystals on the surface of the carbide $Fe_3AlC_{0.66}$ phase

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There were calculated the parameters of unit cells, the enthalpy of formation of the Fe_3AlC, $Fe_{3.125}Al_{0.825}C_{0.5}$, $Fe_{3.5}Al_{0.5}C_{0.5}$, $Fe_{3.5}Al_{0.5}C$, $Fe_3Al_{0.66}C_{0.66}$, $Fe_3AlC_{0.66}$ unit cells and identified the crystallographic planes, on which was possible the epitaxial growth of diamond phase, using density-functional theory as implemented in WIEN2k package.

The possibility of epitaxial growth of diamond crystals on $Fe_3AlC_{0.66}$ (K-phase) substrate was shown. (200) plane was established to be the most suitable plane for the diamond growth having four carbon atoms arranged in a square and a vacancy in the center which can be occupied by carbon during thermobaric treatment. Distances between carbon atoms in the plane differ by only 5% from distances between carbon atoms of a diamond. The electron structure and energetic parameters of a substrate was investigated. It was shown that the substrate with at least four intermediate layers of K-phase exhibits signs of stability such as negative enthalpy of formation and Fermi level falling on minimum of densities of states.