

Calculation of electronic properties of graphene grown on faceted SiC surface as on optimal matrix for the graphene synthesis

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Abstract

It is known that one of the challenges of the digital graphene-based electronics is a difficulty of creating the bandgap ΔE_g in the graphene. Almost none of the ways to generate ΔE_g (graphene nanoribbons NR, stretched graphene, chemical fictionalization, partial reduction of the graphene oxide GO) cannot be considered as satisfactory for the industrial production of graphene.

The arising difficulties are connected here with obtaining a predictable quantity of ΔE_g and, at the same time, with high and predictable quantity of the carrier mobility within a particular technology.

Having an experience in the research of SiC, the authors offer for SiC-Graphene based devices the concept of the graphene growth on accordingly prepared system of SiC faces ("faceted SiC surface"), calculated by some algorithm. This algorithm offers a structure of SiC complicated surface, optimized with using the quantum chemistry methods, analytic methods and non-equilibrium thermodynamics apparatus..

A convenient apparatus for analytical approach to the problem is the Green's functions method in nodal representation, under which the Green's functions matrix elements are looked for in Vannie's function brackets¹.

In this formalism the known linear dispersion law for the infinitive graphene turns to trivial exercise for the Microelectronics Chair students².

The method was mastered by us, then, on several testing calculations: dispersion laws and DOS calculations for the graphene nanoribbons of different width and chirality, and for various graphene superstructures ($(\sqrt{3} \times \sqrt{3})R30^0$, $(\sqrt{3} \times \sqrt{3})R30^0$ etc.).

I plan to tell about the results of the Green's function application to the electron properties calculation for some faceted SiC surfaces.

Within the analytical approach the bandwidth $\Delta E_g \neq 0$ is induced by three factors (Fig.1): by the substrate, by the graphene surface curvature on the faceting-generated SiC protrusions (i.e., the features of the surface), by the superstructure, generated by the system of protrusions.. So, in the zero approximation the ΔE_g is giveb by one dimension quantity (e.g., the protrusion height) and by aspect ratio.

In more realistic calculation (density function theory DFT approach) the faceting details and the indexes of the arisen crystallographic planes is taken into account.

In my report I will show the results of the electronic properties calculation for the graphene, built on such faceted surface.

The principal result is that ΔE_g , determined by the second and by the third factors, can reach 0.5 – 0.7 eV even without immediate contribution of the surface to be substantial for using the graphene on such faceted SiC surface in digital electronics devices.

We succeeded to show, then, that the graphene islands nucleation over the SiC surface protrusions leads to an additional freedom in aligning the island's edges and their mutual orientation at the moment of their stacking. Herewith, the instabilities that generate "terrace –strip" structures of the resulting graphene, are compensate. So, an opportunity arises to synthesize practically ideal graphene with minimal reduction in mobility as compared with the ideally smooth graphene.

The detailed analysis of all such opportunities is a subject of our further research.

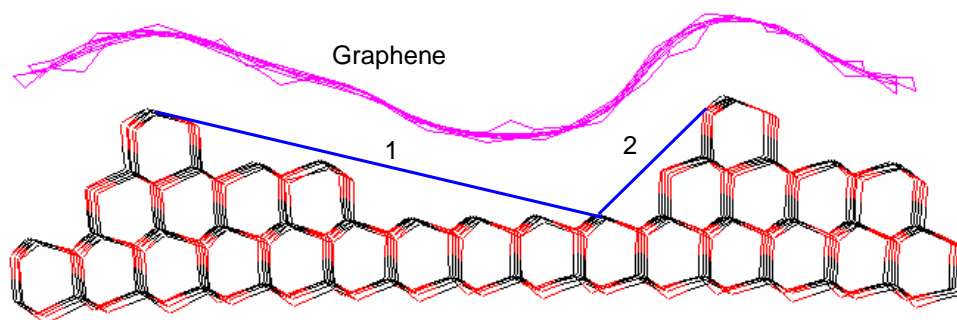


Fig.1. Faceted surface of 2H – SiC and the graphene grown on this surface
The planes 1 and 2 are $\{11\bar{2}7\}$ and $\{11\bar{2}2\}$.

References

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