Calculations of faceted SiC surfaces for production of high-quality graphene with non-zero bandgap

N.I.Alekseyev, V.V.Luchinin

St.-Petersburg ElectroTechnical University LETI.

NIAlekseyev@yandex.ru

The problem of creating the bandgap ΔE_g in graphene is not solved until now qualitatively. None of the methods such as the graphene nanoribbons, stretched graphene, chemical functionalization etc. are not effective enough for the industrial production of the digital electronics devices based on the graphene

We consider the faceted SiC-surfaces in the course of their subsequent sublimation as the graphene source. Such surfaces are really formed when a vicinal SiC face is chemically etched or annealed in H_2. The system of the steps which is formed in this process, depends on the surface preparation technology and can be different.

Nevertheless, we put the problem to calculate the band structure for the surface whose faceting is preset in arbitrary way. This approach allows us to adjust the chart of te experiments to the positive result of calculation instead of trying to calculate the technological details of the real faceting.

The method of the Green's functions in nodal representation was selected as the mean for analytical approach to the problem. In this approach the matrix elements of the Green's functions are sought in the Vannier's function brackets. The whole dispersion low calculation is confined to the linear algebraic system.

We examined two types of the faceted surfaces: the surfaces with sharp- and with smooth fractures in the transition regions from one faceting surface fragment to the adjacent fragment.

In the first case the distortion of the flat graphene structure is wholly concentrated within the limits of one row of the graphene cells. In the second case the distortion on a bend changes fluently, so that the curvature of the envelope surface of SiC has the order of the van-der-Waalse bond lenght.

The calculations results for the first case are predictable. With the small faceting period the ΔE_g quantity can be high. However, to realize such structure in practice is as difficult as to prepare a narrow graphene nanoribbon. Besises that, even with ideal periodicity of the structure the "periods of brightening" of the structure exist, under which $\Delta E_g=0$ even with the small spatial periods of the faceting.

On the contrary, the problem of creating smooth transitions correlates in practice with that of providing the long- and perfect period (not quasiperiod) of the faceted structure. The calculation shows that with sufficient length of the rounding arc $\Delta E_g \neq 0$ and high enough regardless to the period lenght.

The possibilities of technological realizations of this approach are discussed