Graphene elastic moduli in the Keating model

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Now it is generally accepted that the single-layer graphene (SLG) has the most outstanding elastic properties. Hence, the growing intereSt in the problem of the graphene elasticity is not surprising. There are a number of different methods permit one to calculate the elastic moduli for the SLG. Here we demonstrate that the use of well known Keating model permits one to find the analytical expressions for the second- and third-order elastic constants [1,2], which are the direct characteristics of the harmonic and unharmonic sample response to the external mechanical perturbation.

We begin with the expansion of the SLG potential energy in the series using the Keating parameter $(\vec{R}_{0i}\vec{R}_{0j} - \vec{r}_{0i}\vec{r}_{oj})$, where $\vec{R}_{0i}$ 00 $(\vec{r}_{0i})$ is the radius-vector from the reference atom 0 to the deformed (undeformed) position of the nearest-neighbor atom i = 1, 2, 3. Now we take into account only the harmonic central and noncentral terms, which are proportional to $\alpha(\vec{R}_{0i}^2 - \vec{r}_{0i}^2)^2$ and $\beta(\vec{R}_{0i}\vec{R}_{0j} - \vec{r}_{0i}\vec{r}_{oj})^2$ correspondingly, and the anharmonic central term $\propto \gamma(\vec{R}_{0i}^2 - \vec{r}_{0i}^2)^3$. Thus, we arrive at the three force-constant model.

Using the standard procedure, we find two second-order elastic constants: $c_{11} = (A+B)/(3)^{1/2}$, $c_{12} = (A-B)/(3)^{1/2}$, where $A = 4\alpha + \beta$, $B = 18\alpha\beta / A$. For and three third-order elastic constants we get: $c_{111} = C[(1.5-\zeta)^3 + 4\zeta^3]$, $c_{222} = C[(0.5+\zeta)^3 + 4(1-\zeta)^3]$, $c_{112} = C[(1.5-\zeta)^2(0.5+\zeta) + 4\zeta^2(1-\zeta)]$, where the Kleinman internal displacement parameter $\zeta = (2\alpha - \beta)/A$ and $C = 16\gamma/(3)^{1/2}$.

It is worthy to note here that graphene is isotropic only in the harmonic approximation, while the anharmonicity introduces some difference in its response to the deformation along the zigzag and armchair directions. This effect has been also analyzed by the consideration of the hydrostatic pressure effect on the second-order elastic constants.

[1] S.Yu. Davydov, *Phys. Solid State* **52**, 810 (2010).
[2] S.Yu. Davydov, *Phys. Solid State* **53**, 665 (2011).