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Graphene: a nonlinear two-dimensional spring network

Graphene is one of the strongest materials in the world, which has an elastic modulus of 1.0 TPa and an intrinsic strength of 130 GPa (about 100 times of steel). Due to its nanoscale thickness, Graphene can be considered as one of two dimensional (2D) materials. Actually, graphene includes a layer of carbon atoms connected by the chemical bonds, the mechanical behavior of which is essentially similar as that of nonlinear springs, and thus, graphene becomes a hexagonally connected spring network. When graphene is under tension, the springs are stretched; when graphene is under compression, the springs are contracted. Thus, the mechanical properties of graphene depend upon the spring stiffness.

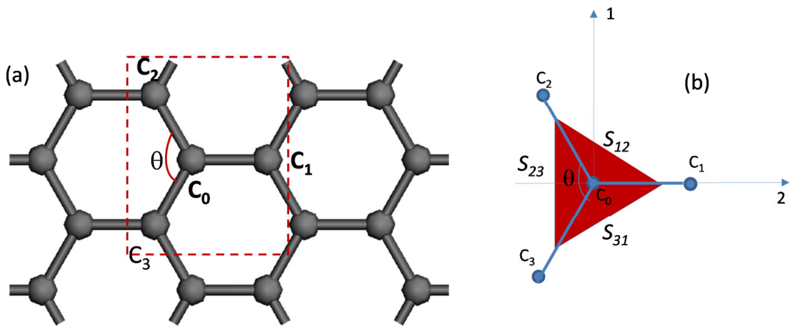

Fig. 1. The represent unit cell of graphene (a) and its simplified represent unit cell of 2D nonlinear spring network (b). C_0C_1, C_0C_2, C_0C_3 are tensile springs and S12, S23 and S31 are compressive springs in (b); and θ is the C-C-C angle in (a) as well the angle between springs in (b).

As a matter of fact, graphene is a more complicated spring network, which includes two types of springs: (I) tensile springs, which only resist the tensile load and cannot support the compressive load (shown as blue color in Figure 1); (II) compressive springs, which only support the compressive load but cannot resist the tensile load. The tensile springs are located at the positions of C-C bonds, which are shows as the sides of hexagons; the compressive springs are spiral type, which resist the decrease in C-C-C angle (θ) ($\theta = 120°$ for the undeformed graphene). Actually, the compressive spiral spring can be easily understood as placing an rubber block (in a triangular shape) in the red area of Figure 1, which makes the decrease of θ highly difficulty but has no effect on the increase of θ.

The stiffness of the tensile-spring k is not a constant, and the spring force (f) can be described as follows:

$$f = k\lambda = \left(A + B\lambda + C\lambda^2\right)\lambda$$

where λ is the stretching ratio of spring ($\lambda = \Delta L/L$, the ratio of the length change of spring to the original length), and A, B and C are constants, in which $A > 0$, $B < 0$ and $C > 0$ (the highest order term's coefficient C is much lower than B). Thus, with the increase of the stretching ratio of spring λ, k decreases. However, the spring force f still increases with λ since the contribution of the increase of λ to f is higher than that caused by the decrease of k, and thus, the tensile-spring can resist the tensile load. When the aforementioned two contributions are equal with each other, the maximum load can be supported by the spring is reached; with continually increasing λ, f decreases but the spring still can support load since k is still larger than zero; the spring is failed when k =0. Therefore, graphene does not show the brittle behavior (it will be failed at the postion with the maximum load) but displays a ductile behavior.

In addition, the stiffness of spiral spring is much higher than that of tensile spring, and thus, the angle between springs (θ) is highly difficult to be changed and the deformation of spring network under the tensile load is undergone by the increase of spring length; for the hexagon network, the spring with a smaller angle with respect to the loading direction will have a larger extension when the angle θ has no noticeable change, which can be seen from Figure 1(a).

From the above analysis, it can be observed that the 2D nonlinear spring network can show the exactly same mechanical response of graphene under external load. Thus, from the mechanical aspect, graphene can be considered to a 2D nonlinear spring network.

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