YOUNG'S MODULUS FOR GRAPHITIC MONO-ATOMIC LAYER (GRAPHENE)

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Recent discovery of perfect two-dimensional crystals [1] revealed a new way for obtaining the strong materials. The conventional wisdom dictates that the rise in a material hardness can be achieved by the increase in the internal energy density by transition to the high mass density phase state with shorter bond length under high pressure-temperature conditions. In 2D crystals the transition to high modulus state occurs in seemingly counter-intuitive way by the diminishing the effective volume per atom due to decrease in the layer thickness down to atomic level, the natural limit of compressibility. It appeared that stiffness of graphene is higher than that of diamond [2]. More than decade ago it was demonstrated that the Young modulus of graphitc monolayer exceeds that for bulk graphite [3]. Simultaneously the modulus of carbon nanotube then was obtained as that for the rolled-up monolayer in agreement with experiments [4].

In what follows the Young (bulk) modulus of a graphitic monolayer is derived from the semi-empirical inter-atomic pseudo-potential for covalently bounded 2D carbon with new experimental evidence taken into account [1,2]. The bulk modulus of a monolayer expresses in a general form through the cohesive energy and effective volume per atom. The extreme stiffness of a monolayer relates to the absence of defects, high cohesive energy and to the minimum effective volume per atom in 2D crystal. I also discuss how this approach applies to the mechanical properties of 2D crystals in general.

It is well known that the linear elasticity predicts well the elastic properties of fullerenes and carbon nanotubes in a good fit to MD calculations and experimental data. Here the modulus of a mono-atomic graphitic sheet is also calculated using the linear elasticity theory. In elasticity theory one can express the modulus through the thermodynamic parameters and the Poisson ratio. One can show that in deformation of a 2D monolayer the Poisson ratio is zero because an atom is incompressible under the force much smaller of atomic forces. Thus for 2D monolayer the homogenous (bulk) modulus, *K*, expresses through the internal energy, *U*, and volume of a system similar to [5] but with different coefficients as the following:

$$K = \frac{2V}{3}\left(\frac{\partial^2 U}{\partial V^2}\right)_{T=0} \quad (1)$$

Relation $K = Y/3$ now connects the bulk and the Young modulii in 2D layer. One can describe in-plane inter-atomic interactions by the simplified semi-empirical pseudo-potential [6] assuming the homogeneity in two dimensions:

$$\phi = Ae^{-\lambda_1 R} - Be^{-\lambda_2 R} \quad (2)$$

The potential (2) reproduces the most important parameters of 2D layer such as inter-atomic distance, R_0, and the binding (cohesive) energy, ε_b, in equilibrium through the condition $(\partial\phi/\partial R)_{R=R_0} = 0$. A molecular volume is presented in the form $V = V_0 N$, where $V_0 = hR_0^2$ is volume per atom, *N* is the number of atoms in a structure, R_0 is in-plane inter-atomic distance in equilibrium and *h* is the effective "thickness" of monolayer that should be extracted from experiment [2]. The total internal energy of a system in equilibrium is $U = \phi(R_0)N$. Now the Young's modulus of a single monolayer expresses through repulsive and attractive gradient

space scales of the potential, the cohesive energy and through the effective "thickness" of monolayer in the following form:

$$Y_{mono} = \frac{\lambda_1 \lambda_2 |\varepsilon_{bind}|}{2h} \quad (3)$$

The physical meaning of (3) is obvious: the Young modulus directly relates to the internal energy density in the characteristic atomic volume. The Young modulus for any 2D crystal with in-plane isotropic properties and known potential can be calculated by formula (3).

Let us apply formula (3) for calculation the Young modulus of graphene taking the following parameters for the potential: A = 1,753.438 eV, B = 452.2 eV, λ_1 = 3.488 Å^{-1} , λ_2 = 2.2 Å^{-1} [6] . Then the binding energy, ε_{bind} = - 7.56 eV is close to the experimentally measured value for graphite. Taking h ~ 2.5- 4 Å from [2] one can calculate the Young's modulus of a defectless mono-atomic graphite sheet, graphene, as Y_{mono} = (1.856-1.16 TPa). One can see that the minimum value is just a little bit higher than that for graphite, c_{11}=1.06 TPa in *a* direction while the maximum value exceeds that for diamond (0.9-1.25 TPa) [7].

One can see that the effective thickness of a monolayer is a crucial parameter defining the strength of 2D crystal. The covalent diameter of carbon of 1.54 Å perhaps gives the upper theoretical limit of the monolayer "thickness" and therefore upper limit for the Young modulus of 2D carbon of 3TPa. Hopefully future smart experiments allow the direct measurement of the graphine Young modulus.

References:

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