Comment on “Nanoindentation models and Young’s modulus of monolayer graphene: A molecular dynamics study” by X. Tan, J. Wu, K. Zhang, X. Peng, L. Sun, and J. Zhong [Appl. Phys. Lett. 102, 071908 (2013)]

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(Dated: 10 April 2017)

The interpretation of the measured load-deflection characteristics from spherical indentation tests on graphene has been a complex issue. In 2013, Tan et al. studied the nanoindentation of monolayer graphene by molecular dynamics simulations, and they found that the response of graphene to indentation is deflection dependent: in small deflection range, the response obeys the response of graphene to indentation is deflection dependent; in small deflection range, the response obeys the response of graphene to indentation is deflection dependent; in small deflection range, the response obeys

\[ F = \left[ \frac{9\pi}{16} \frac{E a}{q} \right] h (R/a)^{1/4} \delta^3 \] (1)

However, according to the sphere model used by Tan et al., the relationship between load and central deflection is as follows:

\[ F = q^2 E a^{-2} h (R/a)^{1/4} \delta^3 \] (2)

where \( q = 1/(0.15 - 0.16\nu^2) \). For monolayer graphene, \( \nu \) is assumed to be 0.165\(^1\)\(^-6\)\(^7\), and therefore, \( q \approx 0.98 \). From Eq. (1) and Eq. (2), it can be seen that without any explanation, the coefficient was changed from 9\(\pi/16 \approx 1.77 \) to \( q^2 \approx 0.94 \).

For monolayer graphene, \( h \) is often assumed to be 0.34 nm\(^1\)\(^6\)\(^-7\). Assuming that \( E = 1.05 \) TPa, the load-deflection curves based on Eq. (1) are plotted in Fig. 1(a), and the load-deflection curves based on Eq. (2) are plotted in Fig. 1(b). It can be seen that \( E = 1.05 \) TPa can be obtained based on the “modified” sphere model, but not on the actual sphere model developed by Begley and Mackin\(^4\). In fact, if \( E = 0.56 \) TPa is assumed, the load-deflection curves obtained from the sphere model match the curves obtained from molecular dynamics simulations very well, as shown in Fig. 1(c). In other words, the sphere model developed by Begley and Mackin predicts that \( E = 0.56 \) TPa, much lower than the experimental results\(^8\)\(^-10\). Since the method proposed by Tan et al. has been widely cited\(^8\)\(^-10\), it is necessary to point out that the “modified” sphere model is not the sphere model developed by Begley and Mackin, and it is not derived based on rigorous study or any sound theoretical basis.

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FIG. 1. Assuming that $E = 1.05$ TPa, the load-deflection curves based on Eq. (1) are plotted in (a), and the load-deflection curves based on Eq. (2) are plotted in (b). If $E = 0.56$ TPa is assumed, the load-deflection curves obtained from the sphere model match the curves obtained from molecular dynamics simulations very well, as shown in (c).