Sharma et al. Reply

Sharma *et al.* Reply: We assume, from literature [1,2], that single bonds are described by a nonlinear potential (i.e., anharmonic), while triple bonds remain well described by a harmonic potential. The pressure (P) chamber works as a reservoir, and P is hydrostatic and discretely spaced between 0.1–4 GPa. The linear carbon chain multiwalled carbon nanotube (LCC@MWCNT) is in equilibrium with each P, and its restoring force ($F_{\text{restoring}}$) is an invariant whose magnitude is set by the reservoir. Therefore, by (i) having $F_{\text{restoring}} = m\omega_{\text{LCC}}^2 \Delta x$, and (ii) realizing that it is not explicitly dependent on P, changes in ω_{LLC} might be balanced by changes in Δx (for each Δx, the LCC has a specific stiffness that pertains to the instantaneous P; Δx depends explicitly on ω and implicitly on P).

Additionally, we assume that P is transmitted from the oil to the MWCNT, and then from the MWCNT to the LCC [3]. The literature [4–16] endorses that, for the P range we consider, P is most relevant in those MWCNT cross sections without LCCs and on MWCNT ends: P is more effective in the LCC's axial direction. Considering our assumptions, $F_{\text{restoring}}$ is, in magnitude, equal to $P_c A_c$ (A_c is the carbon atom cross-section area and P_c is the pressure on the LCC). Additionally, the force applied to the MWCNT is $F_{\text{applied}} = PA$ (A is the inner-tube cross-section area). Since the LCC@MWCNT system is in equilibrium ($F_{\text{restoring}} = F_{\text{applied}}$), $PA = P_c A_c [dP_c = dP(A/A_c)]$.

The LCC's stiffness, in terms of LCC properties, is

$$\Delta x = \frac{\mathrm{F}_{\text{restoring}}}{m\omega_{\text{LCC}}^2}, \tag{1}$$

then,

$$\frac{d(\Delta x)}{d\omega_{\text{LCC}}} = \frac{d(\Delta x)}{dP_c}\frac{dP_c}{d\omega_{\text{LCC}}} = -\frac{2F_{\text{restoring}}}{m\omega_{\text{LCC}}^3}. \tag{2}$$

Therefore,

$$\frac{d(\Delta x)}{dP_c} = -\frac{2F_{\text{restoring}}}{m\omega_{\text{LCC}}^3}\frac{d\omega_{\text{LCC}}}{dP_c}. \tag{3}$$

Alternatively, using the equilibrium condition ($PA = P_c A_c$) we rewrite $[d(\Delta x)/d\omega_{\text{LCC}}] = \{[d(\Delta x)/dP_c](dP_c/dP)\}[(dP_c/d\omega_{\text{LCC}})(dP/dP_c)] = -(2F_{\text{restoring}}/m\omega_{\text{LCC}}^3)$, and $[d(\Delta x)/dP] = [d(\Delta x)/dP_c](dP_c/dP) = -(2F_{\text{restoring}}/m\omega_{\text{LCC}}^3)(d\omega_{\text{LCC}}/dP_c)(dP_c/dP)$. Therefore,

$$\frac{d(\Delta x)}{d\omega_{\text{LCC}}} = \frac{d(\Delta x)}{dP}\frac{dP}{d\omega_{\text{LCC}}} = -\frac{2F_{\text{restoring}}}{m\omega_{\text{LCC}}^3}. \tag{4}$$

and,

$$\frac{d(\Delta x)}{dP} = -\frac{2F_{\text{restoring}}}{m\omega_{\text{LCC}}^3}\frac{d\omega_{\text{LCC}}}{dP}. \tag{5}$$

From the experiment $\omega_{\text{LCC}} = \omega_{\text{LCC}}^0 - (d\omega_{\text{LCC}}/dP)P = \omega_{\text{LCC}}^0 - [d\omega_{\text{LCC}}/(A_c/A)dP_c](A_c/A)P_c = \omega_{\text{LCC}}^0 - (d\omega_{\text{LCC}}/dP_c)P_c$. Therefore, we have the freedom to choose either Eq. (3) or Eq. (5) as long as the proper set of areas and pressures is chosen for the $F_{\text{restoring}}$ magnitude. If Eq. (3) is chosen, $F_{\text{restoring}} = P_c A_c$; if Eq. (5) [also Eq. (5) in Ref. [17]] is chosen, $F_{\text{restoring}} = PA$. The Young's modulus ($E$) is also calculated in terms of LCC properties. Using that $P_c A_c = PA$,

$$E = a_{C-C}\frac{dP_c}{d(\Delta x)} = -a_{C-C}\left(\frac{\mathrm{m}\omega_{\text{LCC}}^3}{2P_c A_c \frac{d\omega_{\text{LCC}}}{dP_c}}\right) = -a_{C-C}\left(\frac{\mathrm{m}\omega_{\text{LCC}}^3}{2PA\frac{d\omega_{\text{LCC}}}{dP}}\right), \tag{6}$$

which is calculated in terms of the monitorable parameters P and A [18] [also Eq. (6) in Ref. [17]]. The LCC's tensile stiffness (K) is also calculated in terms of LCC properties: $K = EA_c = (-a_{C-C}\{m[\omega_{\text{LCC}}(P)]^3/2PA(d\omega_{\text{LCC}}/dP)\})A_c$. Table I summarizes K values using Eq. (6) and A_c's from Refs. [13,15,16]. Table I also includes values reported by Gao *et al.* [19]. For $A_c = 0.47$ Å, our K values are very consistent with Ref. [13].

Finally, if nonlinearities (anharmonicities) are disregarded, decreases of ≈98% in E could be unrealistic. Example: if a Morse (or a Lenard-Jones) potential describes a bond, a 98% reduction would lead to an irreversible strain. However, the assumptions we make for the nonlinearity do not exclude other phenomena. Although not clear in Ref. [17], we are considering an effective potential, where, for example, a Morse potential and a reversible charge transfer could be playing leading roles [20].

TABLE I. Tensile stiffness (K) for several E and A_c. First row: E from our work and A_c from Refs. [13,15], and [16]. Second row: E and A_c from Ref. [13]. Third row: E and A_c from Ref. [15]. Fourth row: E and A_c from Ref. [16].

$E(P)$ (TPa)	A_c (Å) [13]	K [10^{-7} (N/m)]	A_c in Å [15]	K [10^{-7} (N/m)]	A_c in Å [16]	K [10^{-7} (N/m)]
15.0–30.5 ($P \to 0$)	0.47	0.7–1.43	11.7	17.5–35.7	3.14	4.7–9.6
32.7 [13]	0.47	1.53				
1.3 [15]			11.7	1.52		
4.6 [16]					3.14	1.45

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