Breathinglike phonon modes of multiwalled carbon nanotubes

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The breathinglike phonon modes of multiwalled carbon nanotubes are studied within a valence force field model for nanotubes with two and three layers of armchair type and within a continuum model for nanotubes with a large number of layers. A bond-polarizability model is used to calculate the nonresonant Raman intensity of the breathinglike modes. It is obtained that among all breathinglike modes of a given multiwalled tube, the in-phase one has a maximal intensity. The predicted intensity of the breathinglike modes is compared to available low-frequency experimental Raman data. Special attention is given to the comparison with Raman data on double-walled carbon nanotubes.

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I. INTRODUCTION

The discovery of the carbon nanotubes by Iijima¹ in 1991 has inspired experimentalists and theoreticians to study their unique physical properties.² Depending on the production method, the nanotube samples are found to consist of a certain number of nested layers of carbon. Information on the structure of the individual nanotubes in the samples can be derived using direct but expensive experimental techniques such as transmission electron microscopy, atomic force microscopy, scanning tunneling microscopy, and electron and x-ray diffraction methods. On the other hand, experiments on Raman scattering of light can indirectly provide structural data on nanotubes as a cheaper solution to the problem. The main drawback of this method is that the Raman data has to be correlated to the structural properties of the tubes by use of a dynamical model of the tubes. The dynamical properties of single-layer carbon nanotubes [or single-walled carbon nanotubes (SWNT's)] and bundles of SWNT's have been the goal of many papers.³ Extensive theoretical modeling and Raman scattering experiments reveal that the low-frequency (LF) Raman spectrum of a SWNT is dominated by a single high-intensity peak due to the so-called radial breathing mode (BM) of the tube. By simple force-constant arguments, the frequency of this mode in isolated tubes was found to be inversely proportional to the tube radius R .⁴ Recent density-functional theory calculations of achiral SWNT's (Refs. 5,6) confirmed this result within the error bar. In infinite bundles of aligned nanotubes, the model simulations showed that the intertube interactions modify this dependence.^{7–10} These results serve as the basis for assignment of the peaks in the LF region of the Raman spectra of isolated and bundled SWNT's.

The synthesized multilayer (or multiwalled) carbon nanotubes (MWNT's) most often consist of a number of concentric layers. The samples of MWNT's usually have a certain distribution of the number and the radii of the nanotube layers. Due to this complexity of the MWNT systems, the assignment of the LF features in their Raman spectra is difficult. On the other hand, the assignment of the LF Raman

peaks to certain phonons can be carried out successfully only on the basis of theoretical predictions for the vibrational eigenmodes of MWNT's. As far as it is known to the authors, no systematic theoretical study of the dynamical properties of MWNT's has been reported so far. From general arguments, it can be expected that the LF phonons of the isolated layers will be modified significantly when the layers are stacked together in a MWNT and that the packing effect will be negligible for the high-frequency phonons. Again, as in the case of SWNT's, the breathinglike modes are of particular interest because intense Raman peaks are expected to originate from them in the LF region of the spectra.

In this paper we present the results of the theoretical study of the breathinglike phonon modes (BLM's) in ideal MWNT's using a valence force field model and a continuum model. The two models are introduced in Sec. II. The results of the calculation of the BLM's of MWNT's with different number of layers and different radii obtained within both models are given in details and discussed in comparison with available experimental Raman data in Sec. III. The paper ends with conclusions (Sec. IV).

II. DYNAMICAL MODELS

The BLM's of MWNT's are studied here within two models: a microscopic (atomistic) model (model 1) and a continuum model (model 2). Model 1 is based on a lattice-dynamical model developed for isolated infinite nanotubes¹¹ which is extended to bundles of SWNTs by including interlayer interactions.¹² In model 1, a MWNT is considered as consisting of a number of coaxial cylindrical carbon layers. Each layer can be viewed as obtained by rolling of an infinite strip of a graphite sheet into a seamless cylinder and can uniquely be specified by a pair of integers (n, m) , $n \geq m \geq 0$. Model 1 uses the one-dimensional periodicity of the layers and, consequently, can handle only MWNT's with layers of commensurate unit cell lengths. The intralayer carbon-carbon interactions are described by force constants of the valence force field (VFF) type which were obtained by fitting of the phonon dispersion of graphite.¹³ The use of fixed force

constants instead of pair potentials rules out the possibility for the structural optimization of the layers within model 1. While the available experimental structural data are insufficient for the purposes of this study, recent *ab initio* calculations of SWNT's (Refs. 5,6) reveal that the various carbon-carbon bond lengths are nearly equal to each other and that only slight differences are observed between the bond angles. For these reasons, it is assumed here that (1) all bond lengths are equal to 1.42 Å as it is for graphite and is measured in nanotubes (see, e.g., (Refs. 2,14) and (2) all bond angles are equal to each other. The interlayer carbon-carbon interactions are modeled by a potential of the Lennard-Jones (LJ) type $V(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6]$ with parameters $\epsilon = 0.002964$ eV and $\sigma = 3.407$ Å taken from Ref. 15. The intertube interaction energy of a given MWNT is obtained by summing over all pairs of atoms belonging to different layers. This energy is then minimized with respect to the interlayer separations, the relative angles of rotation of the layers around the tube axis and the relative translations of the layers along the same axis. It is implied that the adjacent layers must be of types for which the initial radii difference is close to the optimized interlayer separation so that the change of the bond lengths is small. For the optimized tube, the dynamical matrix is calculated by use of the VFF parameters and the LJ potential. Finally, the vibrational modes of the tube are derived as solutions of the dynamical eigenvalue problem. The computational time increases rapidly with the increase of the number of layers and for this reason nanotubes with more than three layers are treated only within model 2.

The Raman spectra of MWNT's are calculated within model 1 using a nonresonant bond-polarizability model (BPM) (Ref. 16) for backscattering geometry and parallel light polarization with averaging over all tube orientations in space. For most of the MWNT samples the tube diameters are large enough so that the resonant Raman scattering effect is much weaker than for SWNT's.³ For few layer tubes, resonant enhancement of some LF Raman lines may be observed but nevertheless the BPM predictions can be of help in the analysis of the spectra of MWNT samples.

The difficulty to handle tubes with many layers within model 1 are overcome by use of a continuum model (model 2).¹⁷ In this model the tube layers are considered as homogeneous cylindrical surfaces with constant surface mass density. Only uniform radial motion of the layers is allowed with a force constant which is derived from the BM frequency dependence on the tube radius obtained by model 1. The interaction between the layers is described by a LJ potential as above. The total interlayer interaction energy between two layers is obtained by integration over their surfaces. Then, this energy is minimized with respect to the layer radii to find their equilibrium values. Since the interaction energy decreases with the increase of the surface of the layers, the minimum of this energy will be reached for infinite radii. For this reason, the radius of innermost layer is kept fixed in the minimization procedure. This choice corresponds to a layer-by-layer growth of MWNT's. Further on, the force-constant matrix for uniform radial motions of the layers is derived by numerical calculation of the second derivatives of the inter-

FIG. 1. Dependence of the interlayer separations of a MWNT on the innermost layer radius R_{in} and the number of layers obtained within model 2 in comparison with experimentally derived curve from Ref. 19.

layer energy with respect to the layer radii. The BLM's are then found as solutions of the dynamical eigenvalue problem.

III. RESULTS AND DISCUSSION

The stringent restrictions on the layer types in model 1 limit the number of tractable MWNT's. It has been noticed that the tubes of armchair types (5,5) and (10,10) can be nested one within the other to form a two-layer tube with interlayer separation of 3.4 Å.¹⁸ We considered an extension of this case to two- and three-layer tubes with layers of armchair type $(n+5m, n+5m)$ where $m = 1, 2, 3$ enumerates the layers. The integer number n is fixed for a given two- or three-layer MWNT and the following values were used: $n = 0, 1, \dots, 15$ and $n = 0, 1, \dots, 10$, respectively. We carried out structural optimization of these tubes with respect to the separations between the adjacent layers and found that the optimal separations do not deviate more than 0.1% from the difference of the initial layer radii of 3.37 Å. The difference between the BLM frequency of the optimized and the non-optimized MWNT's is below 1 cm^{-1} . It is interesting to note that neither the optimal separations nor the corresponding BLM frequencies are sensitive to the variations of the other two types of structural parameters—the relative angles of rotation and the relative translations of the layers. Therefore, the matching of the layers does not seem to be an important parameter in these calculations.

We utilized a continuum model (model 2) in the study of the BLM's of MWNT's with large layer radii and many layers. The layer radii are optimized for a given number of layers N and a given radius of the innermost layer R_{in} . The obtained interlayer separations for $R_{in} = 10, 15$, and 30 Å and N up to 8, 9, and 14, correspondingly (see Fig. 1), lie in the range from 3.37 to 3.74 Å, in fair agreement with the experimentally derived ones (3.4–3.9 Å).¹⁹ It is seen in Fig.

FIG. 2. Displacements of the unit cell atoms and frequencies for the two BLM's of the two-layer tubes $(5,5)@(10,10)$ and $(20,20)@(25,25)$ obtained within model 1. The BM frequencies of the isolated layers are given in parenthesis. The cross sections of the two layers are depicted schematically by circles.

1 that the interlayer separations decrease in outward direction and reach a value of $3.37 \text{ \AA}$ for the outermost layers and a large number of layers. This behavior is in correspondence with the experimental data¹⁹ where the asymptotic value is $3.44 \text{ \AA}$. As a whole, there is a good agreement between the experimental data and the theoretical predictions bearing in mind that the interlayer interactions are modeled by a simple potential of the LJ type.

The calculated atomic displacements and frequencies of the BLM's for several two- and three-layer tubes within model 1 are shown in Figs. 2 and 3. It is seen in Fig. 2 that for the small radius tube $(5,5)@(10,10)$, each of the two BLM's with frequencies 176 and 340 cm^{-1} has the characteristic features of the BM of one of the layers (167 and 331 cm^{-1}). The reason for this is that the frequencies of the BM's of the separate layers differ significantly from each other and, consequently, the mixing of both modes is negli-

FIG. 3. Same as for Fig. 2 but for the three-layer tubes $(5,5)@(10,10)@(15,15)$ and $(15,15)@(20,20)@(25,25)$.

FIG. 4. Dependence of the frequencies of the BLM's of two-layer tubes on the outer layer radius calculated using models 1 and model 2. The vertical dashed lines pass through the results for the tubes in Fig. 2. The inset shows the estimated Raman intensity of the BLM. The frequency and the Raman intensity of the BM's of isolated layers and the BLM's of two-layer tubes are designated by open symbols and by solid symbols, respectively.

gible. For the large radius tube $(20,20)@(25,25)$, the low- and high-frequency BLM's (77 and 119 cm^{-1}) are in-phase and counterphase collective motions of both layers, respectively, which is due to the closeness of the BM frequencies of the two layers (67 and 84 cm^{-1}). The atomic displacements for two three-layer tubes are displayed in Fig. 3. In the case of the small radius tube $(5,5)@(10,10)@(15,15)$ the displacement pattern of the BLM's (123 , 183 , and 341 cm^{-1}) is characterized by motion of atoms of mainly one layer. For the large-radius tube $(15,15)@(20,20)@(25,25)$, however, the BLM's (77 , 117 , and 146 cm^{-1}) are collective motions of the three layers. The lowest-frequency BLM is an in-phase one, the two higher-frequency ones are of mixed character. The change of the character of the BLM's with the tube radius has a simple explanation considering the layers of a MWNT as coupled oscillators. Indeed, whenever the frequencies of the separate oscillators are nearly equal to each other, the interactions between them lead to vibrational modes of strongly mixed character. For this reason, the BLM's are expected to be of mixed character also for tubes with an arbitrary number of large-radius layers. It is worth pointing out that in some cases the BLM's are not uniform radial motions rather they are strongly mixed with totally symmetric components of doubly degenerate tube modes which split in MWNT's due to the low symmetry of the system (see Figs. 2 and 3). This effect was observed in the case of bundles of SWNT's as well.¹⁷

The results for the frequency and the Raman intensity of the BLM's for a number of two- and three-layer tubes are displayed in Figs. 4 and 5. The comparison of the BLM frequencies (solid symbols) with the BM ones of the isolated

FIG. 5. Same as for Fig. 4 but for three-layer tubes.

layers (empty symbols) reveals a systematic upward shift of the former due to the intertube interactions. While this shift is almost uniform of about 10 cm^{-1} for the in-phase BLM, for the totally and the partially counterphase modes it increases with the increase of the outer layer radius. The BLM frequencies calculated within model 2 for two- and three-layer tubes agree well with those of model 1 as seen in Figs. 4 and 5. The dependence of the frequency (in cm^{-1}) of the in-phase BLM obtained by model 1 (model 2) on the outer layer radius R_{out} (in $\text{\AA}$) was fitted with c/R_{out}^n to yield $c = 1167$ and $n = 0.94$ ($c = 1074$ and $n = 0.94$) for two-layer tubes and $c = 1002$ and $n = 0.90$ ($c = 1068$ and $n = 0.93$) for three-layer tubes (compare to $c = 1148$,¹¹ $c = 1170$,⁵ $c = 1166$,⁶ and $n = 1$ for the BM of a SWNT). The frequencies of the other less intense BLM's of counterphase character cannot be fitted as functions of the layer radii with simple power laws.

The calculated BLM intensity within model 1 and by use of the BPM is shown in the insets of Figs. 4 and 5. It is seen in the inset of Fig. 4 that the intensity ratio for the BLM's of the inner and the outer layers for the small-radius tubes $(5,5)@(10,10)$ is $\approx 1:2$. For small layer radii, the layers behave as nearly independent and for each of them the intensity of the BM is roughly proportional to the radius of the layer. Then, bearing in mind that the normalization volume is the same for both BLM's and that $R_{(5,5)}:R_{(10,10)} \approx 1:2$, we can easily explain the mentioned value of the intensity ratio. The independence of the separate layers is confirmed by the nearly equal intensities of the outer layer BLM in a two-layer tube (solid circles) and the BM of the isolated layer (empty circles). The intensity of small-radius three-layer tubes (see inset of Fig. 5) shows similar behavior except for the middle layer whose BLM is not a pure radial atomic displacement. This is a result of the considerable redistribution of the intensity of the BM of the middle layer among the BLM's of the same layer. For large-radius three-layer tubes, the close-

FIG. 6. Dependence of the frequencies of the BLM's of multilayer tubes calculated within model 2 for fixed radius R_{in} of the innermost layer and different number of layers N .

ness of the frequencies of the BM's of the isolated layers leads to redistribution of the intensity of these modes among all BLM's of the given tube. In particular, with the increase of the layer radii, the intensity of the totally counterphase mode drops rapidly and is negligible for radii larger than $16 \text{ \AA}$. The intensity of the in-phase mode has, on the contrary, a very slow decrease over a wide range of radii.

The calculated frequencies of the BLM's for multilayer tubes are displayed in Fig. 6. In all cases, the lowest frequency mode is an in-phase one, the highest frequency mode is a totally counterphase one, and the remaining modes are of mixed in-phase and counter-phase character and have intermediate frequencies. For a given R_{in} , the frequency of the in-phase mode decreases monotonically to zero with the increase of the number of layers while the frequency of the counterphase mode tends to a constant value of about 130 cm^{-1} . In order to understand the large radii behavior of these two BLM's we take into account that in this case the tube layers are locally parallel to each other. Then, the in-phase layer motion is essentially a parallel translation of the layers which corresponds to the zero-frequency transverse acoustic phonon of graphite. In this limit, the counterphase mode becomes similar in vibrational pattern to the out-of-plane counter-phase B_{2g} of graphite with frequency of 127 cm^{-1} .

In the micro-Raman measurements on a MWNT sample with a mean tube diameter of $10\text{--}20 \text{ nm}$ and predominantly $10\text{--}20$ layers,²⁰ intense peaks were observed in the LF part of the spectra at 166 , 178 , and 205 cm^{-1} . The first and the third of these peaks were tentatively assigned to A_g phonons, possibly BM's of SWNT's (isolated or bundled) or BLM's of few layer MWNT's. In view of the variety of tubes present in the sample, it was impossible to assign these peaks unambiguously. Recent micro-Raman scattering experiments on a MWNT sample reveal that the LF part of the spectra contain

a number of weak features between 100 and 500 cm^{-1} .²¹ The assignment of the Raman lines, based on the $1/R$ law for the BM frequency of isolated layers showed that they originated from the innermost layers of possibly different MWNT's. The wide distributions of the tubes in diameters and in number of layers is an obstacle for the application of our predictions to this case. We note that the LF region of these spectra are in agreement with the arguments that the resonant scattering in large-radius MWNT's should be much weaker than in SWNT's.³

For MWNT's with a few layers, however, it can be expected that the Raman scattering could be resonant under certain conditions and intense peaks may be observed in the LF part of the spectra. Recently, two Raman spectra measurements on double-layer nanotubes (DWNT's) have been reported.^{22,23} In Ref. 22, the Raman spectra of a sample with 90% SWNT's and DWNT's showed several peaks in the region below 250 cm^{-1} (inset of Fig. 5 in Ref. 22). It was concluded that the strong peaks at about 180 and 200 cm^{-1} were due to SWNTs which was supported by the measured diameter distribution of the tubes. The remaining weaker peaks below and above these two peaks are not discussed in the mentioned paper. In the light of our results, we can assign the pair of peaks at 145 and 250 cm^{-1} by use of Fig. 4 to the BLM's of a DWNT with layer radii of 7.9 and 4.5 Å. The intensity ratio for those two peaks is close to the predicted one in the inset of Fig. 4. The lack of sufficient structural data will make the assignment of the remaining peaks to BLM's rather uncertain.

In Ref. 23, DWNT's were prepared in a two-stage procedure: (1) C_{60} molecules were inserted efficiently in the interior of SWNT's by vapor phase reaction of C_{60} with SWNT's at 400 °C and (2) the C_{60} molecules coalesced after heating the sample up to 1200 °C to form an inner layer of the SWNT's. The measured Raman spectrum of the nanotube sample shows many, well-resolved peaks (see Fig. 3 in Ref. 23) which were assigned using the $1/R$ law to BM's of the separate layers. It is interesting to check the validity of our predictions for the peak positions and intensities in this case as well, although the measured peaks are resonantly enhanced. First, we notice that for initially fully packed C_{60} molecules inside the nanotubes, after coalescence, theoretically only about 2/3 of the nanotubes will be filled by an inner layer and the remaining space will be emptied. Then, the Raman spectrum can be considered as consisting of contributions of a given number of SWNT's (with radii equal to the outer layer radii of the DWNT's) and twice as more DWNT's. Therefore, we supposed that the peaks below $\approx 200 \text{ cm}^{-1}$ are due to BM's of SWNT's and in-phase BLM's of DWNT's while the peaks above $\approx 200 \text{ cm}^{-1}$ are due to counterphase BLM's of DWNT's. Since the diameter distribution of the tubes in the measured spot of the sample is unknown, we fitted the peaks in the higher-frequency band with Lorentzians with full width at half maximum of 5 cm^{-1} . The centers of the best-fit Lorentzian were taken as the frequencies of the counterphase BLM's. The frequencies of the corresponding in-phase BLM's and BM's were obtained from Fig. 4. Finally, the lower-frequency part of the Raman spectrum was drawn by means of Lorentzians, cen-

FIG. 7. The predicted Raman spectrum by model 1 in comparison with the experimental spectrum of a DWNT sample prepared by heating of C_{60} -filled SWNT's up to 1200 °C.²³ See text for details.

tered at the latter frequencies, whose heights were determined by use of the inset of Fig. 4. The so-estimated Raman spectrum is shown in comparison with the measured one in Fig. 7. It is evident that (a) the peaks of the theoretical spectrum are close in intensity to those of the experimental one except for the missing peak at 143 cm^{-1} and (b) there is a systematic underestimation of the frequencies in LF band. The latter disagreement may be explained by charge transfer from the tube layers to the interlayer region²⁴ possibly accompanied by softening of the carbon-carbon bonds and thus lowering of the BLM frequency, and by modification of the interlayer interactions. The clarification of this phenomenon requires, however, a more sophisticated approach than the one adopted here.

IV. SUMMARY

The results of the theoretical study of the BLM's of MWNT's using two different models are presented. The BLM's of two- and three-layer tubes are calculated within a valence force-field model and the Raman intensity of these modes is obtained via a bond-polarizability model. Due to computational restrictions, tubes with many layers are handled by a continuum model. The derived dependence of the optimized interlayer separations on the radius of the internal layer and the number of layers is in good agreement with estimations based on experimental data. In particular, the interlayer separation is largest for the innermost layers and decreases with the increase of the layer radius. The results of the dynamical calculations show that the atomic displacement pattern of the BLM's is modified on passing from small to large layer radii. As a consequence, for small layer radii, the BLM's are uniform radial displacements of mainly one layer. In the large layer radius case, the BLM's represent

collective motions of many layers of mixed in-phase and counterphase types. In the very large radius limit, the highest frequency BLM is a counterphase motion similar to the out-of-plane counter-phase B_{2g} mode in graphite. The lowest frequency BLM is an in-phase mode and its frequency decreases with the radius of the outmost layer as $1/R_{\text{out}}^n$. The Raman intensity of all BLM's decreases rapidly with the increase of the layer radius with the exception of the in-phase BLM that has a very slowly decreasing intensity over a large interval of radii. We compare our results to available experimental Raman data on MWNT's. In the case of tubes with many layers, the variety of the tubes in the sample hinders the unambiguous application of our results to the assignment of LF Raman peaks. Although our model simulations are restricted to the non-resonant Raman intensity, it is shown

that their predictions correspond well to the experimental resonant Raman spectrum of two-layer tubes.

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