Rapid Research Note

Low-frequency vibrational modes of viruses used for nanoelectronic self-assemblies

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Viruses of cylindrical shape have recently attracted attention as templates for assembly of nanostructured materials and as elements of nanoelectronic circuits. We have calculated the dispersion relations for the lowest vibrational frequencies of the tobacco mosaic virus (TMV) and M13 bacteriophage immersed in air or water. The radial breathing modes of TMV and M13 viruses in air (water) are 1.85 cm^{-1} and 6.42 cm^{-1} (2.10 cm^{-1} and 6.12 cm^{-1}), respectively. Elastic vibrations of the two viruses in water are damped with the quality factor of 3.6 for the radial breathing modes.

Recently, rod-shaped viruses, such as tobacco mosaic virus (TMV) and M13 bacteriophage, have been utilized as biological templates in the synthesis of semiconductor and metallic nanowires [1–3]. They were also proposed as elements in the biologically-inspired nanoelectronic circuits. Genetically modified TMV and M13 viruses have been successfully used for self-assembly of nanomaterials into liquid crystals, films, and fibers [2]. It is expected that genetically programmed viruses will contribute to the next generation of nanoelectronic circuits and optoelectronic devices. Both TMV and M13 viruses have cylindrical shape: M13 is 860 nm long and 6.5 nm in diameter, while TMV is 300 nm long, 18 nm in diameter and with a 4 nm in diameter axial canal [1, 2]. Since the two viruses have the diameters of the same order of magnitude as diameters of semiconductor nanocrystals and nanowires, elastic vibrations of TMV and M13 viruses should manifest themselves in ultra-low-frequency Raman scattering spectra. The knowledge of the low-frequency vibrational modes of the viruses is important for interpretation of Raman spectra and monitoring the aforementioned self-assembly processes. If functionalised viruses are used in the assembly of hybrid inorganic-organic nanoelectronic circuit, their vibrational modes, i.e. phonon spectra, will significantly affect the properties of the inorganic-organic interface.

There are only few reports on the estimation of vibrational modes in organic nanostructures: spherical virus particles have been considered in Ref. [4] and thin-wall microtubules have been studied in Ref. [5]. Here, we present results of our calculations of phonon spectra of TMV and M13 viruses immersed in air and water. Due to the fact that the length of the viruses is much larger than their diameter, we model TMV and M13 as infinite cylinders. The complex-frequency approach is employed to take into account the effect of exterior medium [6, 7]. The elastic parameters of viruses are assumed to be equal to the parameters of the lysozyme protein crystal: longitudinal speed of sound $V_l = 1817$ m/s, Poisson's ratio $\sigma = 0.33$, and mass density $\rho = 1.21$ g/cm^3 [8]. For water one has $V_l = 1483$ m/s, $\sigma = 0.5$, $\rho = 1$ g/cm^3.

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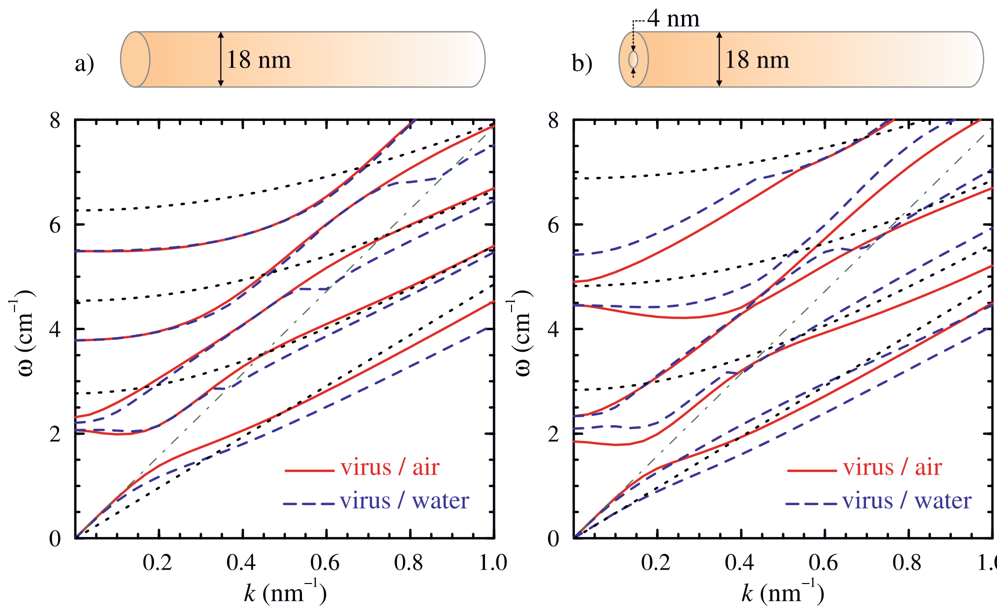

Fig. 1 (online colour at: www.pss-b.com) Dispersion of the lowest vibrational frequencies with $m = 0$ for cylindrical viruses a) without and b) with an axial canal. Solid (dashed) lines correspond to radial-axial vibrations of the virus in air (water). Dotted lines correspond to torsional vibrations. Dash-dotted lines mark the speed of sound in water.

We find the low-frequency vibrational modes of cylindrical viruses as eigenmodes of the equation of motion for the displacement vector $\boldsymbol{u}$. Due to the axial symmetry of the problem, the equation of motion can be solved analytically in cylindrical coordinates and the displacement vector can be written as

$$\boldsymbol{u}(r,\phi,z,t) = \boldsymbol{w}_{m,k}(r)\exp(im\phi + ikz - i\omega_{m,k}t), \quad (1)$$

where m is the angular quantum number and k is the axial wavenumber [9]. We only consider the Raman-active vibrational modes with $m = 0$. When $m = 0$, the vibrational modes can be divided into radial-axial and torsional modes. The k-dependences of the lowest vibrational modes are shown in Fig. 1a for a simple cylindrical virus and in Fig. 1b for a cylindrical virus with an axial canal. While the torsional vibrations have the same frequencies for the viruses immersed in air and water, the radial-axial vibrations are different. The main difference consists in the fact that radial-axial vibrations in air are harmonic while radial-axial vibrations in water are damped when $\omega > k\ V_l^{(\mathrm{water})}$, i.e. the frequency has a nonzero imaginary part that is equal to the inverse lifetime and also defines the broadening of the Raman peak.

When $k = 0$, the radial-axial vibrations split into purely axial and purely radial, which include the radial breathing mode. Like torsional modes, axial modes with $k = 0$ are not damped and are the same when the exterior medium is air or water. On the contrary, the damping is maximal for radial modes with $k = 0$. Comparing Figs. 1a and b, one can see that the presence of an axial canal substantially changes the low-frequency vibrational modes. For example, the lowest radial-axial acoustical branch of a simple virus in water splits in two parts for the virus with an axial canal. Moreover, there is only one radial mode in Fig. 1a, while there are two such modes in Fig. 1b. Finally, the radial mode is the mode with the lowest nonzero frequency for the virus with an axial canal, while it is the second lowest nonzero frequency for the simple virus. Note that the dispersion plot in Fig. 1a is calculated for the virus with diameter 18 nm. Other diameters can be considered by a simple rescaling of Fig. 1a, e.g., both axes of the plot should be multiplied by 18/6.5 to get the dispersion curves of the M13 virus. Figure 1b corresponds to the TMV.

Radial modes are particularly important since they have the maximal intensity in the Raman scattering spectra. Figure 2 shows the eigenfrequencies and the corresponding displacement fields for the radial

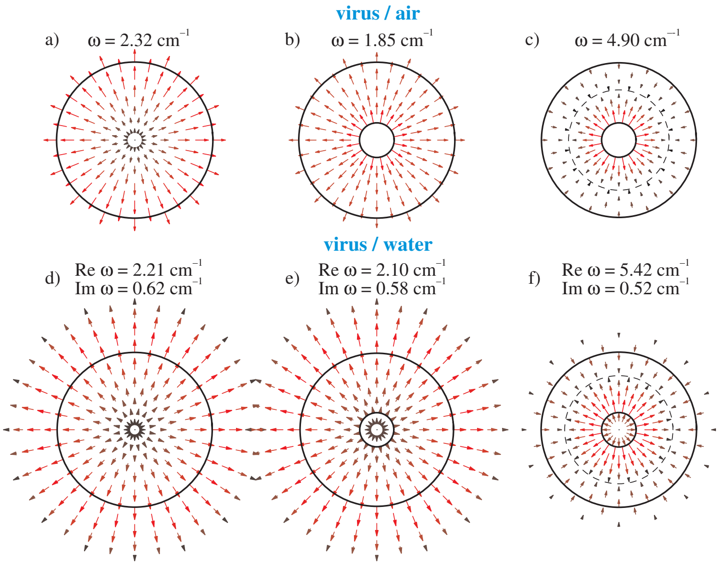

Fig. 2 (online colour at: www.pss-b.com) Radial modes of the lowest frequencies with $m = 0$ and $k = 0$ for a cylindrical virus in air (a–c) and in water (d–f). The viruses without (a, d) and with (b, c; e, f) an axial canal are considered. The sizes of the viruses are the same as in Fig. 1. The length of arrows is proportional to the magnitude of the displacement vector.

modes shown in Fig. 1. As seen from Figs. 2a, b and d, e, the frequency of the radial breathing mode in air is 25% less for the virus with an axial canal than it is for the simple virus. However, the above difference decreases to 5% when the viruses are immersed in water. Note that the second radial mode (see Figs. 2c and f) reveals two synchronized vibrations. The quality factor Re (ω)/Im (ω) for radial vibrations in water is about 3.6 for the first mode and about 10 for the second mode.

In conclusion, we have theoretically studied the low-frequency vibrational modes of TMV and M13 viruses used for nanoelectronic self-assemblies. The radial breathing modes of TMV and M13 viruses in air are found to be 1.85 cm^{-1} and 6.42 cm^{-1}, respectively. If the viruses are in water, the above frequencies become 2.10 cm^{-1} and 6.12 cm^{-1}, respectively. The results are important for Raman spectra interpretation and control of the self-assembly process.

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