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Low frequency vibrational modes of nano-metric spherical viruses

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The low frequency dynamics has been investigated by using an elastic body approximation for a spherical virus with free surface. The frequencies for spheroidal mode are obtained in terms of their eigen values. The effect of aqueous surrounding medium is also observed by incorporating the acoustic impedance factor. The damping time, frequency and quality factor are evaluated for a virus-medium system.

Keywords: Acoustic vibrations, Phonons, Protein, Nano-metric spherical viruses
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1 Introduction

Viruses with size range lying in few nanometers (20-3000 nm diameters) are the largest aggregates of biological macromolecules whose structures are determined by using soft X-ray crystallography[1]. Most of these biological objects prefer icosahedral which is nearly spherical in shape[2]. However, they also occur in nature with other shapes[3]. A virus is a tinier micro-organism which consists of mainly, single stranded or double stranded genomic material (i.e. either RNA or DNA) to form its core and is surrounded by a symmetrically organized protective shell of proteins (i.e. a capsid). The basic shapes of viruses are rod-like for example, tobacco mosaic viruses (TMV) and M13 Bacteriophage viruses, or spherical (i.e. icosahedral) for example polyoma viruses, adenoviruses, etc[3].

One of the most recent examples is the utilization of biological objects, such as viruses, as nano-templates for the nano-fabrication[4]. Such miniscule pockets of proteins, namely viruses, have a notable importance since their excitations of very low energy could have applications in either diagnosis or treatment of viral diseases. As viruses have sizes of the order of those of quantum dots and nanocrystals, one can expect a close analogy in their low energy elastic vibrations. The elastic vibrations of these spherical viruses should manifest themselves in the low frequency Raman scattering spectra and interpretation of these spectra requires the theoretical understanding of their low frequency vibrational modes. There are only few reports on the estimation of vibrational frequencies of viruses[5]. The detection of viruses by acoustic oscillations has also been recently reported by Cooper *et al*[6]., which involves a mechanism distinct from the excitation of the vibrational modes of virus particle itself. In a very recent report on tobacco mosaic virus (TMV) and M13 bacteriophage immersed in air and water, Balandin *et al*[3]. discuss the dispersion relations for their lowest vibrational frequencies. L H Ford has also reported the theoretical estimates of vibrational frequencies of spherical virus particles in his recent paper by using liquid drop model and an elastic sphere model[5]. Saviot *et al*[7]. later gave a direction to calculate the damping of these modes for embedded elastic sphere.

In the present paper, we report our estimates of low frequency vibrational modes of a spherical virus particle, under the framework of an elastic continuum model along with appropriate boundary conditions at the surface of a spherical virus, where a virus is treated as a uniform elastic sphere. The vibrations of a spherical body give rise to the spheroidal and the torsional (not reported) modes. Since, the viruses exist in some medium, to ensure specific function of the virus particles, the effect of surrounding medium on Raman spectrum is also studied. The coupling constant, which is a parameter depending on coupling between the capsid of a virus particle and medium, is also studied for different surrounding environment.

2 Experimental Details

The finiteness of the size of a virus particle is manifested in the discrete set of its vibrational frequencies, which can be achieved using the above-mentioned approach under stress-free boundary conditions at surface of virus particle. The vibrational modes of a virus particle are calculated by using an equation of motion of a three dimensional spherical elastic body, which was first given by Lamb[8] and later by Tamura *et al*[9]. This methodology has been quite successfully used for the description of phonons in several nanostructured systems by Murray *et al*[10]. and recently by the authors[11].

Lamb theory starts with an equation of motion of a three dimensional spherical elastic body in the differential form as:

$$\rho\ddot{\mathbf{u}} = (\lambda+\mu)\text{ grad div }\mathbf{u} - \mu\text{ rot rot }\mathbf{u} \quad \ldots (1)$$

where **u** is a lattice displacement vector, the two parameters μ and λ are also known as Lame's constants and ρ is the mass density, which are related to the longitudinal and transverse sound velocities in bulk.

$$V_l = [(\lambda + \mu)/\rho]^{1/2} \text{ and } V_t = (\mu/\rho)^{1/2} \quad \ldots (2)$$

Energy eigen values for a spherical virus with radius R are obtained by using following stress free boundary conditions in Eq. (1) at the surface of the spherical virus.

$$\sigma_{rr}\big|_{r=R} = 0\ ;\ \sigma_{r\theta}\big|_{r=R} = 0\ ;\ \sigma_{r\psi}\big|_{r=R} = 0 \quad \ldots (3)$$

The eigen values of Eq. (1) for both spheroidal and torsional modes are described by orbital angular momentum quantum no l and harmonic n. The eigen values of the spheroidal modes, ξ and η are then obtained[12] as :

$$\xi = \omega d/2V_l \text{ and } \eta = \omega d/2V_t \quad \ldots (4)$$

where ξ and η are the dimensionless eigen values and ω is the angular frequency and d is the diameter of a spherical virus. The breathing and quadrupolar modes corresponding to l = 0 and l = 2 for n = 0 harmonic, are Raman active according to the group theoretical analysis[13]. The l = 0 mode is purely radial with spherical symmetry and produces totally polarized spectra, while l = 2 mode produces partially depolarized spectra. The frequencies of the Raman lines are estimated from Eq. (4) following the procedure adopted in Ref. (11) with the help of the solution of the previous equations and using average sound velocities of proteins, V_l and V_t.

3 Results and Discussion

The low frequency vibrational modes of spherical virus particles immersed in a liquid medium have been obtained using the above approach considering the elastic properties of viruses to be close to the parameters of protein crystals[14,15]. We assume for the definiteness, that the elastic parameters of viruses coincide with the parameters of lysozyme protein crystal from Ref.(15) and their values are summarized in Table 1. The energy eigen values of low frequency spheroidal vibrational modes are calculated from the above-mentioned approach and the corresponding eigen values for some harmonics n for this mode are presented in Table 2. The angular frequencies for the various virus size and surrounding media can be deduced from these computed eigen values by using Eq. (4).

Since water or any other aqueous environment is a medium required for the virus synthesis, purification and assembly processes, the theoretical results on the vibrational modes are significantly important. In the present paper, we investigate the effect of water and glycerol media on low frequency vibrational modes of spherical viruses which is manifested in the computed values of their damping time and quality factor. We

Table1— Acoustic parameters for spherical virus embedded in surrounding medium

System	V_l (m/s)	V_t (m/s)	ρ (g/cm^3)	ρ_m/ρ_{Virus}
Water	1483	0	1.00	0.826
Virus	1817	915	1.21	1
Glycerol	1904	0	1.26	1.041

Table2—Eigen values and frequency (cm^{-1}) of a free standing spherical virus of 50 nm radius

		SPH	
l	n	Eigen Values	Frequency (cm^{-1}) (ν = ω/2π)
0	0	1.693	0.326
	1	2.369	0.456
	2	4.539	0.874
	3	5.133	0.988
	4	8.490	1.635
	5	11.640	2.242
	6	12.580	2.423
	7	17.610	3.392
	8	19.380	3.732
	9	19.650	3.784
1	0	3.500	0.674
	1	4.863	0.936
	2	8.030	1.546
	3	10.570	2.035
	4	13.670	2.633
	5	16.050	3.091
	6	19.400	3.736

Table3—Frequency (cm^{-1}), damping time (*p* sec) and quality factor (*Q*) for spherical virus of 100 nm diameter

Medium	Frequency (cm^{-1})	Damping Time (*p* sec)	Quality Factor
Water	1.5393	17.3	0.7978
Glycerol	1.495	34.4	1.5447

incorporate the effect of the surrounding media by introducing a parameter namely, acoustic impedance (*Z*) at the interface of the medium. This modifies the equation for the spheroidal modes as given in Ref. (11). The energy eigen values of modified spheroidal equation is given by expression, $s = \omega d/2V_{lp}$. The acoustic impedance (*Z*) is simply density times the sound velocity for a plane interface, however, for a spherical interface it is a complex number. The value of *s* is then used to evaluate the complex angular frequency ω, which can further be related with the damping time τ_D. The damping time (τ_D) is an inverse of the imaginary part of the complex angular frequency ω. Table 3 describes damping time (τ_D) for virus particle of 100 nm diameter immersed in different media. It is clear from Table 3 that damping time of a virus particle is significantly affected by the medium in which virus resides. For less dense medium (i.e. water in the present case), the low frequency vibrations of virus dampen faster than in more dense medium (i.e. glycerol in this case). The small damping time for virus-water system is due to the stronger mechanical coupling of virus with the water medium. The strength of mechanical coupling is reflected in the computed vibrational frequency given in Table 3. The calculated values of damping time of a confined virus system are observed to have similar order for other water-protein systems[16]. We also report our results of quality factor (*Q*) estimated by using expression $Q = \omega \tau_D$ for a confined virus in different media in Table 3. Quality factor should be as high as possible in order to get maximum efficiency of this embedded biological system. It is seen from Table 3 that quality factor (*Q*) for water-embedded virus is less than that for glycerol embedded virus.

In a summary, we have investigated the confined acoustic phonon modes, namely the spheroidal and the effect of medium on the damping time and quality factor of virus. The damping time decreases with decrease in the density of surrounding medium. However, the quality factor increases for less dense elastic medium. We emphasize the need for new experimental data in particular, Raman scattering by acoustic phonons to check the results of the present study.

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References

1 Stuart D I, Grimes J M & Burroughs N *et al.*, *Microbiology Today*, 26 (1999) 59.
2 Zandi R, Reguera D & Bruinsma R F *et al.*, *PNAS*, 101 (2004) 15556.
3 Balandin A A & Fonoberov V A, *J Biomed Nanotech*, 1 (2005)1; Lidmar J, Mirny L & Nelson D R, arXiv: cond-mat/0306741, 2003.
4 Shenton W, Douglas T & Young M *et al*., *Adv Mater*, 11 (1999) 253.
5 Ford L H, *Phys Rev E,* 67 (2003) 051924:1; Sirenko Y, Stroscio M A & Kim K W, *Phys Rev E,* 69 (2004) 023901:1
6 Cooper M A, Dultsev F N & Minson T *et al*., *Nat Biotechnol,* 19 (2001) 833.
7 Saviot L, Murray D B & Mermet A, *Phys Rev E*, 69 (2004) 023901.
8 Lamb H, *Proc London Math Soc* ,13 (1982)189.
9 Tamura A & Ichniokawa T, *J Phys C*, 16 (1983) 4779 and references there in.
10 Saviot L, Murray D B & M del Carmen Marco de Lucas, *Phys Rev B***,** 69 (2004) 113402.
11 Talati M & Jha P K, *Physica E,* 28(2005) (17) and references there in.
12 Tanaka A, Onari S & Arai T, *Phys Rev B,* 47 (1993)1237.
13 Duval E, *Phys Rev B,* 46 (1992) 5795.
14 Tachibana M, Kojima K & Ikuyama R *et al*,. *Chem Phys Lett*, 332 (2000) 259.
15 Edwards C, Palmer S B & Emsley P *et al*,. *Acta Crystallogr Sect A: Found Crystallogr A*, 46 (1990) 315.
16 Mizoguchi K, Hori Y & Tominaga Y, *J Chem Phys,* 97 (1992) 1961.