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Transverse Inertia, Poisson Ratio and Layer Number Effect on Relaxation and Retardation Time of Wave Propagation in Simulated Microbiology Structures

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The transverse inertia effect considered and in terms of the principle of energy equilibrium in viscoelastic mechanics, the 6 order partial differential wave equation and universe solutions for the dimensionless relaxation and retardation time of wave propagation in simulated microbiology structures subjected to a uniaxial stress are deduced. The general solutions for the dimensionless relaxation and retardation time of wave propagation can converge to the classical results of Maxwell rheological model and Kelvin solid model separately when transverse inertia effect is not been taken into account. The transverse inertia effect leads to the increase of relaxation time of wave propagation with increasing Poisson ratio, ratio of diameter to wave length and layer number. The transverse inertia effect induces the decrease of retardation time of wave propagation with increasing Poisson ratio, ratio of diameter to wave length and layer number.

Key words: Simulated microbiology structures, Transverse Inertia, Longitudinal Wave, Relaxation Time, Retardation Time.

It took the Daedalus' "hollow molecules" two decades to become incarnated in a family of fullerenes. Carbon nanotubes (CNTs) that are also an important member in a family of fullerenes possess cylindrical hollow macromolecules consisted of carbon atoms in a periodic hexagonal structure. The past 21 years have witnessed an intense international research in the field of CNTs which were discovered by Iijima in 1991 (Iijima, 1991). Some analytic solutions for CNTs mechanical behavior have been proposed in addition to experimental works. The modeling for the analysis of CNTs is mainly classified into two categories. The first one is the atomic modeling, including the techniques such as classical molecular dynamics (MD) (Yakobson *et al*., 1997), tight binding molecular dynamics (TBMD) (Hernandez *et al*., 1998) and density functional theory (DFT) (Portal *et al*., 1999), which is only limited to systems with a small number of molecules and atoms and therefore only restrained to the study of small-scale modeling. On the other hand, continuum modeling is[1] practical in analyzing CNTs with large-scale sizes. Ru (Ru, 2000) proposed a double-walled carbon nanotube (DWNT) axial buckling load via the local elastic shell model. Zhang *et al*. (Zhang *et al*., 2006) investigated the small effect on elastic buckling of multi-walled carbon nanotubes (MWNT) under radial pressure. Wang (Wang *et al*., 2007) allowed for transverse inertia effect on static deformation of single walled carbon nanotube (SWNT). Wang (Wang, 2005) took into account transverse inertia effect on the wave phase velocity of CNTs. Yoon *et al*. (Yoon *et al*., 2004) considered transverse inertia effect on the wave

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phase velocity and critical frequency of CNTs.

The attenuation of the displacement amplitude in wave propagation due to the multiple scattering of CNTs is negligible because the size of CNTs is much smaller than the wave length. Therefore, the attenuation of the displacement amplitude in wave propagation is mostly induced by the viscous characteristic of CNTs. CNTs are remarkably resilient, sustaining extreme strain with no signs of brittleness, plasticity, or atomic rearrangements. CNTs are rolled up from some sheets of graphite (Yakobson *et al*., 1997) which is considered as a viscoelastic material. Two important parameters of relaxation and retardation time of one-dimensional stress wave propagation are needed for the study of the constitutive laws of CNTs. Ordinarily, relaxation and retardation time could be obtained via split Hopkinson pressure bar (SHPB) techniques (Zhao, 2003). Indeed transverse inertia has influence on relaxation and retardation time. Techniques of inverse analysis (Inoue *et al*., 2001) are adopted to estimate transverse inertia effect.

When CNTs are subjected to bending, torsion or axial compression, they snap from one shape to the next, emitting acoustic waves along its walls at every "crunch". These "crunchy molecules" never actually break, but reversibly accommodate to external stress. At large deformations of CNTs an abrupt release of energy is accompanied by a reversible transformation into a different morphological pattern. The manuscript derives the 6 order partial differential wave equation and analytic solutions of relaxation and retardation time of wave propagation in *N*-layered CNTs under an axial stress, which allow for transverse inertia effect. Such analytic solutions, hitherto unavailable in this form, are useful to how to eliminate transverse inertia effect when experimentally measuring relaxation and retardation time of CNTs.

Order partial differential wave equation in *n*-layered CNTS

One of the outstanding features of CNTs is their hollow circular cirque structure; they consist of atoms densely packed along a closed surface that defines the overall shape. The proposition for the material properties used in continuum viscoelastic bar model for wave propagation in CNTs will be studied through an analysis of N-layered CNTs shown in Fig.1. do and di are the diameters of outer and inner surfaces. The diameter of the mid surface circle is d. $h = Nt$ is the thickness, N layer number, t the equilibrium interlayer space of adjacent CNTs.

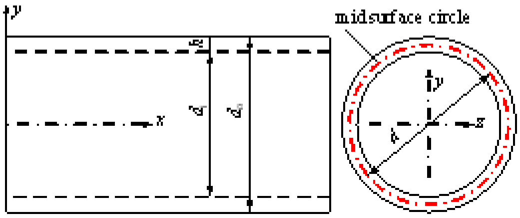


Fig. 1. Layout of *N*-layered CNTs.

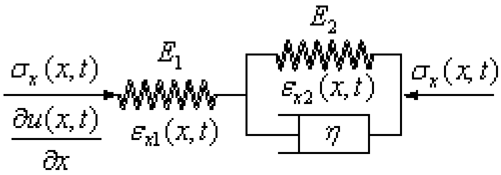


Fig. 2. Three-parameter solid of *N*-layered CNTs

Viscoelastic model of N-layered CNTs subjected to a uniaxial external stress $\sigma_x(x,t)$ is platted in Fig.2. The subscription x stands for the stress direction.

In the Love theory, the radial motion of a rod was postulated by a simple relation with the axial motion as (Wu et al., 1998)

$$v(x,y,t) = -\mu y \frac{\partial u(x,t)}{\partial x} \quad \text{...(1)}$$

$$w(x,z,t) = -\mu z \frac{\partial u(x,t)}{\partial x} \quad \text{...(2)}$$

where $u(x,t)$, $v(x,y,t)$ and $w(x,z,t)$ are the displacements of N-layered CNTs in the axial and radial directions respectively, μ Poisson ratio. Transverse inertial kinetic energy of an infinitesimal element $A\,dx$ in Fig.1 can be expressed as follows

$$T(x,t) = \frac{1}{2}\rho A dx \frac{\int_A \left\{\left[\frac{\partial v(x,y,t)}{\partial t}\right]^2 + \left[\frac{\partial w(x,z,t)}{\partial t}\right]^2\right\} dy dz}{A} = \frac{1}{2}\rho\mu^2 \frac{I_p}{A}\left[\frac{\partial^2 u(x,t)}{\partial x \partial t}\right]^2 A dx = \frac{1}{8}\rho\mu^2(d^2 + N^2t^2)\left[\frac{\partial^2 u(x,t)}{\partial x \partial t}\right]^2 A dx \quad \text{...(3)}$$

where $I_p = \pi N d t (d^2 + N^2 t^2)/4$ (not $I_p \overset{d \gg Nt}{\approx} \pi N d^3 t/4$ proposed by Wang and Varadan (Wang *et al.*, 2006) is an exact expression of the second polar moment of area for N-layered CNTs with no approximation, $A = \pi N d t$ the cross area of circular cirque, ρ the density.

Table 1 lists the relative error of second polar moment of area between Ref. (Wang *et al.*, 2006) and the manuscript at different values of N (Yu *et al.*, 2000).

Table 1. Error between reference (Wang *et al.*, 2006) and the manuscript

N	1	2	5	6
error/%	0.4337	1.7126	9.8205	13.5558
N	10	15	18	19
error/%	30.3427	49.4975	58.5294	61.1275

As is seen in table 1 that the larger N is, the larger the relative error becomes. Of course, such a surprising large error 61.1275% and essentially the hypothesis of $d \gg Nt$ are unacceptable with the increase of N.

From Fig.1 Newton second law of N-layered CNTs subjected to a uniaxial stress $\sigma_x(x,t)$ in x-axis direction can be written as

$$\frac{\partial \sigma_x(x,t)}{\partial x} = \rho \frac{\partial^2 u(x,t)}{\partial t^2} \quad \text{...(4)}$$

From the free body diagram of the infinitesimal element in Fig.1 or Fig.2, the work $A\sigma_x(x,t)\frac{\partial u(x,t)}{\partial x}\mathrm{d}x$ done by the external stress switches into the longitudinal strain energy $AE_1\varepsilon_{x1}(x,t)\frac{\partial u(x,t)}{\partial x}\mathrm{d}x$ in Fig.2 and transverse inertial dynamic energy expressed by Eq. (3), namely

$$A\sigma_x(x,t)\frac{\partial u(x,t)}{\partial x}\mathrm{d}x = AE_1\varepsilon_{x1}(x,t)\frac{\partial u(x,t)}{\partial x}\mathrm{d}x + \frac{1}{8}\rho\mu^2(d^2+N^2t^2)\left[\frac{\partial^2 u(x,t)}{\partial x \partial t}\right]^2 A\mathrm{d}x \quad \text{... (5)}$$

Differentiating Eq. (5) with respect to *t* once infers

$$\sigma_x(x,t)\frac{\partial^2 u(x,t)}{\partial x \partial t} = E_1\varepsilon_{x1}(x,t)\frac{\partial^2 u(x,t)}{\partial x \partial t} + \frac{1}{4}\rho\mu^2(d^2+N^2t^2)\frac{\partial^2 u(x,t)}{\partial x \partial t}\frac{\partial^3 u(x,t)}{\partial x \partial t^2} \quad \text{...(6)}$$

From Eq. (6) it is easy to obtain that

$$\sigma_x(x,t) = E_1\varepsilon_{x1}(x,t) + \frac{1}{4}\rho\mu^2(d^2+N^2t^2)\frac{\partial^3 u(x,t)}{\partial x \partial t^2} \quad \text{...(7)}$$

The constitutive relations in Fig.2 can be expressed as

$$E_1\varepsilon_{x1}(x,t) = E_2\varepsilon_{x2}(x,t) + \eta\frac{\partial \varepsilon_{x2}(x,t)}{\partial t} \quad \text{...(8)}$$

$$\varepsilon_{x1}(x,t) + \varepsilon_{x2}(x,t) = \frac{\partial u(x,t)}{\partial x} \quad \text{...(9)}$$

Substitution of Eq. (8) into Eq. (7) and using Eq. (9) yield

$$E_1\eta\frac{\partial \varepsilon_{x2}(x,t)}{\partial t} = (E_1+E_2)\sigma_x(x,t) - E_1E_2\frac{\partial u(x,t)}{\partial x} - \frac{1}{4}\rho\mu^2(d^2+N^2t^2)(E_1+E_2)\frac{\partial^3 u(x,t)}{\partial x \partial t^2} \quad \text{...(10)}$$

Substituting Eq. (8) into Eq. (7) results in

$A\mathrm{d}x$

$$\eta\frac{\partial \varepsilon_{x2}(x,t)}{\partial t} = \sigma_x(x,t) - \frac{1}{4}\rho\mu^2(d^2+N^2t^2)\frac{\partial^3 u(x,t)}{\partial x \partial t^2} - E_2\varepsilon_{x2}(x,t) \quad \text{...(11)}$$

Differentiating Eq. (7) with respect to *t* once and using Eq. (9) derive

$$\frac{\partial \sigma_x(x,t)}{\partial t} = E_1\frac{\partial^2 u(x,t)}{\partial x \partial t} - E_1\frac{\partial \varepsilon_{x2}(x,t)}{\partial t} + \frac{1}{4}\rho\mu^2(d^2+N^2t^2)\frac{\partial^4 u(x,t)}{\partial x \partial t^3} \quad \text{...(12)}$$

It is simple to deduce from Eqs. (11)-(12)

$$E_1E_2\eta\varepsilon_{x2}(x,t) = \eta^2\frac{\partial \sigma_x(x,t)}{\partial t} + E_1\eta\sigma_x(x,t) - E_1\eta^2\frac{\partial^2 u(x,t)}{\partial x \partial t} - \frac{1}{4}\rho\mu^2(d^2+N^2t^2)\eta^2\frac{\partial^4 u(x,t)}{\partial x \partial t^3} - \frac{1}{4}\rho\mu^2(d^2+N^2t^2)E_1\eta\frac{\partial^3 u(x,t)}{\partial x \partial t^2} \quad \text{...(13)}$$

By differentiating Eq. (10) with respect to *x* once and employing Eq. (4) it can acquire that

$$E_1\eta\frac{\partial^2\varepsilon_{x2}(x,t)}{\partial x\partial t}=\rho(E_1+E_2)\frac{\partial^2 u(x,t)}{\partial t^2}-E_1E_2\frac{\partial^2 u(x,t)}{\partial x^2}-\frac{1}{4}\rho\mu^2(d^2+N^2t^2)(E_1+E_2)\frac{\partial^4 u(x,t)}{\partial x^2\partial t^2}\quad ...(14)$$

Differentiating Eq. (13) with respect to *x* and *t* once simultaneously and using Eq. (4) can result in

$$E_1E_2\eta\frac{\partial^2\varepsilon_{x2}(x,t)}{\partial x\partial t}=\rho\eta^2\frac{\partial^4 u(x,t)}{\partial t^4}+\rho E_1\eta\frac{\partial^3 u(x,t)}{\partial t^3}-E_1\eta^2\frac{\partial^4 u(x,t)}{\partial x^2\partial t^2}-\frac{1}{4}\rho\mu^2(d^2+N^2t^2)\eta^2\frac{\partial^6 u(x,t)}{\partial x^2\partial t^4}-\frac{1}{4}\rho\mu^2(d^2+N^2t^2)E_1\eta\frac{\partial^5 u(x,t)}{\partial x^2\partial t^3}\quad ...(15)$$

By Eq. (15) dividing Eq. (14), the 6 order partial differential wave equation in *N*-layered CNTs is derived as

$$\rho\eta^2\frac{\partial^4 u(x,t)}{\partial t^4}+\rho E_1\eta\frac{\partial^3 u(x,t)}{\partial t^3}-\rho(E_1+E_2)E_2\frac{\partial^2 u(x,t)}{\partial t^2}=\frac{1}{4}\rho\mu^2(d^2+N^2t^2)\eta^2\frac{\partial^6 u(x,t)}{\partial x^2\partial t^4}+\frac{1}{4}\rho\mu^2(d^2+N^2t^2)E_1\eta\frac{\partial^5 u(x,t)}{\partial x^2\partial t^3}+[E_1\eta^2-\frac{1}{4}\rho\mu^2(d^2+N^2t^2)(E_1+E_2)E_2]\frac{\partial^4 u(x,t)}{\partial x^2\partial t^2}-E_1E_2^2\frac{\partial^2 u(x,t)}{\partial x^2}\quad ...(16)$$

For a harmonic longitudinal wave propagation in the infinite *N*-layered CNTs governed by the wave equation (16), one solution can be written in complex form as (Zhao *et al*., 1995)

$$u(x,t)=U\,e^{-(\alpha+i\omega/c)x}\,e^{i\omega t}\quad ...(17)$$

$$\omega=2\pi c/\lambda\quad ...(18)$$

where , and *c* are the angular frequency, attenuation coefficient of displacement amplitude and phase velocity in CNTs wave propagation respectively, the wave length.
Substitution of Eq. (17) into Eq. (16) concludes

$$\rho\omega^4\eta^2-i\rho\omega^3E_1\eta+\rho\omega^2(E_1+E_2)E_2=\frac{1}{4}\rho\mu^2(d^2+N^2t^2)\omega^4(\alpha^2-\omega^2/c^2+i2\omega\alpha/c)\eta^2+\frac{1}{4}\rho\mu^2(d^2+N^2t^2)\omega^3[2\omega\alpha/c+i(\omega^2/c^2-\alpha^2)]E_1\eta+[E_1\eta^2-\frac{1}{4}\rho\mu^2(d^2+N^2t^2)(E_1+E_2)E_2]\times\omega^2(\omega^2/c^2-\alpha^2-i2\omega\alpha/c)+(\omega^2/c^2-\alpha^2-i2\omega\alpha/c)E_1E_2^2\quad ...(19)$$

From the real and imaginary part of Eq. (19) one can obtain two identities as below

$$\rho\omega^4\eta^2+\rho\omega^2(E_1+E_2)E_2=\frac{1}{4}\rho\mu^2(d^2+N^2t^2)\omega^4(\alpha^2-\omega^2/c^2)\eta^2+\frac{1}{2}\rho\mu^2(d^2+N^2t^2)\omega^4\alpha E_1\eta/c+[E_1\eta^2-\frac{1}{4}\rho\mu^2(d^2+N^2t^2)(E_1+E_2)E_2]\omega^2(\omega^2/c^2-\alpha^2)+(\omega^2/c^2-\alpha^2)E_1E_2^2\quad ...(20)$$

$$-\rho\omega^3E_1\eta=\frac{1}{2}\rho\mu^2(d^2+N^2t^2)\omega^5\alpha\eta^2/c+\frac{1}{4}\rho\mu^2(d^2+N^2t^2)\omega^3(\omega^2/c^2-\alpha^2)E_1\eta-2[E_1\eta^2-\frac{1}{4}\rho\mu^2(d^2+N^2t^2)(E_1+E_2)E_2]\omega^3\alpha/c-2\omega\alpha E_1E_2^2/c\quad ...(21)$$

In the first instance, introduction of assuming $E_2=0$ into Eqs. (20)-(21) yields

$E_1=+\infty$

$$\frac{\omega^2/c^2-\alpha^2}{\rho\omega^2}E_1\eta=\eta+\frac{1}{4}\mu^2(d^2+N^2t^2)(\omega^2/c^2-\alpha^2)\eta-\frac{1}{2}\mu^2(d^2+N^2t^2)\alpha E_1/c\quad ...(22)$$

$$\frac{2\alpha}{\rho c}E_1\eta=E_1+\frac{1}{2}\mu^2(d^2+N^2t^2)\omega^2\alpha\eta/c+\frac{1}{4}\mu^2(d^2+N^2t^2)(\omega^2/c^2-\alpha^2)E_1\quad ...(23)$$

Eq. (22) dividing Eq. (23) and adopting Eq. (18) lead to the dimensionless relaxation time of *N*-layered CNTs as below

$$\tau_M^*=\frac{\eta/E_1}{\frac{\omega^2-c^2\alpha^2}{2\omega^2c\alpha}}=1+\frac{\pi^2\mu^2(d^2+N^2t^2)(\omega^2+c^2\alpha^2)^2}{\lambda^2\omega^2(\omega^2-c^2\alpha^2)}\quad ...(24)$$

As can be seen that Eq. (24) reduces to the classical result of Maxwell rheological model when transverse inertia effect is not been considered, viz. $(d^2+N^2t^2)/\lambda^2$ is so small that it can be taken as zero. Physical interpretation is that the parameter $i_p=(d^2+N^2t^2)/4$ that can reflect transverse inertia effect is the polar gyration radius of the *N*-layered CNTs.

In the second instance, substitution of assuming into Eqs. (20)-(21) results in

$$\frac{\omega^2/c^2-\alpha^2}{\rho\omega^2}(\omega^2\eta^2+E_1^2)=E_1-\frac{1}{2}\mu^2(d^2+N^2t^2)\omega^2\alpha\eta/c+\frac{1}{4}\mu^2(d^2+N^2t^2)(\omega^2/c^2-\alpha^2)E_1 \quad ...(25)$$

$$\frac{2\alpha}{\rho\omega c}(\omega^2\eta^2+E_2^2)=\frac{1}{4}\mu^2(d^2+N^2t^2)\omega(\omega^2/c^2-\alpha^2)\eta+\frac{1}{2}\mu^2(d^2+N^2t^2)\omega\alpha E_2/c+\omega\eta \quad ...(26)$$

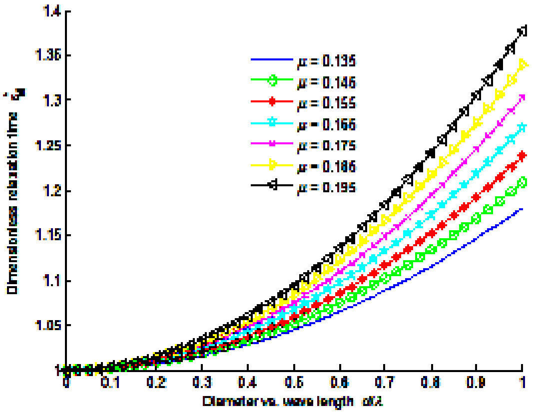
Eq. (25) dividing Eq. (26) and using Eq. (18) lead to the dimensionless retardation time of N-layered CNTs as follows

$$\tau_K^*=\frac{\eta/E_2}{\dfrac{2c\alpha}{\omega^2-c^2\alpha^2}}=\frac{\lambda^2\omega^2(\omega^2-c^2\alpha^2)}{\lambda^2\omega^2(\omega^2-c^2\alpha^2)+\pi^2\mu^2(d^2+N^2t^2)(\omega^2+c^2\alpha^2)^2} \quad ...(27)$$

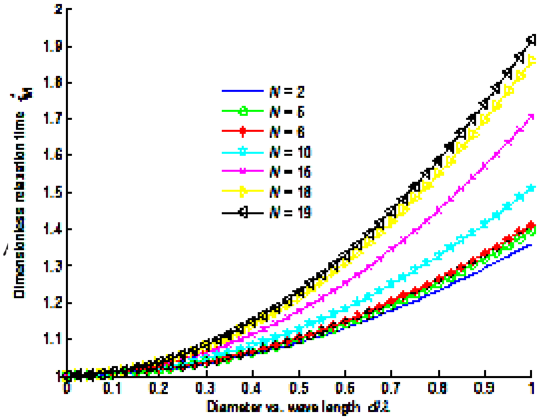
Similarly, as can be observed that Eq. (27) reduces to the classical result of Kelvin solid model when transverse inertia effect is not been allowed for, namely $(d^2+N^2t^2)/\lambda^2$ becomes so small that it can be tackled as zero.

Relaxation and retardation time of wave equation in *n*-layered CNTS

As an example, isotropic N-layered CNTs are studied. Such parameters are given below as $\rho=2.3\times10^3$ kg/m³, (Wang *et al.*, 2006), $\mu_2=0.19$ (Yakobson *et al.*, 1996, Zhu *et al.*, 2008), elastic modulus $E=5.5$ TPa, nm, flexural rigidity $D=Et^3/[12(1-\mu^2)]=0.85$ eV, in-plane stiffness $C=Et=59$ eV/atom $=360$ J/

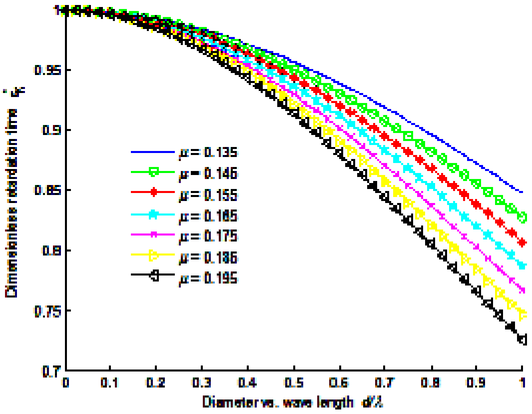


(a) Dimensionless relaxation time at N =1

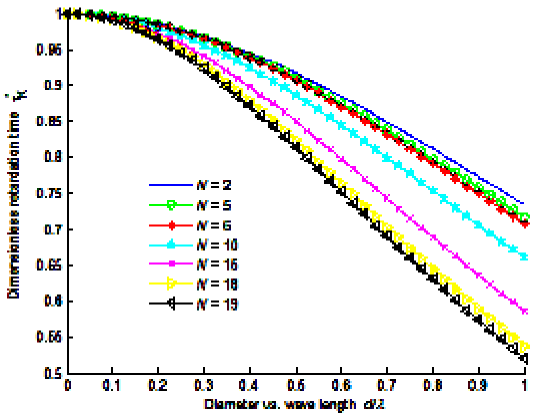


(b) Dimensionless relaxation time at μ = 0.19

Fig. 3. Dimensionless relaxation time of CNTs



(a) Dimensionless relaxation time at N =1



(b) Dimensionless relaxation time at μ = 0.19

Fig. 4. Dimensionless relaxation time of CNTs

m^2 as a virtually constant parameter, $d = 1$ nm, $\omega = 1$ THz, $c = 11795$ m/s (Yoon *et al*., 2004), $\alpha = 1.36$ m^{-1}, $\lambda = 1 \sim 60$ nm.

Fig.3 provides the dimensionless relaxation time of wave propagation in *N*-layered CNTs at different Poisson ratios and layer numbers. The transverse inertial effect results in the increase of relaxation time of wave propagation with increasing Poisson ratio, ratio of diameter to wave length and layer number.

Fig.4 shows the dimensionless retardation time of wave propagation in *N*-layered CNTs at different Poisson ratios and layer numbers. The transverse inertial effect induces the decrease of retardation time of wave propagation with increasing Poisson ratio, ratio of diameter to wave length and layer number.

CONCLUSIONS

The transverse inertia effect taken into account, the general solutions for the dimensionless relaxation and retardation time of wave propagation in *N*-layered CNTs subjected to a uniaxial stress are deduced. The general solutions for the dimensionless relaxation and retardation time of wave propagation can reduce to the classical results of Maxwell rheological model and Kelvin solid model separately when transverse inertia effect is not been allowed for.

The transverse inertial effect results in the increase of relaxation time of wave propagation with increasing Poisson ratio, ratio of diameter to wave length and layer number. The transverse inertial effect induces the decrease of retardation time of wave propagation with increasing Poisson ratio, ratio of diameter to wave length and layer number.

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