# Nonlinear Oscillations of a Double-Walled Carbon Nanotube

Muhammad A. Hawwa[a] & Hussain M. Al-Qahtani[b*]

Department of Mechanical Engineering

King Fahd University of Petroleum & Minerals

Dhahran 31261, Saudi Arabia

Fax: (+9663) 860 2949

E-mails:

(a) drmafh@kfupm.edu.sa

(b) qahtanih@kfupm.edu.sa

*corresponding author

## Abstract

An elastic continuum approach for modeling the nonlinear vibration of a double-walled carbon nanotubes under harmonic excitation is presented. The carbon nanotube is modeled as two doubly clamped beams coupled through nonlinear continuous springs representing Van der Waal bonds. Geometric nonlinearity is included due to mid-plane stretching. A Galerkin approach is used to discretize the integro-partial differential equation leading to two nonlinear coupled second-order ordinary differential governing equations. The numerically obtained dynamic response to a primary-resonance exciting the co-axially first and second vibration modes is investigated through frequency response, periodic and chaotic motions characteristics.


**Keywords:** Carbon Nanotubes; Continuum modeling; Nonlinear Oscillations; Chaotic Behavior

# 1 Introduction

Double-walled carbon nanotubes are interesting special cases of multi-walled carbon nanotubes, each consisting of two concentrically nested seamless graphene cylinders bonded together by van der Waal forces. Double-walled carbon nanotubes can be simply generated by breaking the C60 molecules encapsulated in single-walled carbon nanotubes[1]. The uniqueness of double-walled carbon nanotubes stems from the fact that they are more resistant to chemicals than single-walled carbon nanotubes[2]. As promising building blocks for emerging nanoelectronics, nanodevices, and nanocomposites, double-walled carbon nanotubes have recently received the attention of several researchers. Raman experimental studies have been performed on double-walled carbon nanotubes to identify the modes associated with inner and outer tubes[3–9].

The dynamic behavior of double-walled carbon nanotubes has been also explored theoretically using molecular dynamics simulations and elastic continuum mechanics modeling. The utilization of the continuum approach is computationally less involved than the molecular approach. Continuum models are considered important in studying nano-vibration where it is proved to be difficult to measure physical parameters. The utilization of elastic continuum theories has been gaining more momentum over the past few years. In a series of papers, Zhang et al.[10–12] utilized a nonlocal double-elastic beam model for studying the free transverse vibrations of double-walled carbon nanotubes, considering the effects of a small length scale, a compressive axial load, and a temperature change. Xu et al.[13] used the harmonic balance method to analyze the amplitudes-frequency relationship for free nonlinear vibrations of a double-walled carbon nanotube having nonlinear interlayer van der Waals forces. Ece and Aydogdu[14] used a nonlocal elasticity Timoshenko-beam theory to study the influence of in-plane loads on the natural frequencies of simply supported double-walled carbon nanotubes. Xu et al.[15] calculated the first seven order resonant frequencies and their relative vibration modes for a double-walled carbon nanotube under the assumption of different boundary conditions between the inner and outer tubes. Yan et al.[16] modeled the nonlinear free vibration behaviors of double-walled carbon nanotubes in the context of the Donnell's cylindrical shell and used the harmonic balance method to find the amplitudes-frequencies relationship. Natsuki et al.[17] analyzed the vibration characteristics of double-walled carbon nanotubes with simply supported boundary conditions using the Euler-Bernoulli beam theory.

In this paper, the forced vibration problem of a double-walled carbon nanotube is modeled under the context of the continuum theory. The nano structure is represented by two parallel beams coupled by nonlinear springs representing Van der Wall bonds and clamped at both ends. The two coupled elastic beams model is made general to encompass geometric nonlinearity due to mid-plane stretching. A transverse harmonic load is applied at the outer wall of the double-walled carbon nanotube. A single-mode Galerkin approximation is used to convert nonlinear integral-differential equations governing the motion of the nanotube into a system of two second-order nonlinear ordinary differential equations. A shooting numerical method is used to integrate the equations and investigate periodic as well as chaotic behavior of the system.

## 2 Mathematical Formulation

Carbon nanotubes can by schematically thought of as rolled graphene layers. To mathematically express the way of rolling, a chirality vector is defined. Depending on chirality, nanotubes are classified into the arm-chair, the zig-zag, or the chiral type. In addition, carbon nanotubes can be made to have different inner radii. The chirality and radius of a carbon nanotube are important factors in deciding its physical properties such as density ($\rho$) and modulus of elasticity ($E$)[18,19]. Hence, each of the two nested carbon nanotubes will be modeled as an individual elastic beam with different density and stiffness. The two beams are coupled by Van der Waal bonds, which are modeled as distributed nonlinear elastic springs as shown in Fig. 1. The elastic beams, representing the nested carbon nanotubes are considered to be doubly clamped at both ends which represent a source and a drain. The fixed-fixed boundary conditions are assumed to cause bending induced tension, which gives rise to a nonlinear mid-plane stretching effect. The outer carbon nanotube is excited by a time dependent driving force. Then, the equations of motion are:

$$E_1 I_1 \frac{\partial^4 w_1}{\partial x^4} + c_1(w_1 - w_2) + c_3(w_1 - w_2)^3 + A_1\rho_1 \frac{\partial^2 w_1}{\partial t^2} = \frac{A_1 E_1}{L}\left(\int_0^L \frac{1}{2}\frac{\partial w_1}{\partial x}^2 dx\right)\frac{\partial^2 w_1}{\partial x^2} \quad (1)$$

$$E_2 I_2 \frac{\partial^4 w_2}{\partial x^4} + 2\xi\frac{\partial w_2}{\partial t} + c_1(w_2 - w_1) + c_3(w_2 - w_1)^3 + A_2\rho \frac{\partial^2 w_2}{\partial t^2} = \frac{A_2 E_2}{L}\left(\int_0^L \frac{1}{2}\frac{\partial w_2}{\partial x}^2 dx\right)\frac{\partial^2 w_2}{\partial x^2} + F\cos(\Omega t) \quad (2)$$

where $E_j$, $j = 1, 2$ is the moduli of elasticity, $I_j$ is the area moment of inertia, $\rho_j$ is the mass densities, $A_j$ is the cross sectional area, $F$ is the spatial distribution of the transverse load, $\Omega$ is the frequency of transverse loading, $L$ is the length of the carbon nanotube, and $x$ and $t$ are the spatial and time coordinates, respectively. $c_1$ and $c_2$ are the Van der Waal interlayer interaction coefficients. Note that a phenomenological viscous damping is included in the problem formulation, and is represented by the coefficient $\xi$. The integral-differential equations of motion contain a nonlinear mid-plane stretching effect due to a bending induced tension.

At the supports, the nested carbon nanotubes are subjected to the following boundary conditions:

$$w_1 = \frac{\partial w_1}{\partial x} \quad \text{at} \quad x = 0, L \quad (3)$$

$$w_2 = \frac{\partial w_2}{\partial x} \quad \text{at} \quad x = 0, L \quad (4)$$

In order to solve the system defined by Eqs. (1-4) to obtain the first mode resonance case, a Galerkin procedure is followed. Assuming a coaxial deflection in the two nested nanotubes; the displacements can be written as $w_i = X_i(x)T_i(t)$, $i = 1, 2$, where the basis function $X_i(x)$ takes a very close profile to the first-order mode shape. i,e. $X(x) = (1 - \cos(2\pi x/L))$. We substitute this into Eqs. (1) and (2), multiply the result by $X(x)$, then integrate over the domain [0-L]. Afterwards, the obtained equations are normalized using $R$ (the inner radius of the inner nanotube) as a characteristic length and $1/\omega_0$ ($\omega_0$ is the fundamental frequency) as a characteristic time to get the following nondimensional governing equations:

$$\ddot{T}_1 + \hat{a_1}T_1 + \hat{c_1}T_1^3 + \hat{d_1}T_2 + \hat{e_1}T_2^2T_1 + \hat{f_1}T_2T_1^2 + \hat{h_1}T_2^3 = 0 \quad (5)$$

$$\ddot{T}_2 + \mu\dot{T}_2 + \hat{a_2}T_2 + \hat{c_2}T_2^3 + \hat{d_2}T_1 + \hat{e_2}T_2T_1^2 + \hat{f_2}T_2^2T_1 + \hat{h_2}T_1^3 = \cos(\Omega t)\hat{g} \quad (6)$$

where the coefficients are explicitly written in the Appendix.

# 3 Numerical Results and Discussion

For numerical illustrations, let us consider a double-walled carbon nanotube having a length $L = 60$ nm and the properties given in Table (1).

The areas and the moments of inertia are calculated using $A = \frac{\pi}{4}(d_o^2 - d_i^2)$ and $I = \frac{\pi}{64}(d_o^4 - d_i^4)$, respectively. The Van der Waal interaction coefficients are $c_1 = 71.11$GPa and $c_3 = 2.57 \times 10^4$ GPa/nm$^2$. The damping coefficient is taken to be 0.1.

In order to investigate the frequency response curves of the two coupled beams system, let us monitor the vibration amplitudes, while fixing all parameters and slowly varying the excitation frequency as a control parameter. It is observed in Fig. 2 that the amplitudes of the first and second modes vary as smooth functions of the excitation frequency; the two curves bend to the right side which indicates a hardening spring behavior; but a clear jump phenomena occurs.

The analysis of periodic and chaotic motions is then performed using a fourth-order Runge-Kutta algorithm. The Matlab ® subroutine `ode45` was used to solve the differential equations since it is recommended in the Matlab manual to be the first choice due to its accuracy. The time window used for integrating the differential equation is $t = 300\,T$ where the period $T = 2\pi/f$ with a time step $\Delta t = T/3000$. It is worthy to note that all the figures were developed for nondimensional quantities.

The excitation amplitude is used as a controlling parameter over a wide (though practical) range of variation, while keeping the excitation frequency fixed. The bifurcation diagrams for the case of a uniform harmonic excitation whose nondimensional frequency $\omega = 1.0$ is shown in Fig. 3. By increasing the excitation amplitude, the response of the first and second modes undergoes the following stages: Period doubling bifurcation, Subharmonic response, Quasi-periodic response and, Chaotic behavior.

Figure 4 shows the phase plane (portrait), the Poincaré map (section), and the time history for the first and second modes. A period-one motion prevails at $f = 10$, a period-three motion occurs at $f = 15$, while a chaotic behavior takes place as clear at $f = 30$.

## 4 Conclusion

The nonlinear response of a double-walled carbon nanotube excited at its primary resonances was considered. The problem was modeled in the context of an elastic continuum beam theory, where the double-walled carbon nanotube was looked at as two coupled beams clamped at a source and a drain. Geometric nonlinearity in the form of mid-plane stretching and physical nonlinearity in the form of nonlinear VdW forces were included. The mathematical model was reduced to two governing integro-partial differential equations and associated boundary conditions. Using an approximate linear vibration mode as a trial function, Galerkin procedure led to a set of two nonlinearly coupled second-order ordinary differential equations in time. Utilizing numerical integration, the dynamic response of the double-walled carbon nanotube illustrated hardening nonlinear characteristics. The transition from quasiperiodic to chaotic behavior was analyzed showing nonlinear jump phenomena and nonlinear bifurcations leading to chaos.

# Appendix

$$\hat{a_1} = \frac{c_1}{a_1\rho\omega_0^2} + \frac{16EI_1\pi^4}{3a_1L^4\rho\omega_0^2} \qquad \mu = \frac{2\xi}{a_2\rho\omega_0}$$

$$\hat{c_1} = \frac{35c_3L^2}{12a_1\rho\omega_0^2} + \frac{4E_1\pi^4}{3\rho\omega_0^2L^2} \qquad \hat{a_2} = \frac{c_1}{a_2\rho\omega_0^2} + \frac{16EI_2\pi^4}{3a_2L^4\rho\omega_0}^2$$

$$\hat{d_1} = -\frac{c_1}{a_1\rho\omega_0^2} \qquad \hat{c_2} = \frac{35c_3L^2}{12a_2\rho\omega_0^2}$$

$$\hat{e_1} = \frac{35c_3L^2}{4a_1\rho\omega_0^2} \qquad \hat{d_2} = -\frac{c_1}{a_2\rho\omega_0^2}$$

$$\hat{f_1} = -\frac{35c_3L^2}{4a_1\rho\omega_0^2} \qquad \hat{e_2} = \frac{35c_3L^2}{4a_2\rho\omega_0^2}$$

$$\hat{h_1} = -\frac{35c_3L^2}{12a_1\rho\omega_0^2} \qquad \hat{f_2} = -\frac{35c_3L^2}{4a_2\rho\omega_0^2}$$

$$\hat{g} = \frac{2F}{3a_2L\rho\omega_0^2} \qquad \hat{h_2} = -\frac{35c_3L^2}{12a_2\rho\omega_0^2}$$

# References


[1] D. E. Luzzi and B. W. Smith. *Science and Applications of Nanotubes*, page 67. Kluwer Academic Press, 2000.

[2] E. Flahaut, R. Bacsa, A. Peigney, and C. Laurent. Gram-scale ccvd synthesis of double-walled carbon nanotubes. *Chemical Communications*, 12:1442–1443, 2003.

[3] S. Bandow, M. Takizawa, K. Hirahara, M. Yudasaka, and S. Iijima. Raman scattering study of double-wall carbon nanotubes derived from the chains of fullerenes in single-wall carbon nanotubes. *Chemical Physics Letters*, 337:48–54, 2001.

[4] W. Ren, F. Li, and H. M. Cheng. Polarized raman analysis of aligned double-walled carbon nanotubes. *Physical Review B*, 71:115428: 1–5, 2005.

[5] S. Bandow, G. Chen, G. U. Sumanasekera, R. Gupta, M. Yudasaka, S. Iijima, and P. C. Eklund. Diameter-selective resonant raman scattering in double-wall carbon nanotubes. *PHYS. REV. B*, 66:075416: 1–8, 2002.

[6] Ci Lijie, Zhenping Zhou, Xiaoqin Yan, Dongfang Liu, Huajun Yuan, Li Song, Yan Gao, Jianxiong Wang, Lifeng Liu, Weiya Zhou, Gang Wang, and Sishen Xie. Resonant raman scattering of double wall carbon nanotubes prepared by chemical vapor deposition method. *Journal of Applied Physics*, 94:5715–5719, 2003.

[7] J. Wei, B. Jiang, X. Zhang, H. Zhu, and D. Wu. Raman study on double-walled carbon nanotubes. *Chemical Physics Letters*, 376:753–757, 2003.

[8] J. Maultzsch, S. Reich, P. Ordejan, R. R. Bacsa, W. Bacsa, E. Dobardi, M. Damnjanovi, and C. Thomsen. Vibrational properties of double-walled carbon nanotubes. volume 685, pages 324–327. AIP Conf., October 2003.

[9] F. Li, S. G. Chou, W. Ren, J. A. Gardecki, A. K. Swan, M. S. Unlu, B. B. Goldberg, and M. S. Dresselhaus. Identification of the constituents of double-walled carbon nanotubes using raman spectra taken with different laser-excitation energies. *Journal of Materials Research*, 18:1251–1258, 2003.

[10] Y. Q. Zhang, G. R. Liu, and X. Y. Xie. Free transverse vibrations of double-walled carbon nanotubes using a theory of nonlocal elasticity. *Physical Review B*, 71:195404: 1–7, 2005.

[11] Y. Q. Zhang, X. Liu, and G. R. Liu. Thermal effect on transverse vibrations of double-walled carbon nanotubes. *Nanotechnology*, 18:445701: 1–7, 2007.

[12] Y. Zhang, G. Liu, and X. Han. Transverse vibrations of double-walled carbon nanotubes under compressive axial load. *Physics Letters A*, 340:258–266, 2005.

[13] K. Y. Xu, X. N. Guo, and C. Q. Ru. Vibration of a double-walled carbon nanotube aroused by nonlinear intertube van der waals forces. *Journal of Applied Physics*, 99:064303: 1–7, 2006.

[14] M. C. Ece and M. Aydogdu. Nonlocal elasticity effect on vibration of in-plane loaded double-walled carbon nanotubes. *Acta Mechanica*, 190:185–195, 2007.

[15] K. Y. Xu, E. C. Aifantis, and Y. H. Yan. Vibrations of double-walled carbon nanotubes with different boundary conditions between inner and outer tubes. *Journal of Applied Mechanics*, 75:131–139, 2008.

[16] Y. Yan, L. X. Zhang, and W. Q. Wang. Dynamical mode transitions of simply supported double-walled carbon nanotubes based on an elastic shell model. *Journal of Applied Physics*, 103:113523: 1–6, 2008.

[17] T. Natsuki, Q. Q. Ni, and M. Endo. Analysis of the vibration characteristics of double-walled carbon nanotubes. *Carbon*, 46:1570–1573, 2008.

[18] M. Meo and M. Rossi. Prediction of young's modulus of single wall carbon nanotubes by momolecular -mechanics based finite element modeling. *Composite Science and Technology*, 66:1597–1605, 2006.

[19] K. Chandraseker and S. Mukherjee. Atomistic-continuum and ab initio estimation of the elastic moduli of single-walled carbon nanotubes. *Computational Materials Science*, 40:147–158, 2007.

# List of Tables

## List of Figures

# Figures

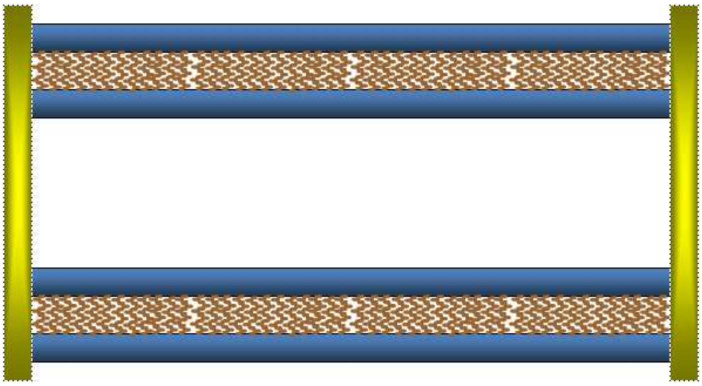

Figure 1: The double-walled carbon nanotube cross section.

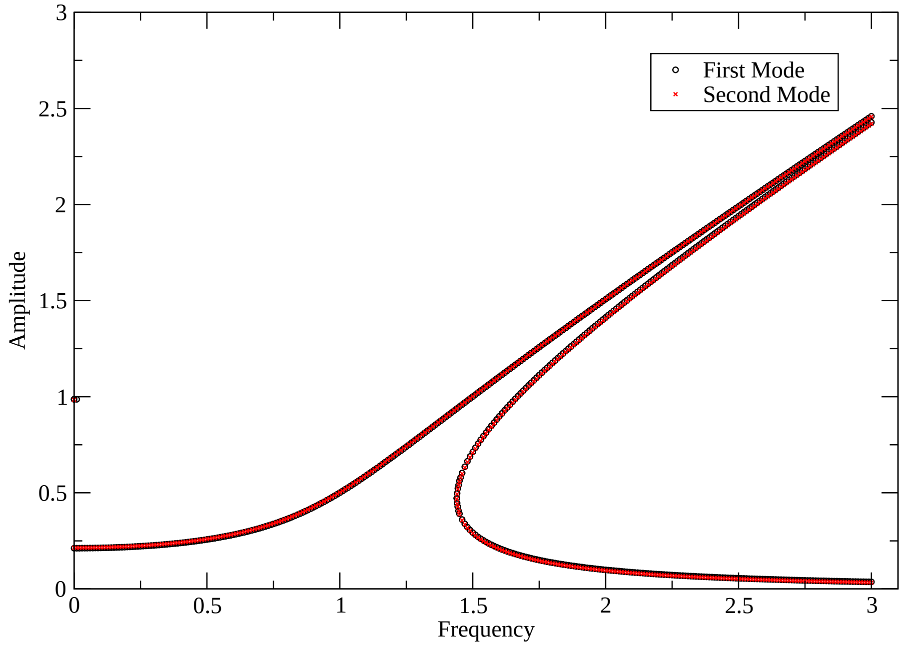


Figure 2: Frequency response of the double CNT.

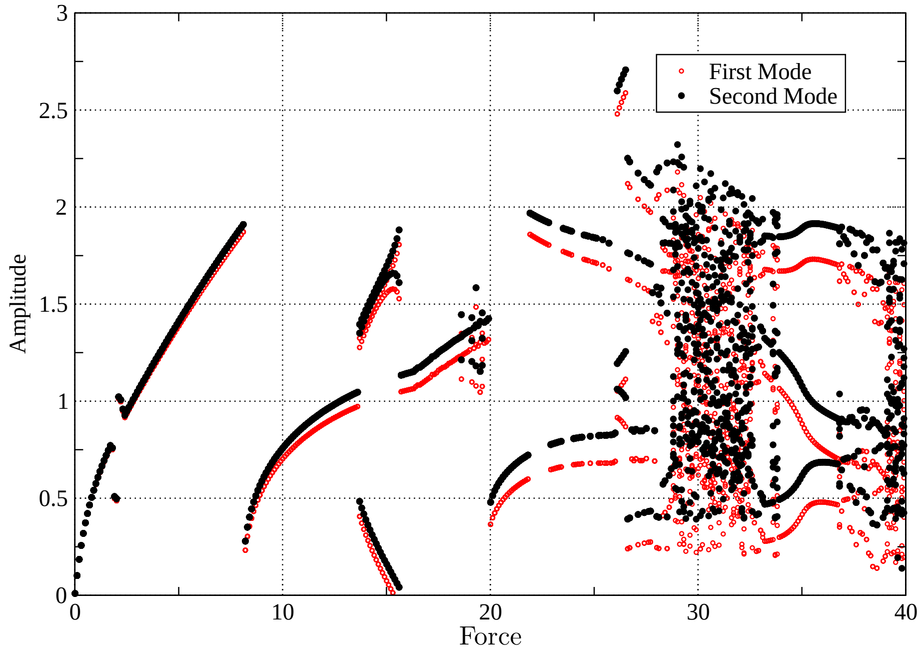


Figure 3: Bifurcation diagram of CNT first mode.

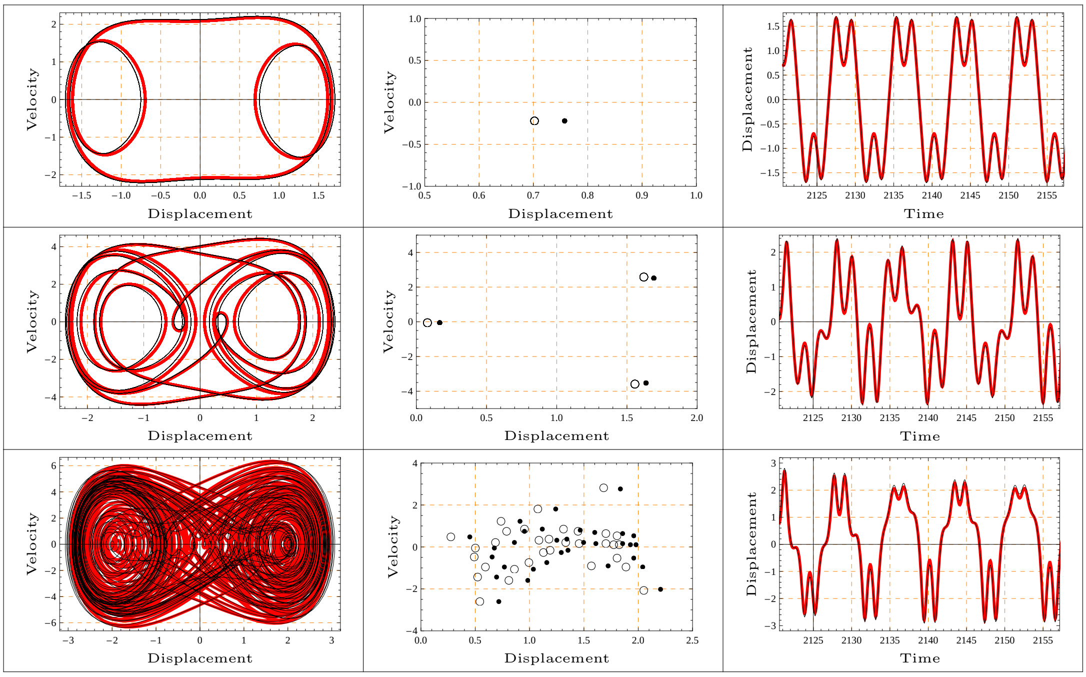


Figure 4: Phase portrait, Poincare section and time history of CNT second mode at $f = 10, 15, 30$.

## Tables

Table 1: Physical and geometrical data of the double-walled CNT

| $\rho_1$( kg/m$^3$) | $\rho_2$ (kg/m$^3$) | $E_1$ (TPa) | $E_2$ (TPa) | $D_i$ (nm) | thickness (nm) | annulus (nm) |
|---|---|---|---|---|---|---|
| $1.13 \times 10^3$ | $1.13 \times 10^3$ | 0.926 | 0.923 | 5 | 0.34 | 0.142 |