Molecular investigation of the mechanical properties of single actin filaments based on the vibration analysis

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ABSTRACT: The continuum beam model had been used to predict the mechanical properties of single actin filaments on continuum mechanics level. However, this continuum model clearly has limitations to represent the nanoscale single actin filaments. In this paper, the mechanical vibration properties of single actin filaments with lengths from 50 to 288 nm are numerically investigated by the molecular simulation, i.e., the Coarse Grain Molecular Dynamics (CGMD) simulations. The Fast Fourier Transform (FFT) power spectrum analysis is then applied to the periodic motion information from the molecular simulations to extract the natural frequencies of the simulated single actin filaments. The natural frequencies obtained from the molecular simulations are compared with the Normal Mode Solution (NMS) of the equivalent Euler-Bernoulli beams, and the mechanical properties including the flexural rigidity and the Young's modulus are then evaluated. Based on the convergence study of the mechanical properties with respect to the filament length, it has found that the Euler-Bernoulli beam model can only be reliably used when the aspect ratio of the single actin filament is larger than 17. Hence, this molecular investigation not only provides the evidence for the use of the continuum beam model in characterizing the mechanical properties of single actin filaments, but also clarifies the criteria for the effective use of the Euler-Bernoulli beam model.

Keywords*: Actin filament; Mechanical vibration; Flexural rigidity; Young's modulus; Coarse-Grained Molecular Dynamics*

Introduction

The cytoskeleton is the structural fundament for an eukaryotic cell to resist deformations due to external loads (Fletcher and Mullins 2010). Microfilament, intermediate filament and microtubule are three principal cytoskeleton elements (Cossart 2005). Among these three cytoskeleton components, microfilament is discovered in non-muscle cells, which indicates that the mechanical behaviours of the microfilament networks may regulate the cellular change and the force generation in cell migration and division (Stossel et al. 2001; Pollard 1976; Pantaloni et al. 2001; Pollard et al. 2000). As the principal component of microfilaments, mechanical properties of single actin filaments should be focused to understand the mechanical performances of the microfilament.

As the development of experiment techniques in last few decades, scholars experimentally studied the flexural rigidity and the Young's modulus of single actin filament by either directly stretching tests (Shin et al. 2004; Dupuis et al. 1997; Liu and Pollack 2002; Kojima et al. 1994), or thermal fluctuation analysis (Gittes et al. 1993; Janmey et al. 2001; Huxley et al. 1994). By employing the mechanical properties from experiments, the continuum beam model has been used to predict the mechanical and thermal dynamics performances of single actin filaments and microfilament networks. Based on the continuum beam assumption, You et al. presented a mathematical model for the strain amplification in the actin cytoskeleton of osteocytes (You et al. 2001), Mogilner and Oster proposed a model to explain the force generation by actin polymerization (Mogilner and Oster 2003), Chen and Shenoy explained the myosin II induced strain stiffening of actin filament networks (Chen and Shenoy 2010). However, the reliability of continuum beam model being employed in the predictions on nanoscale is still unclear, and this calls for further studies.

The molecular characterization of the mechanical performances provides a way to unravel the physical basis of biological phenomena in living cells (Karplus 2002). In the nanoscale biotechnology, the performance of a structural protein is decided by the atomic configuration. With the high resolution atomic configuration of actin filament (Holmes 2009; Oda et al. 2009), molecular dynamics (MD) simulations are executed on single actin filaments, and the structural properties are estimated (Splettstoesser et al. 2010; Pfaendtner et al. 2010). Deriu et al. and Matsushita et al. independently studied the thermal dynamics behaviours of single actin filaments by molecular dynamics and elastic networks model simulation, and estimated the mechanical

properties of the single actin filaments (Deriu et al. 2011; Matsushita et al. 2010). However, to the best of our knowledge, the study of direct MD simulations of mechanical performances of single actin filaments is limited.

In this paper, the molecular simulations of mechanical vibrations of single actin filaments are conducted to validate the reliability of continuum beam model in the nanoscale single actin filaments modelling. Due to the challenge in reaching a fully equilibrated atomic configuration of single actin filaments in all-atom MD simulation using today's computational power, it is hard to evaluate the mechanical properties directly by MD simulations of the quasi static stretching or bending tests of single actin filaments. However, the mechanical vibration, as the dynamics motion, can also reflect the mechanical constitutive information of the system. Therefore, in this paper, the free vibrations of single actin filaments after direct mechanical excitations are investigated by the molecular simulations.

The MARTINI force field for the molecular simulations of biological systems is proposed by Marrink and Mark (Marrink and Mark 2003), and has been validated by the results of all-atom MD simulation (Marrink et al. 2007). With the MARTINI Coarse Grain Molecular Dynamics (CGMD) technique, the overall particle number can be reduced to only 25% of the original atom number, which will significantly save the computational cost. The Fast Fourier Transform (FFT) is subsequently applied to the periodic motion information from the CGMD simulations to find out the natural frequencies of the single actin filaments. The natural frequencies obtained from the molecular technique are compared with the Normal Mode Solution (NMS) of the equivalent Euler-Bernoulli beams, and the flexural rigidity and the Young's modulus can be then evaluated. Based on the mechanical properties evaluations from the molecular technique, the reliability of continuum beam model can be studied correspondingly.

Methods

In order to investigate the mechanical performances of single actin filaments, the molecular simulation technique is employed in this paper. Numerical simulations are conducted to study the mechanical vibration properties of the actin filament molecular system by the CGMD (MARTINI force field) method. The power spectrum analysis is used to extract the natural frequencies from the molecular simulations. The natural frequencies are compared with those obtained from the

analytical solutions of the Euler-Bernoulli beam theory, and the flexural rigidity and the Young's modulus of single actin filaments can be then evaluated. The CGMD simulation technique, the power spectrum analysis and the analytical solutions of the natural frequencies based on the Euler-Bernoulli beam model will be detailed in this section.

Atomic structure of the single actin filaments

The atomic structure of a globular actin is obtained from Protein Data Base (PDB) under the ID 2ZWH which is classified in contractile protein family (Oda et al. 2009). The 'Oda 2009' actin filament model is developed based on the nature of the globular actin to the filamentous actin transition (Oda et al. 2009) by an original code. There are 13 globular actin subunits in every actin filament repeat, the rotation for every monomer is 166.2^{o} and the length of one actin filament repeat is 35.9 nm (Dominguez and Holmes 2011). The rotation mechanism makes the actin filament appear to be a turning right-hand double helix structure. Fig. 1 shows the detailed configuration of a single filamentous actin repeat.

The CGMD simulation of free vibration

The CGMD simulations (MARTINI force field) are employed on the actin filaments with lengths from 50 to 288 nm to investigate the mechanical properties of single actin filaments, and the molecular simulations are all performed on the platform of non-commercial package of GROMACS (Van Der Spoel et al. 2005).

The CGMD simulation is divided into two parts: the simulation of the mechanical excitation and the simulation of the free vibration. In the simulation of the mechanical excitation, 10 ns CGMD simulation with a mechanical excitation is performed in an NPT ensemble (pressure 1 bar, temperature 303K), in which both pressure and temperature are controlled by the Berendsen method (Berendsen et al. 1984). Both of the ends of the simulated actin filament are fixed, and a transverse step force (from 75 to 1500 kJ/mol·nm, with respect to the filament length) is applied to excite an initial deformation for the free vibration of the filament. Langevin dynamics (Car and Parrinello 1985) is used in this part to mimic the friction from water. Subsequently, 20-40 ns CGMD simulations without external force besides the fixed-fixed boundary condition are performed in an NVE ensemble after the mechanical excitation simulation to mimic the free

vibration of single actin filaments. Note that the free vibration simulations are performed in vacuum to avoid the damping effect from water molecules.

The Root Mean Square Deviation (RMSD) of certain atoms in a molecule with respect to a reference structure is defined by least-square fitting (David et al. 2006):

$$RMSD(t_1,t_2)=[\frac{1}{M}\sum_{i=1}^{N}m_i \square p_i(t_1)-p_i(t_2)\square^2]^{\frac{1}{2}},\ M=\sum_{i=1}^{N}m_i \quad (1)$$

where $p_i(t)$ is the position of atom *i* at the time *t*, m_i is the mass of atom *i*, *N* is the atom number and the reference structure in this paper is the initial structure (t_2=0). Because there are millions of freedoms in a complex biological molecular system, it is hard to summarize total energy or a single atom's motion as a vibration signal of the whole system's vibration. However, the system's homogenized motion information can be then evaluated from the value of RMSD.

The CGMD simulation in the second part can be taken as the free vibration after an initial mechanical excitation has been applied and then withdrawn. With the help of the FFT power spectrum analysis, the discrete data with different vibration modes from the molecular simulations can be processed to distinguish the vibration modes from the complex system motions.

The NMS of the Euler-Bernoulli beam model

In the vibration theory, the NMS is the process to solve the frequencies of the normal modes of a system known as natural frequencies. To validate the reliability of the beam model in the mechanical behaviours prediction of single actin filaments, equivalent beams with the same geometry and material constants of single actin filaments are analysed through the NMS of the classic beam model. To be comparable with the experimental studies, the radius of the single beam cross section is assumed to be 2.82 nm, which is the same as literatures (Kojima et al. 1994). The actin filaments simulated in this paper are with lengths from 50 to 288 nm. It is noteworthy that, the length of the single actin filament is different from the beam length because the actin molecules on the ends of the filament are frozen as fixed boundary condition. Therefore, the beam length is shorter than the real filament length. The aspect ratios of the equivalent beam model are from 6.9 to 49.1, The Euler-Bernoulli beam model is employed to represent the single actin filaments (Boresi et al. 1993). Fig. 2(a) shows the equivalent beam model with the same geometry as the single actin filaments. Fig. 2(b) shows the deformed configuration of the beam under the

transverse excitation. The analytical NMS of a Euler-Bernoulli beam can be found in Rao's book (Rao 2007). For a uniform Euler-Bernoulli beam, the governing equation of free vibration is:

$$\frac{d^4w}{dx^4} - \beta^2 w = 0 \quad (2)$$

where, w is the deflection, and β is a constant for frequency according to the boundary conditions. Therefore, the natural frequency f can be calculated for this equivalent beam based on its geometry and material constants:

$$f = \frac{\beta}{2\pi L^2}\sqrt{\frac{EI}{\rho A}} \quad (3)$$

where E is the Young's modulus, I is the moment of inertia of the cross section, ρ is the density of the material and A is the area of the beam cross section. L is the effective beam length, which is 11 nm (the length of four actin molecules) smaller than the real filament length as the four actin molecules on the ends of the filament are fixed. Note that, EI is defined as the flexural rigidity of the beam. Under the circular cross section assumption, the moment of inertia I is supposed to be $\pi r^4/4$, where r is the radius of the cross section (2.82 nm) (Kojima et al. 1994). The homogenized constant ρA can be estimated by dividing the mass of one filament repeat by the repeat length as $\rho A = Mn/N_A l$. Where n=13, which is the number of globular actin monomers in one repeat of the filamentous actin. N_A is the Avogadro's number, M is the molar mass of an globular actin which is 42 kDa and l is the length of one actin filament repeat, which is 35.9 nm. With these constants, ρA is estimated to be 2.53×10^{-14} kg/m. The flexural rigidity (EI) and the Young's modulus (E) of single actin filaments can be then evaluated from the NMS results by comparing the natural frequencies obtained from the molecular simulations and the corresponding NMS of the Euler-Bernoulli beam model.

Results and discussion

Herein, the molecular technique is employed to characterize the mechanical vibrations of single actin filaments. Based on the evaluations of the key mechanical properties, we studied the reliability of the Euler-Bernoulli beam model in the nanoscale single actin filaments modelling.

The free vibration of single actin filaments

The free vibration simulation of CGMD (MARTINI force field**)** for the 144 nm actin filament is specifically extended to 40 ns, which is 20 ns longer than the other filament length cases, to study the duration dependency of the characterization result from the molecular simulations. The FFT analyses are independently applied to the RMSD results within four different free vibration simulation stages, including 0-10 ns, 10-20 ns, 20-30 ns and 30-40 ns. Fig. 3 shows the results of the power spectrum analyses obtained from different simulation stages. All the natural frequencies obtained have identical values of 2.53 GHz in different simulation stages, indicating that the natural frequency is insensitive with the simulation time durations. Therefore, the vibration simulation technique developed in this paper is reliable during the whole simulation procedure. This is an attractive advantage of this technique because the reliable results can be extracted by employing a short free vibration simulation time duration (i.e., 10 ns for this case), which will significantly save the computational cost.

Fig. 4 shows the deformation configurations of a 144 nm single filament at different time in the free vibration simulation. In the CGMD simulation, the step force is applied in a short duration of 10 ns in the first simulation part of the mechanical excitation. As a result of the dynamic excitation, the deformation of the single filament is not in the absolute bending status. Based on the deformation configurations obtained from the simulation as shown in Fig. 4, it can be concluded that the initial mechanical excitation has led to the third order free vibration mode, and the corresponding natural frequency constant β in Eq. (3) is 120.9 (Rao 2007). It should be mentioned here that the order of the free vibration mode to be excited depends on the boundary conditions at the two ends and the external excitation force. The third order free vibration mode obtained in this study is because we consider a fixed-fixed filament under a transverse step excitation force.

The free vibration investigations are performed on different actin filaments with lengths from 50 to 288 nm. By employing a typical Young's modulus (2.5 Gpa) of single actin filaments obtained from experiments (Dupuis et al. 1997; Gittes et al. 1993; Higuchi et al. 1995; Janmey et al. 2001), the analytical solution of the natural frequency of these actin filaments can be evaluated using Eq. (3), which is derived based on the Euler-Bernoulli beam model. Fig. 5 shows the frequencies evaluated theoretically by the beam model and obtained numerically by the CGMD simulation, respectively. The frequencies obtained by these two approaches agree with each other. These identical results indicate that the Euler-Bernoulli beam model can be a reasonable candidate to

describe the mechanical vibration properties of single actin filaments. From Fig. 5, it can be also found that the natural frequencies decrease while the length of the single actin filament increases.

The reliability of the Euler-Bernoulli beam model

The numerical characterization technique can also be employed as an effective approach for the estimation of the key material properties of single actin filaments. Take the flexural rigidity as example, the flexural rigidity of single actin filaments can be derived from Eq. (3), i.e.,

$$EI = 4\pi^2 \rho A L^4 \frac{f^2}{\beta^2} \quad (4)$$

With the provided geometry and material constants of the single actin filament, for a 144 nm filament, the natural frequency obtained by the CGMD and the FFT is 2.53 GHz, as shown in Fig. 3 and Fig. 5. Therefore, the flexural rigidity can be calculated using Eq. (4), i.e., EI=13.3×10^{-26} N·m^2. According to literatures, the flexural rigidity evaluated from the experimental studies varied between 3×10^{-26} N·m^2 to 10×10^{-26} N·m^2 (Deriu et al. 2011; Dupuis et al. 1997; Gittes et al. 1993; Janmey et al. 2001). The characterization result obtained in this study by the molecular investigation of the free vibration is on the same order with the experimental results.

It is noteworthy that, the solution environment is important to the experiment results and theoretical evaluations (Janmey et al. 2001). To avoid the damping effect from water molecules in the vibration analysis, in the studies of this paper, the molecular simulation of the free vibration is performed in vacuum, while previous experiments and thermal dynamics evaluation were taken in solution environment. In other words, the undamped free vibration is studied in this paper while previous experiments and thermal dynamics evaluation considered an underdamped system. Based on the mechanical vibration theory (Rao 2007), the undamped natural frequency will be larger than the underdamped natural frequency, which explains why the flexural rigidity obtained from our studies is in the upper limit for the range of the flexural rigidity obtained from the experimental studies.

Single actin filaments were assumed to be Euler-Bernoulli beams on the continuum mechanics level to understand the biomechanics of the microfilament networks in living cells including strain amplification (You et al. 2001), force generation (Mogilner and Oster 2003) and strain hardening (Chen and Shenoy 2010). In order to validate the reliability of the Euler-Bernoulli beam model in predicting the mechanical vibration behaviours of single actin filaments on nanoscale, mechanical

properties of single actin filaments with different lengths are evaluated to investigate the size dependency of the beam model. Fig. 6 shows the flexural rigidity and the Young's modulus evaluated from the NMS of Euler-Bernoulli beam model by using the natural frequencies from the molecular simulations with respect to the actin filament lengths. The flexural rigidity, which is evaluated based on the Equation (4), increases with the length of the filament and converges to 13.3×10^{-26} N·m^2 when the length of the single actin filament is on the order of hundreds nano meter scale. The Young's modulus presents a same trend which converges to 2.6 GPa. According to the mechanics of materials, for the continuum material, the flexural rigidity and Young's modulus should not be related to the length of beam. However, the mechanical properties of the filaments evaluated from the classic beam model do not converge until the beam aspect ratio of the equivalent beam exceeds 17, which means the Euler-Bernoulli beam model is not applicable when the aspect ratio of the single actin filament is less than 17. This is an important finding because complex single actin filaments exist with a wide range of lengths in living cells(Oda et al. 1998), and the beam models should be carefully selected to accurately characterize the mechanical properties of the single actin filaments whose lengths vary from nanoscale to microscale.

Conclusion

The mechanical vibration properties of single actin filaments are studied by a comprehensive numerical technique based on the Coarse-Grained Molecular Dynamics simulations, the Fast Fourier Transform power spectrum analysis and the Normal Mode Solution of the Euler-Bernoulli beam. The frequency results are found to have no dependence on the duration of the simulations, which can significantly save the computational cost by conducting only short duration molecular simulations. For single actin filaments with lengths from 50 to 288 nm, the natural frequencies obtained by the numerical simulations match the analytical solutions of the Euler-Bernoulli beam model, which proves that the continuum beam model can be a good candidate in the nanoscale single actin filaments modelling. The evaluations of the flexural rigidity and the Young's modulus agree with those obtained by the experiments, Through the study on the convergences of the evaluations with respect to the filament length, it can be found that the Euler-Bernoulli beam model can be only reliably used for continuum mechanics analyses of single actin filaments when the aspect ratio is larger than 17, which is different from the mechanics of traditional materials (Boresi et al. 1993).

In summary, the investigation of the mechanical vibration provides the evidence for the use of continuum beam model in nanoscale single actin filaments modelling from the microscopy point of view. The molecular simulation of the mechanical behaviours of single actin filaments provides a way to evaluate the mechanical properties of single actin filaments which are needed in the continuum mechanics level study to predict the performances of the cytoskeleton. It has also clarified the criteria of the aspect ratio of the single actin filaments for the effective use of the Euler-Bernoulli beam model. This will eventually contribute to understand the biomechanics and mechanobiology of the microfilament networks in living cells.

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References

Berendsen HJC, Postma JPM, Van Gunsteren WF, DiNola A, Haak J (1984) Molecular dynamics with coupling to an external bath. The Journal of Chemical Physics 81:3684

Boresi AP, Schmidt RJ, Sidebottom OM (1993) Advanced mechanics of materials, vol 5. Wiley,

Car R, Parrinello M (1985) Unified approach for molecular dynamics and density-functional theory. Physical Review Letters 55 (22):2471-2474

Chen P, Shenoy VB (2010) Strain stiffening induced by molecular motors in active crosslinked biopolymer networks. Soft Matter 7 (2):355-358

Cossart P (2005) Cellular microbiology. Amer Society for Microbiology,

David S, Erik L, Hess B (2006) Gromacs user manual. version 4.0. Netherlands: University of Groningen

Deriu MA, Bidone TC, Mastrangelo F, Di Benedetto G, Soncini M, Montevecchi FM, Morbiducci U (2011) Biomechanics of actin filaments: A computational multi-level study. Journal of Biomechanics 44 (4):630-636. doi:10.1016/j.jbiomech.2010.11.014

Dominguez R, Holmes KC (2011) The Structure of G and F Actin Filaments. Annual Review of Biophysics 40 (1)

Dupuis DE, Guilford W, Wu J, Warshaw D (1997) Actin filament mechanics in the laser trap. Journal of muscle research and cell motility 18 (1):17-30

Fletcher DA, Mullins RD (2010) Cell mechanics and the cytoskeleton. Nature 463 (7280):485-492

Gittes F, Mickey B, Nettleton J, Howard J (1993) Flexural rigidity of microtubules and actin filaments measured from thermal fluctuations in shape. The Journal of cell biology 120 (4):923-934

Higuchi H, Yanagida T, Goldman YE (1995) Compliance of thin filaments in skinned fibers of rabbit skeletal muscle. Biophysical journal 69 (3):1000-1010

Holmes KC (2009) Structural biology: actin in a twist. Nature 457 (7228):389-390

Huxley HE, Stewart A, Sosa H, Irving T (1994) X-ray diffraction measurements of the extensibility of actin and myosin filaments in contracting muscle. Biophysical journal 67 (6):2411-2421. doi:10.1016/s0006-3495(94)80728-3

Janmey PA, Tang JX, Schmidt CF (2001) Actin filaments. Supramolecular Assemblies

Karplus M (2002) Molecular dynamics simulations of biomolecules. Accounts of Chemical Research 35 (6):321-323

Kojima H, Ishijima A, Yanagida T (1994) Direct measurement of stiffness of single actin filaments with and without tropomyosin by in vitro nanomanipulation. Proceedings of the National Academy of Sciences 91 (26):12962

Liu X, Pollack GH (2002) Mechanics of F-actin characterized with microfabricated cantilevers. Biophysical journal 83 (5):2705-2715
Marrink SJ, Mark AE (2003) Molecular dynamics simulation of the formation, structure, and dynamics of small phospholipid vesicles. Journal of the American Chemical Society 125 (49):15233-15242
Marrink SJ, Risselada HJ, Yefimov S, Tieleman DP, De Vries AH (2007) The MARTINI force field: coarse grained model for biomolecular simulations. The Journal of Physical Chemistry B 111 (27):7812-7824
Matsushita S, Adachi T, Inoue Y, Hojo M, Sokabe M (2010) Evaluation of extensional and torsional stiffness of single actin filaments by molecular dynamics analysis. Journal of Biomechanics 43 (16):3162-3167
Mogilner A, Oster G (2003) Force generation by actin polymerization II: the elastic ratchet and tethered filaments. Biophysical journal 84 (3):1591-1605
Oda T, Iwasa M, Aihara T, Maéda Y, Narita A (2009) The nature of the globular-to fibrous-actin transition. Nature 457 (7228):441-445
Oda T, Makino K, Yamashita I, Namba K, Maéda Y (1998) Effect of the length and effective diameter of F-actin on the filament orientation in liquid crystalline sols measured by x-ray fiber diffraction. Biophysical journal 75 (6):2672-2681
Pantaloni D, Clainche CL, Carlier MF (2001) Mechanism of actin-based motility. Science 292 (5521):1502
Pfaendtner J, Lyman E, Pollard TD, Voth GA (2010) Structure and Dynamics of the Actin Filament. Journal of molecular biology 396 (2):252-263. doi:10.1016/j.jmb.2009.11.034
Pollard TD (1976) Cytoskeletal functions of cytoplasmic contractile proteins. Journal of supramolecular structure 5 (3):317-334
Pollard TD, Blanchoin L, Mullins RD (2000) Molecular mechanisms controlling actin filament dynamics in nonmuscle cells. Annual Review of Biophysics and Biomolecular Structure 29 (1):545-576
Rao SS (2007) Vibration of continuous systems. Wiley Online Library,
Shin JH, Mahadevan L, So P, Matsudaira P (2004) Bending stiffness of a crystalline actin bundle. Journal of molecular biology 337 (2):255-261
Splettstoesser T, Holmes KC, Noé F, Smith JC (2010) A Comparison of Actin Filament Models by Molecular Dynamics Simulation. Biophysical journal 98:154
Stossel TP, Condeelis J, Cooley L, Hartwig JH, Noegel A, Schleicher M, Shapiro SS (2001) Filamins as integrators of cell mechanics and signalling. Nat Rev Mol Cell Biol 2 (2):138-145
Van Der Spoel D, Lindahl E, Hess B, Groenhof G, Mark AE, Berendsen HJC (2005) GROMACS: fast, flexible, and free. Journal of computational chemistry 26 (16):1701-1718
You L, Cowin SC, Schaffler MB, Weinbaum S (2001) A model for strain amplification in the actin cytoskeleton of osteocytes due to fluid drag on pericellular matrix. Journal of Biomechanics 34 (11):1375-1386

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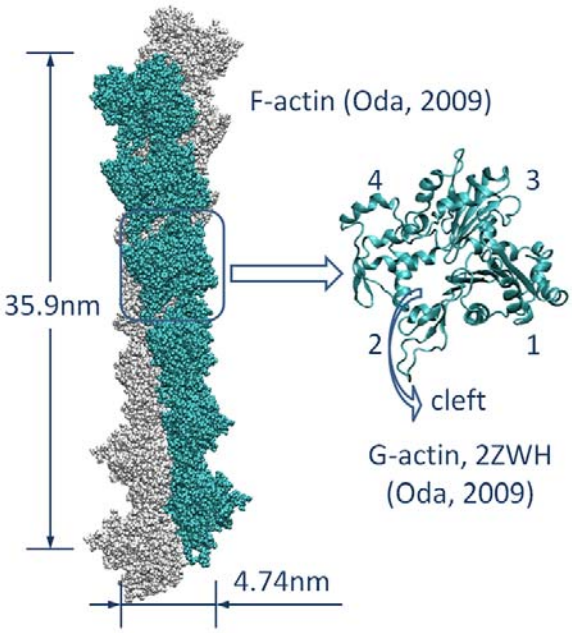

Fig. 1 Actin filament repeat built from globular actin (‘Oda 2009’). 13 globular actin monomers build one actin filament repeat with the length of 35.9 nm.

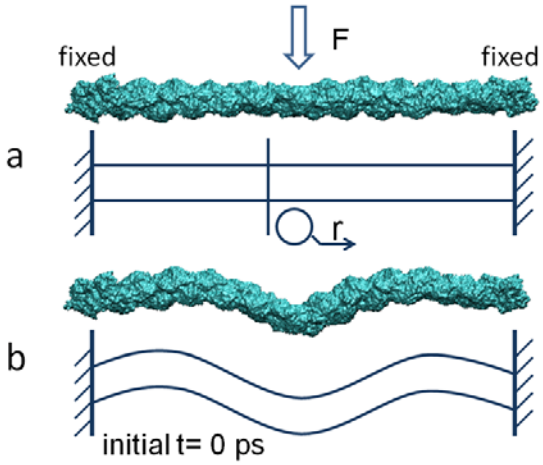

Fig. 2 Schematic of initial transverse excitation applied on the single actin filament. a: the transverse step force loading on a both ends fixed actin filament. b: the initial atomic configuration after the transverse excitation. The beam length is L and the cross section radius is r; there are 26 actins in this case, and each end has two actins monomers being fixed.

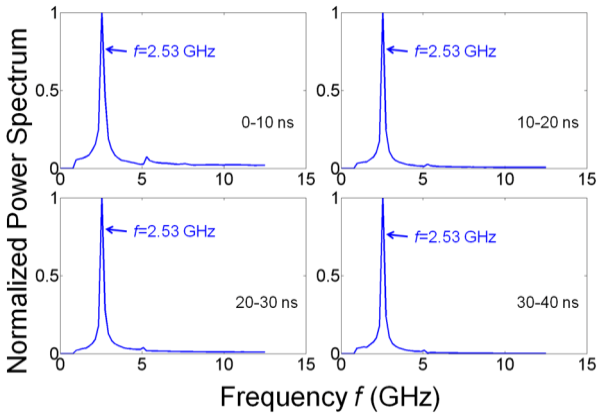

Fig. 3 Power spectrum analyses within different simulation stages of a 144 nm actin filament. The results in different simulation stages all present the same natural frequency of 2.53 GHz.

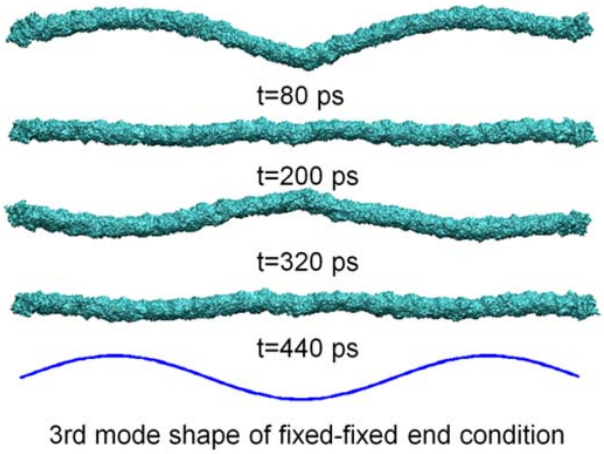

Fig. 4 The deformation of a both ends fixed single actin filament (144 nm) during free vibration. The deformations with respect to simulation time match the third mode shape of free vibration from analytical solution.

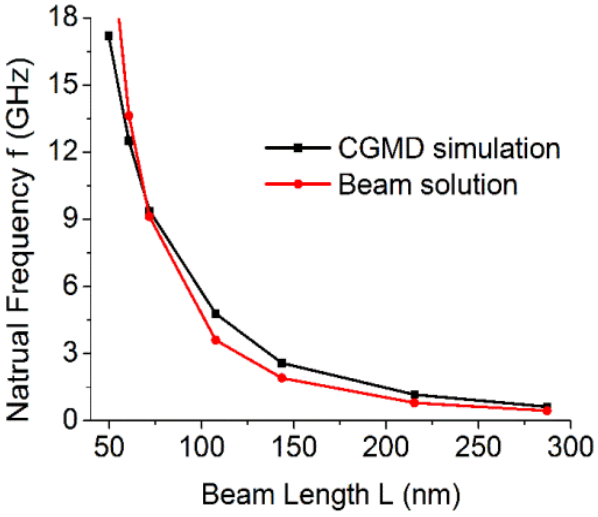

Fig. 5 Frequency from CGMD simulation compared with the theoretical beam solution derived from the NMS of the Euler-Bernoulli beam model. The frequencies are obtained from the first 10 ns CGMD simulations of the free vibration of single actin filaments.

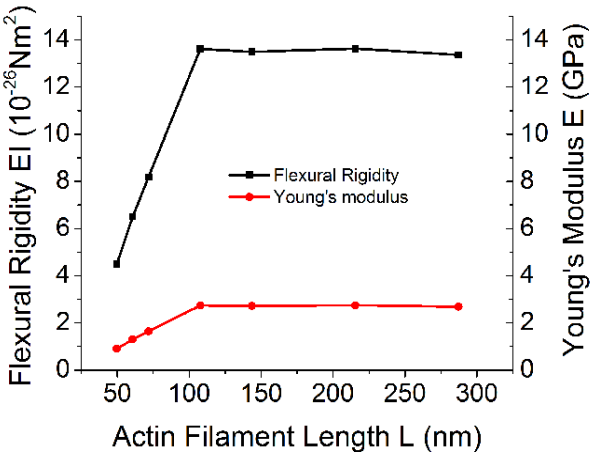

Fig. 6 The flexural rigidity and the Young's modulus evaluations of filaments based on beam model. The flexural rigidity converges to 13.3×10^{-26} N·m^2, and the Young's modulus converges to 2.6 GPa when the length is on the order of hundreds nano meter scale.