Effect of Diameter, Length, and Chirality on the Properties of Silicon Nanotubes

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Abstract
The mechanical properties of nanostructures are a researcher’s favorite topics. In the meantime, the mechanical and physical properties of the two dimensional structures and the nanotubes have attracted greater attention due to their wide application. Si (Si) nanotubes are structures consisting of Si atoms that are arranged as honeycombs. This structure has created some special properties in Si nanotubes. In this paper, Young’s modulus values and stress strain diagrams of Si nanotubes are investigated using molecular dynamics method and the Tersoff potential. Then, the changes effect of size and dimension was investigated for a closer look. For this purpose, the effect of nanotube diameter, length, and chirality shift from zigzag to armchair were studied. The results showed that the fracture stress of nanotube decreased with increasing the length of Si nanotube. It was also shown that the armchair structure was stronger than the zigzag. The effect of diameter change on the mechanical properties was also investigated and it was observed that no specific order could be found between the diameter changes with the Si nanotube strength. The results were in good agreement with other studies.

Keywords Silicon nanotube · Chirality · Mechanical properties · Molecular dynamics

1 Introduction

Much of the changes we can make at the material structure to improve their performance are in the nano dimension, and these properties in the nanostructure are not industry specific and exist in nature, and these nanostructures with useful features are always being produced [1–5] such as self-cleaning lotus leaves [6] and butterfly wings colors [7], photoreceptor in brittlestar [8], and anti-reflection eyes of moth [9]. Nanostructures especially Si nanotubes are used at the production of sensors and biosensors [10–15], anode of cells [16–19], solar cell [20, 21], transistors [22–25], fuel batteries and biological materials [26, 27], energy storages [28], rechargeable lithium batteries [29–31], drug delivery systems [32]. Furthermore, Fahad et al. [23] have pointed out the usefulness and effectiveness of using Si nanotubes in tunnel field-effect transistor. Kunjie et al. [14] found that Si nanotube had a stronger interaction with carbon monoxide (CO) and nitrogen monoxide (NO) compared to carbon nanotube, which could increase the sensitivity of detection and recognition of Si nanotube to these two CO and NO. Si nanotube converts to metallic state after absorption of carbon monoxide and, if Si nanotube is combined with nitrogen monoxide (NO), will have magnetism properties. Si nanotube is a good option for use in sensors of detection and recognition a carbon monoxide and nitrogen monoxide. Park et al. [17] studied the importance of Si nanotube as a battery anode due to its high charge capacity as well as 89% columbic efficiency and 10 fold capacity per each 200 cycles. Lan et al. [33] studied the Si nanotube and carbon nanotube and compared the capacity of these nanotubes for hydrogen absorption at room temperature (298 K) and pressure of 1 to 10 MPa. In that study, Si nanotube was introduced as a better option for hydrogen absorption. They had found by studying the structure of Si nanotube that rhombic structure (state) of Si nanotube was more capable of hydrogen absorption. They studied the three armchair nanotubes (5–5), (7–7), and (9–9) at 298 K and pressure of 4 to 10 MPa to predict the behavior of the Si nanotube with the
changes of the diameter. They found that diameter alone did not alter the rate of hydrogen absorption.

In this study, tubes with chirality 7–7 have the highest rate of hydrogen uptake. With the advancement of tool science towards material shrinkage, low heat transfer tools are expanding and becoming more widely used [34].

Li [35] studied Si nanowire and Si bulk with the molecular dynamics method, and found that the heat transfer in Si nanowires is about half of a Si bulk. Chen [36] found at his investigation using molecular dynamics method that the Si nanotube had 33% heat transfer of Si nanowire at room temperature. He showed that it was possible to reduce the heat transfer capability by increasing the surface to the volume of nanotube, and they introduced Si nanotube as a suitable option for thermoelectric devices. Szczech et al. [37] have introduced Si as a high capacity anode of battery and they stated increasing the Si volume when lithiating and delithiating has prevented its commercial application. Furthermore, the other problem of using Si at battery is the poor recovery capability. These problems can be solved by using Si nanostructures. Isfahani et al. [38] have studied the effect of pore shape on the behavior of single crystalline Si np structures using molecular dynamics method. In that paper, the pore with shapes of circular, elliptical, square and hexagonal were investigated and the elastic modulus, ultimate strength, fracture stiffness and hardness are measured. They stated that the H ellipse pore has the highest strength (stiffness). Chan [39], Pozot [40] and Kasavajjula [41] have proposed nanostructures with holes as a suitable option to eliminate and improve the problems of stability and performance. Bai et al. [42] investigated the various structures of single dimensional Si and Si nanotube had introduced as a good alternative to wide bandgap semiconductor.

Most of the stress of Nano dimension tools is due to thermal inconsistencies and networking between different materials. The reliability of many devices in these dimensions depends on the response of nanostructures to mechanical loading. Therefore, a deep and comprehensive understanding of the deforming of mechanisms under external mechanical forces is needed for technology future of nanostructures. Fagan et al. [43] have theoretically investigated the similarities and differences between Carbon and Silicon structures using two methods, i.e., DFT and Monte Carlo (which employs the Tersoff potential). They had investigated the electrical and structural properties of the two material by DFT method and found that these properties were dependent on diameters and chirality. They had shown that Si nanotubes can play both metal (armchair) and semiconductor (zigzag) roles. They had also investigated the thermal behavior of these two structures using the Monte Carlo method. Palaria [44] has investigated the structural properties of Si nanotubes including atomic structure and elastic properties using molecular dynamics and first principle force field theory and density functional theory. He measured and published the Si Nanotube Young’s modulus at various structural scales. He had shown according the structure that this number varies between 50 and 493 MPa. Zhang et al. [45] investigated the electronic and structural properties of Si nanotube using DFT and found that the structure of Si nanotube in small diameters is metallic and armchair structure of Si nanotube is more stable. San Paulo [46] investigated the mechanical structure of Si nanowires using the AFM method using the vapor solid liquid method, and he found experimentally that the Young’s modulus was 186 GPa. Kang et al. [47] studied Si nanowire using the molecular dynamics method and with applying the MEAM potential and investigated the relationship between temperature and fracture mechanism and he found that the failure

Table 1 Value of parameters in Tersoff potential

| Parameters | C       | Si       | Ge       |
|------------|---------|----------|----------|
| A (eV)     | 1.3936*10^3 | 1.8308*10^3 | 1.769*10^3 |
| B (eV)     | 3.467*10^2   | 4.7118*10^2  | 4.1923*10^2 |
| λ (Å⁻¹)    | 3.4879           | 2.4799           | 2.4451           |
| μ (Å⁻¹)    | 2.2119           | 1.7322           | 1.7047           |
| β          | 1.5724*10⁻⁷     | 1.1000*10⁻⁶     | 9.0166*10⁻⁷     |
| n          | 1.5724*10⁻⁷     | 7.8734*10⁻⁷     | 7.5627*10⁻⁷     |
| C          | 3.8049*10⁴     | 1.0039*10⁵     | 1.0643*10⁵     |
| d          | 4.384*10⁰     | 1.6217*10¹     | 1.5652*10¹     |
| h          | -5.7058*10⁻¹   | -5.9825*10⁻¹   | -4.3884*10⁻¹   |
| R (Å)      | 1.8          | 2.7          | 2.8          |
| S (Å)      | 2.1          | 3.0          | 3.1          |
| χC−Si=0.9776 |           |             |             |
| χSi−Ge=1.0061 |           |             |             |

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mechanism is related to both the diameter of the Si nanowire and the temperature.

Therefore at this paper, according the importance of the effect of nanotube diameter on the mechanical properties, the stress and strain behavior and Si nanotube Young’s modulus are investigated using molecular dynamics method and the chirality effect and nanotube length are discussed.

### 2 Simulation

Molecular dynamics is a powerful method that involves solving the classical many-body problem in contexts relevant to the study of matter at the atomistic level [48]. This simulation is carried out based on the Tersoff potential [49]. Tersoff shows that if this function is used for pair terms, it can be a good starting point for prediction because

| length | Atomicity | chirality | Diameter(A) | Critical stress (GPa) | Young’s modulus(GPa) |
|--------|------------|-----------|-------------|-----------------------|----------------------|
| 100    | 936        | (9–9)     | 19.32       | 27.62                 | 168.13 ± 1.06        |
| 200    | 1854       | (9–9)     | 19.32       | 25.53                 | 197.52 ± 0.6         |
| 300    | 2790       | (9–9)     | 19.32       | 24.75                 | 205.37 ± 0.58        |

![Fig. 1 Schematic of length comparison of Si nanotube](image)

![Fig. 2 Stress strain diagram for lengths 100, 200 and 300A](image)

![Fig. 3 schematic comparison of diameters 12.3, 17.3 and 23.5 A](image)
this potential included a large range of structural features of Si. Earlier, Kang [47] had used this potential to investigate the effect of temperature and size changes of nanowires on the fracture mechanism using molecular dynamics method. As well as Verma and Jeong Won Kang have separately studied Si nanotube structure using this potential [50–52]. This potential follows the following equations:

\[ E = \sum_i E_i = \frac{1}{2} \sum_{i\neq j} V_{ij}, \]

\[ V_{ij} = f_C(r_{ij})[f_R(r_{ij}) + b_{ij}f_A(r_{ij})]; \]

\[ f_C(r_{ij}) = A_{ij}\exp(-\lambda_{ij}r_{ij}), \]

\[ f_A(r_{ij}) = -B_{ij}\exp(-\mu_{ij}r_{ij}); \]

\[ b_{ij} = X_i(1 + \beta_i n_{ij})^{-1/n_{ij}}, \]

\[ g(\theta_{ik}) = 1 + c_i^2 d_i^2 - c_i^2 \left[ d_i^2 + (b_{ik}\cos(\theta_{ik}))^2 \right], \]

\[ \lambda_{ij} = (\lambda_i + \lambda_j)/2, \]

\[ \mu_{ij} = (\mu_i + \mu_j)/2, \]

\[ A_{ij} = (A_iA_j)^{1/2}, \]

\[ B_{ij} = (B_iB_j)^{1/2}, \]

\[ S_{ij} = (S_iS_j)^{1/2}. \]

Table 3  Mechanical properties of nanotubes with different diameters

| Chirality | Atomicity | Length(A) | Diameter(A) | Critical stress (GPa) | Young’s modulus(GPa) |
|-----------|-----------|-----------|-------------|----------------------|---------------------|
| 10–0      | 890       | 150       | 12.3        | 10.65                | 182.5456 ± 1       |
| 14–0      | 1246      | 150       | 17.3        | 10.86                | 183.481 ± 1.038    |
| 19–0      | 1691      | 150       | 23.5        | 11.66                | 185.173 ± 0.01     |

Fig. 4 Stress strain diagram for Si nanotube with diameters 12.3, 17.3 and 23.5 Å

Fig. 5 Structure schematic comparison of tubes with same diameters and different chirality
Labels of system atoms are i, j and k and r_{ij} is the bond length and \( \theta_{ijk} \) is the angle between the bonds. \( n_i \) and \( \lambda_{i,o} \) only depend on the type of atom (carbon, Si, Ge). \( E \) is the total energy of the system and \( E_i \) is the site energy. \( V_{ij} \) is bond energy between atoms i and j. The function \( f_R \) states a repulsive pair potential, which includes the orthogonalization energy when atomic wave functions overlap. \( f_A \) displays an attractive pair potential associated with bonding. Function of \( f_A \) and \( f_R \) represents the repulsion and attraction potential between two atoms, respectively. The extra term \( f_C \) is merely a smooth cutoff function to limit the range of the potential. The function \( b_{ij} \) is the sole novel feature of the potential. It represents a measure of the bond order, and is for now assumed to be a monotonically decreasing function of the coordination of atoms i and j. Parameter of \( \omega_{ij} \) (where \( \omega_{ii} = 1 \)) are available for possible future use that permit greater flexibility when dealing with more drastically different types of atoms.

The value of 1 is considered for \( \chi \) and \( \omega \) in this calculation. Other values are shown at Table 1.

## 3 Results and Discussion

In this simulation, we try to predict the behavior of stretched Si nanotubes in different shapes. In this process, the nanotube is first relaxed and then the two its sides are fixed at the appropriate sizes and moves with a rate of 0.012 Å/ps in the opposite direction and a fillet stress in the nanotube is created by increasing the tension and the nanotube is divided into two parts when the tension reaches to the critical stress limit. In these nanotubes, the distance between the two Si atoms is considered 2.248 Å [28, 36].

The investigation of changes effect of sizes and shapes is divided to three parts:

### 3.1 The Effect of Length Change on Strength

In the first part, three nanotubes with lengths of 100, 200 and 300 Å and with chirality of (9–9) and diameter of 19.32 Å were simulated in box with \( 30 \times 30 \times 110, 30 \times 30 \times 210 \) and \( 30 \times 30 \times 310 \) Å dimension and number of atoms of 936, 1854 and 2790 to study the effect of nanotube length on their strength. Fig. 1 shows the schematic of length comparison of Si nanotube.

Previously, Peng et al. [53] had investigated the effect of length change on tension strength of multiwall carbon nanotube. They found that tension strength reduced with increasing the length of the nanotube sample. In this simulation, we also obtained similar results and we observed a reduction of critical stress with increasing length of the nanotube sample (Fig. 2). The values are also presented in Table 4.

### Table 4 Mechanical properties of nanotubes with chirality of zigzag and armchair

| Chirality | Atomicity | Length(A) | Diameter(A) | Critical Stress (GPa) | Young’s Modulus (Gpa) |
|-----------|------------|-----------|-------------|-----------------------|-----------------------|
| 7–7       | 1092       | 150       | 15          | 15.05                 | 185.07 ± 1.258        |
| 12–0      | 1068       | 150       | 14.8        | 10.39                 | 175.09 ± 0.01         |
| 8–8       | 1248       | 150       | 17.17       | 14.38                 | 183.98 ± 1.159        |
| 14–0      | 1246       | 150       | 17.3        | 10.86                 | 183.481 ± 1.038       |

Fig. 6 Si nanotube stress strain diagrams with different chirality

![Si nanotube stress strain diagrams with different chirality](image-url)
Table 2. As expected, the value of the critical stress decreases from 27.6 to 24.7 GPa by increasing the nanotube length from 100 to 300 Å.

3.2 The Effect of Diameter Change on the Strength

In the second part, the purpose is to find the effect of nanotube diameter on its strength. For this purpose, four nanotubes with a length of 150 Å and diameters of 12.3, 17.3 and 23.5 Å and chirality of (10–0), (14–0) and (19–0), respectively are stretched at simulation boxes with dimensions of 20 × 20 × 160, 30 × 30 × 160 and 40 × 40 × 160, and the number of atoms of 890, 1246 and 1691 (Fig. 3).

The stress strain diagram is shown in Fig. 4. The results are also presented in more detail in Table 3. As can be seen in Table 3, by increasing nanotube diameter from 12.3 Å to 23.5 Å, The Young’s modulus increased. However, this increase is slight.

Genoese et al. [47], studied behavior of several nanotubes and found that by increasing diameter of nanotubes, the Young’s modulus increased slightly. For example, in CNT, by changing chirality from (14–0) to (20–0), the Young’s modulus increased about 0.6%. Also, in SiCNT, by changing chirality from (14–0) to (20–0), the Young’s modulus increased about 0.77%.

In this work, in silicon nanotube, by changing chirality from (14–0) to (19–0), the Young’s modulus increased about 0.8% which shows good agreement with previous works.

3.3 Effect of Chirality on Strength

In this part, four nanotubes will be used that each pair have the same diameter and length, and just have different chirality, one zigzag and the other armchair. The nanotubes have a length of 150 Å, a diameter of 14.8 and 17.3 Å, and with chirality of [(12–0) and (7–7)] and [(14–0) and (8–8)] (Fig. 5). The size of the simulation boxes are (30 × 30 × 160), (30 × 30 × 155) and (30 × 30 × 160) and (30 × 30 × 160) and the number of atoms are 1092 and 1068 and 1248 and 1246.

The stress strain diagram for both states is shown in Fig. 6. The results of these figures are analyzed and presented in Table 4 completely. As can be seen, under the same geometrical conditions, the critical stress of the zigzag nanotube (12–0) is lower than the critical stress of the armchair nanotube (7–7) and furthermore, it has less Young’s modulus. The same results are for the zigzag and armchair of nanotubes (0–14) and (8–8), respectively. Therefore, it can be concluded that Si nanotubes with chirality of armchair have more strength and their Young’s modules is higher than zigzag structure.

Ranjbartoreh et al. [45] showed in their study that carbon nanotubes with armchair structure is more strength. Also, Genoese et al. [47] studied some nanotubes. Their results showed that for three kind of nanotubes, Carbon nanotubes (CNTs), boron nitride nanotubes (BNNTs), and silicon carbide nanotubes (SiCNTs), the Young’s modulus of armchair structures are more strength. So, our results have good agreement with previous works.

4 Conclusion

In this paper, the Young’s modulus values and stress strain diagrams of Si nanotubes are investigated using molecular dynamics method and the Tersoff potential. Then, for a closer look, the changes effect of size and dimension was examined. For this purpose, the change effect of diameter and length of nanotube and the shift effect of chirality from zigzag to armchair were investigated. The results showed that the fracture stress decreased from 27.6 to 24.7 GPa with increasing the length of Si nanotube from 100 to 300 Å.

Furthermore, it was shown that the armchair structure has more strength than the zigzag. For example, the elastic modulus of armchair and zigzag were 185 and 175 GPa, respectively for two Si nanotubes with the same diameter and length. The change effect of diameter on the mechanical properties was also investigated and it was observed that no specific order could be found between the diameter change with the strength of Si nanotube and other parameters such as temperature may be involved which should be investigated in future research. The results were in good agreement with other studies.

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Code Availability The LAMMPS package is free and open-source software.

Authors’ Contributions Both authors contributed to the design and implementation of the research, to the analysis of the results and to the writing of the manuscript.

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Data Availability The datasets generated and/or analyzed during the current study are not publicly available but are available from the corresponding author on reasonable request.

Declarations

Ethics Approval and Consent to Participate Not applicable

Consent for Publication Not applicable

Competing Interests The authors declare that they have no competing interests.
References

1. Huang Y, Chattopadhyay S, Jen Y, Peng Y, Liu T, Hsu Y, Pan C, Lo H, Hsu C, Chang Y, Lee C, Chen K, Chen L (2007) Improving broadband and quasiomnidirectional anti-reflection properties with biomimetic silicon nanostructures. Nat Nanotechnol. 2:770–774

2. Lee LP, Szeema R (2005) Inspirations from biological optics for advanced photonic systems. Science. 310:1148–1150

3. Vukusic P, Sambles JR (2003) Photonic structures in biology. Nature. 424:852–855

4. Parker AR, Townley HE (2007) Biomimetics of photonic nanostructures. Nat Nanotechnol. 2:347–353

5. Potyrailo R, Ghiradella H, Vertiatchikh A, Dovidenko K, Courmoyer J, Olson E (2007) Morpho butterfly wing scales demonstrate highly selective vapour response. Nature Photon: 1:123–128

6. Neinhuis C, Barthlott W (1997) Characterisation and distribution of water-repellent, self-cleaning plant surfaces. Ann Bot 79:67–79

7. Ghiradella H, Aneshansley D, Eisinger T, Silberring RE, Hinton HE (1972) Ultraviolet reflection of a male butterfly: interference color caused by thin-layer elaboration of wing scales. Science. 178:1214–1217

8. Aizenberg J, Tkachenko A, Weiner S, Addadi L, Hendler G (2001) Calcitic microcrystals as part of the photoreceptor system in brittlestars. Nature. 412:819–822

9. Bernhard CG (1967) Structural and functional adaptation in a visual system. Endeavour. 26(98):79–84

10. Singh A, Chaudhury S, Chanda M, Sarkar CK (2020) Split gated silicon nanotube FET for bio-sensing applications. IET Circuits, Devices & Systems 14(8):1289–1294

11. Hibst N, Steinbach AM, Strehe S (2016) Fluidic and electronic transport in silicon nanotube biosensors. MRS Advances 1(56):3761–3766

12. Mu C, Zhao Q, Xu D, Zhuang Q, Shao Y (2007) Silicon nanotube array/gold electrode for direct electrochemistry of cytochrome c. J Phys Chem B 111(6):1491–1495

13. Camilli L, Passacantando M (2018) Advances on sensors based on carbon nanotubes. Chemosensors. 6(4):62

14. Kunjie L, Wang W, Cao D (2011) Novel chemical sensor for CO and NO: silicon nanotube. J Phys Chem C 115(24):12015–12022

15. Ji X, Wang H, Song B, Chu B, He Y (2018) Silicon nanomaterials for biosensing and bioimaging analysis. Frontiers in chemistry 6:38

16. Wijayantha C, Zhang G, Li B (2010) Remarkable reduction of thermal conductivity in silicon nanotube. J Mol Struct Theochem 539:101–106

17. Szczech JR, Jin S (2011) Nanostructured silicon for high capacity lithium battery anodes. ChemElectroChem 8(12):1901–1905

18. Tesfaye AT, Gonzalez R, Coffler JL, Djenizian T (2015) Porous silicon nanotube arrays as anode material for Li-ion batteries. ACS Appl Mater Interfaces 7(37):20495–20498

19. Wu H, Chan G, Choi J, Ryu I, Yao Y, McDowell MT, Lee S, Jackson A, Yang Y, Hu L, Cui Y, Cho J (2009) Silicon nanotube battery anodes. Nano Lett 9(11):3844–3847

20. Tesfaye AT, Gonzalez R, Coffler JL, Djenizian T (2015) Porous silicon nanotube arrays as anode material for Li-ion batteries. ACS Appl Mater Interfaces 7(37):20495–20498

21. Pop E, Sinha S, Goodson KE (2006) Heat generation and transport in silicon nanotube arrays. J Phys Chem B 111(6):1491–1495

22. Li D, Wu Y, Kim P, Shi L, Young’s P (2003) Thermal conductivity of individual silicon nanowires. Appl Phys Lett 83(14):2934–2936

23. Chen J, Zhang G, Li B (2010) Remarkable reduction of thermal conductivity in silicon nanotubes. Nano Lett 10(10):3978–3983

24. Szczecz JR, Jin S (2011) Nanostructured silicon for high capacity lithium battery anodes. Energy Environ Sci 4(5):1578–1601

25. Huang Y, McDowell MT, Jackson A, Cha JJ, Hong SS, Cui Y (2010) New nanostructured Li2S/LiSi2O3 rechargeable battery with high specific energy. Nano Lett 10(4):1486–1491

26. Li D, Wu Y, Kim P, Shi L, Young’s P (2003) Thermal conductivity of individual silicon nanowires. Appl Phys Lett 83(14):2934–2936

27. Chen J, Zhang G, Li B (2010) Remarkable reduction of thermal conductivity in silicon nanotubes. Nano Lett 10(10):3978–3983

28. Szczecz JR, Jin S (2011) Nanostructured silicon for high capacity lithium battery anodes. Energy Environ Sci 4(5):1578–1601

29. Huang Y, McDowell MT, Jackson A, Cha JJ, Hong SS, Cui Y (2010) New nanostructured Li2S/LiSi2O3 rechargeable battery with high specific energy. Nano Lett 10(4):1486–1491

30. Li D, Wu Y, Kim P, Shi L, Young’s P (2003) Thermal conductivity of individual silicon nanowires. Appl Phys Lett 83(14):2934–2936

31. Chen J, Zhang G, Li B (2010) Remarkable reduction of thermal conductivity in silicon nanotubes. Nano Lett 10(10):3978–3983

32. Szczecz JR, Jin S (2011) Nanostructured silicon for high capacity lithium battery anodes. Energy Environ Sci 4(5):1578–1601

33. Huang Y, McDowell MT, Jackson A, Cha JJ, Hong SS, Cui Y (2010) New nanostructured Li2S/LiSi2O3 rechargeable battery with high specific energy. Nano Lett 10(4):1486–1491

34. Li D, Wu Y, Kim P, Shi L, Young’s P (2003) Thermal conductivity of individual silicon nanowires. Appl Phys Lett 83(14):2934–2936

35. Chen J, Zhang G, Li B (2010) Remarkable reduction of thermal conductivity in silicon nanotubes. Nano Lett 10(10):3978–3983

36. Szczecz JR, Jin S (2011) Nanostructured silicon for high capacity lithium battery anodes. Energy Environ Sci 4(5):1578–1601

37. Huang Y, McDowell MT, Jackson A, Cha JJ, Hong SS, Cui Y (2010) New nanostructured Li2S/LiSi2O3 rechargeable battery with high specific energy. Nano Lett 10(4):1486–1491

38. Li D, Wu Y, Kim P, Shi L, Young’s P (2003) Thermal conductivity of individual silicon nanowires. Appl Phys Lett 83(14):2934–2936

39. Chen J, Zhang G, Li B (2010) Remarkable reduction of thermal conductivity in silicon nanotubes. Nano Lett 10(10):3978–3983

40. Szczecz JR, Jin S (2011) Nanostructured silicon for high capacity lithium battery anodes. Energy Environ Sci 4(5):1578–1601

41. Huang Y, McDowell MT, Jackson A, Cha JJ, Hong SS, Cui Y (2010) New nanostructured Li2S/LiSi2O3 rechargeable battery with high specific energy. Nano Lett 10(4):1486–1491

42. Li D, Wu Y, Kim P, Shi L, Young’s P (2003) Thermal conductivity of individual silicon nanowires. Appl Phys Lett 83(14):2934–2936

43. Chen J, Zhang G, Li B (2010) Remarkable reduction of thermal conductivity in silicon nanotubes. Nano Lett 10(10):3978–3983

44. Szczecz JR, Jin S (2011) Nanostructured silicon for high capacity lithium battery anodes. Energy Environ Sci 4(5):1578–1601

45. Huang Y, McDowell MT, Jackson A, Cha JJ, Hong SS, Cui Y (2010) New nanostructured Li2S/LiSi2O3 rechargeable battery with high specific energy. Nano Lett 10(4):1486–1491

46. Li D, Wu Y, Kim P, Shi L, Young’s P (2003) Thermal conductivity of individual silicon nanowires. Appl Phys Lett 83(14):2934–2936

47. Chen J, Zhang G, Li B (2010) Remarkable reduction of thermal conductivity in silicon nanotubes. Nano Lett 10(10):3978–3983

48. Szczecz JR, Jin S (2011) Nanostructured silicon for high capacity lithium battery anodes. Energy Environ Sci 4(5):1578–1601

49. Huang Y, McDowell MT, Jackson A, Cha JJ, Hong SS, Cui Y (2010) New nanostructured Li2S/LiSi2O3 rechargeable battery with high specific energy. Nano Lett 10(4):1486–1491

50. Li D, Wu Y, Kim P, Shi L, Young’s P (2003) Thermal conductivity of individual silicon nanowires. Appl Phys Lett 83(14):2934–2936

51. Chen J, Zhang G, Li B (2010) Remarkable reduction of thermal conductivity in silicon nanotubes. Nano Lett 10(10):3978–3983

52. Szczecz JR, Jin S (2011) Nanostructured silicon for high capacity lithium battery anodes. Energy Environ Sci 4(5):1578–1601
clamped silicon nanobeams fabricated by the vapor-liquid-solid method. Appl Phys Lett 87(5):053111
47. Genoese A, Genoese A, Salerno G (2019) On the nanoscale behaviour of single-wall C, BN and SiC nanotubes. Acta Mech 230:1105–1128
48. Rapaport, D. “The art of molecular dynamics simulation”, Cambridge University press 1995, UK (2004)
49. Tersoff J (1986) New empirical model for the structural properties of silicon. Phys Rev Lett 56:632–635
50. Verma V, Dharamvir K, Jindal VK (2008) Structure and Elastic Modulii of Silicon Nanotubes. J Nano Res 2:85–90
51. Kang JW, Seo JJ, Hwang HJ (2002) Molecular Dynamics Study of Hypothetical Silicon Nanotubes Using the Tersoff Potential. J Nanosci Nanotechnol 2:687–691
52. Jeong Won Kang, Jae Jeong Seo, Ho Jung Hwang. “A Study on Silicon Nanotubes based on the Tersoff potential” (2002)
53. Lv P, Feng Y-y, Zhang P, Chen H-m, Zhao N, Feng W (2011) Increasing the interfacial strength in carbon fiber/epoxy composites by controlling the orientation and length of carbon nanotubes grown on the fibers. Carbon. 49(14):4665–4673

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