Deformation independent thermal conductivity of the designed Si nanobeam

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Abstract

The thermal properties of nanostructures have been widely focused due to their broad applications. Generally, applying deformation or strain is an effective way to tune thermal transport. However, deformation independent thermal conductivity is less reported. This work investigates the thermal conductivity of a designed curved Si nanobeam with quasi-zero stiffness feature by molecular dynamics simulation. Interestingly, it is found that the designed Si nanobeam has both unchanged thermal conductivity and quasi-zero stiffness feature under deformation. Besides, the designed Si nanobeam can reduce thermal conductivity up to 35.6% compared with the corresponding straight beam. The analyses show that the stress in the designed Si nanobeam is ultra-small compared with that in bulk Si and Si nanowires with strain, and the phonon density of states are little changed when deformation is applied, which lead to the deformation independent thermal conductivity. This work provides valuable insights on multifunctional applications of designed nanostructures, such as both stable thermal and stable mechanical properties.

Keywords: Curved nanobeam, deformation effect, thermal conductivity, stress and strain
1. Introduction

Thermal properties of nanostructures are critical for a broad range of applications, such as thermoelectric\cite{1-3} and thermal management of nanoelectronics\cite{4}. Especially, flexible electronics and many other functional applications involve large deformation, which demands nanostructures with the ability of working well with deformation\cite{5}. On the other hand, deformation or strain is inevitable for devices in practical applications or experimental characterization. Therefore, deformation or strain effect on the properties of nanostructures is meaningful to be studied.

Different from widely used scattering effects such as defects and interfaces\cite{6-9} and coherent effects such as nanophononics\cite{10,11}, deformation or strain/stress is another effective mechanisms to tune the thermal conductivity (\(\kappa\))\cite{12-15}. On the other hand, designing morphologies of nanostructures provides new degrees of freedom to manipulate properties of nanostructures\cite{16-18}, which is different from previous preliminary designs such as periodic nanostructure\cite{10,19,20}, and random structure\cite{2,21}. It was found that curved nanostructures with designed morphologies like kinked nanowires can be used to manipulate thermal transport\cite{22}. Therefore, designed curved nanostructures under deformation which couple the designed morphology and strain/stress are worthy to be investigated.

Most previous researches demonstrated that the deformation or strain/stress can affect the thermal conductivity of nanostructures\cite{12-15,23}. For example, the \(\kappa\) of the strained silicon nanowires (SiNW) and thin films is shown to decrease continuously when the strain changes from compressive to tensile\cite{24}. The measured \(\kappa\) of the 50 nm thick silicon nitride films is decreased from 2.7 W/mK at zero strain to 0.34 W/m-K at about 2.4% tensile strain\cite{25}. However, just few works reported the unchanged \(\kappa\) under deformation or strain conditions. Murphy et al. found that the SiNW with diameter in the range of 170-180 nm is largely unaffected by uniform uniaxial tensile strain below 1% studied by situ Raman piezothermography method\cite{26}, unlike the defect effect which reduces the \(\kappa\) by over 70%. Another work also observed the unchanged \(\kappa\) in the strained SiNW, which is measured to be similar in value to the unstrained SiNW of between 0.3-1.0 W/mK\cite{27}. Other nanostructures with stable thermal transport properties under various deformation or strain/stress conditions...
are less investigated.

Curved nanostructures in designed morphologies can effectively manipulate thermal transport.\[22\] It was found that the kinked SiNW has smaller $\kappa$ compared with that of the straight SiNW because of the interchanging effect between longitudinal and transverse phonon modes and the pinching effect.\[28\] Further, experimental measurements found that kinks in boron carbide nanowires can pose a thermal resistance up to \~30 times larger than that of a straight wire segment.\[18\] Later, a simulation work attributed the additional kink resistance to the back scattering of phonons from the free surface of the kink.\[29\] Similarly, Si nanoribbons with multiple kinks can reach a maximum reduction of 21% of $\kappa$.\[30\] It was also found that curvature of nanowires can impede ballistic phonon transport causing the reduction of effective $\kappa$.\[31\] The curved SiNW obtained by applying deformation can relate curvature and deformation or strain/stress,\[32\] importantly, its $\kappa$ is reduced by 10% because of the inhomogeneous topological and stress distribution due to the curvature.\[32\]

Interestingly, a recent work reported that optimally designed curved macroscale beams can achieve quasi-zero stiffness (QZS) by realizing a plateau in their force-displacement curve, which is the requirement as QZS isolator.\[33\] Such QZS isolators with sufficient load bearing capacity are of interest in many fields such as precision instruments, suspensions and sensors for isolating undesirable vibrations.\[34-37\] However, curved nanostructures with QZS feature are rarely reported.

Considering that curved structure can realize QZS in macroscale beam \[33\] and tune $\kappa$ in nanostructures\[31\], optimally designed curved nanostructures probably have both the QZS feature and the tuned $\kappa$, however, it is rarely demonstrated theoretically or experimentally. In addition, the deformation or strain effect on curved nanostructures has not been systematically studied, which is important for many devices like flexible electronics. Recent experiment work showed that Si nanowire can possess “deep ultra-strength”, when it is pristine, defect-scarce, nanosized single-crystalline structure with atomically smooth surfaces.\[5\] Therefore, nanostructured Si can be possibly created in designed curve and work under various deformation conditions to achieve multifunction.
In this work, a designed curved Si nanobeam (DCSiNB) with quasi-zero stiffness feature is investigated by nonequilibrium molecular dynamics (NEMD) simulations. The $\kappa$ of DCSiNB is calculated and compared with the corresponding straight beam. Importantly, the trend of $\kappa$ versus the deformation is systematically studied. The stress and phonon density of states are calculated to understand the underlying mechanism.

2. Design and Method

![Figure 1. Structure of the designed curved Si nanobeam. (a) The Si block used to create the DCSiNB. The solid black lines are the designed curves, which are linearly scaled from the geometry of the macroscale beam in Ref. [33] The length (L) and height (H) of the block is 173.79 Å and 84.46 Å, respectively. (b) The structure of the DCSiNB-I. The DCSiNB is created by removing the atoms in (a) outside of the curves. It is the initial state of the DCSiNB-I before it is deformed. The thickness of the DCSiNB-I is 10.86 Å. The solid black lines are kept to lead the eye. (c) The structure of the deformed DCSiNB-I with displacement of 0, 16.97, 33.94 and 50.92 Å, respectively. The DCSiNB-I with $D_x=0$ Å is the initial state in (b).](image)

The DCSiNB is created from a Si block based on the designed curve, which is shown in Figure 1. The curve is linearly scaled from the geometry of the macroscale beam in Ref. [33],
which is optimized for the prescribed QZS feature by genetic algorithm. Firstly, a Si block with length of 173.79 Å and height of 84.46 Å is created (Figure 1 (a)), which is 32×15 conventional cell (CC) of Si. The lattice constant (La) of Si is 5.431 Å. Secondly, the atoms outside of the curves are removed, meanwhile, the atoms inside of the curves are kept, which is the DCSiNB (Figure 1 (b)). It is the initial state of the DCSiNB before it is deformed. The thickness of the DCSiNB in Figure 1 (b) is 10.86 Å (2CC of Si), this structure is noted as DCSiNB-I.

The deformed DCSiNB is obtained by displacing the right end of the DCSiNB in -x direction. During this process, the force-displacement curve is calculated by recording the displacement (Dx) and the force on the right end of the DCSiNB. The left end of the DCSiNB is fixed, and periodic boundary condition is applied in z direction. The size of the DCSiNB in z direction is set as 5.431 Å (1 CC of Si). For the deformation, first the atoms on the top of the right end are displaced by La/64 in -x direction, then the atom coordinates of the DCSiNB are optimized by performing energy minimization with stopping tolerance of force of 1.0×10^{-12} ev/Å, finally, the force of the atoms on the top of the right end is calculated. The DCSiNB is deformed successively step by step. The force-displacement curve of the DCSiNB-I is shown in Figure S1 (a) in the Supplementary Material. The plateau in its force-displacement curve indicates the QZS feature of the DCSiNB-I.

The structures of the deformed DCSiNB-I with Dx of 0, 16.97, 33.94 and 50.92 Å are shown in Figure 1 (c). The interaction between Si atoms are described by Stillinger-Weber potential,[38] which has been widely applied in Si nanostructures. The energy minimization is performed by LAMMPS.[39] The force-displacement of the DCSiNB-I with 2 CC of Si in z direction are presented in Figure S2 in the Supplementary material. After the DCSiNB is deformed, it also can recover if the right end is displaced reversely (in x direction). The force-displacement curve for the reverse direction is shown in Figure S3 in the Supplementary Material.

The thermal conductivity of the DCSiNB is calculated by NEMD method. The fixed boundary conditions are applied at the two ends. Periodic boundary condition is applied in z direction, the size of DCSiNB-I in z direction is set as 6 CC of Si to obtain converged \( \kappa \). Langevin heat baths[40] with temperature of 310 K and 290 K are applied at the left and right ends of the DCSiNB, respectively. The time step of NEMD simulation is set as 0.5 fs. In the
beginning, the simulation runs 4 ns to reach a steady state. Then, the simulation runs 5 ns to get an averaged heat flux and temperature profile. The effective $\kappa$ is calculated from

$$
\kappa = \frac{J l}{A \Delta T}
$$

where $J$ is the heat current, $A$ is the cross-section area of the DCSiNB, and $\Delta T$ is the temperature difference between the two ends of DCSiNB. $l$ is the length of the DCSiNB. The final results of $\kappa$ are averaged over six simulations with different initial conditions. The error bar is the standard deviation of the six simulations.

3. Results

The thermal conductivity of the DCSiNB-I is calculated according to Eq. (1). The corresponding straight Si beam is studied for comparison. The straight Si beam has the same thickness and number of atoms as that of the DCSiNB-I. The length $l$ of the straight Si beam and the DCSiNB-I are both 24.4 nm. The temperature profile for the DCSiNB-I at initial and straight Si beam along $x$ direction are shown in Figure 2 (a). The black dashed line is the linear fit for the temperature profile of straight Si beam. The temperature distributions in both $x$ and $y$ directions are shown in Figure S5 in the Supplementary Material. There are temperature jumps at the two ends for the straight Si beam, but no obvious temperature jump appears for the DCSiNB-I. The temperature jumps are considered for the straight Si beam in the calculation of $\kappa$. The heat flux and $\kappa$ are shown in Figure 2 (b) and (c), respectively. The heat flux and $\kappa$ for the straight Si beam are $2.18\pm0.18 \times 10^9$ W/m$^2$ and $2.86\pm0.24$ W/m-K, respectively, which are represented by the black dashed lines. The reduction of heat flux and $\kappa$ of the DCSiNB-I at initial state ($D_x=0$ Å) is around 15.8% and 21.7%, respectively, which is consistent with the findings of the curvature effect on the $\kappa$ of Si nanowire$^{31,32}$. However, the $\kappa$ of the deformed DCSiNB-I with $D_x$ from 0 to 51 Å are little changed, which indicates the deformation independent $\kappa$ of the DCSiNB. Therefore, the DCSiNB has relatively stable thermal properties under deformation.
Figure 2. (a) Temperature profile of the DCSiNB-I at initial state ($D_x=0$ Å) and the corresponding straight Si beam along $x$ direction. The black dashed line is the linear fit for the straight Si beam. Heat flux (b) and thermal conductivity (c) for the deformed DCSiNB-I with displacement from 0 to 51 Å. The dashed line in (b) and (c) is for the corresponding straight Si beam. (d) Phonon density of states of straight Si beam and the DCSiNB-I with $D_x=0$, 27.32 and 46.67 Å.

To further understand the underlying mechanisms, phonon density of states (DOS) of the deformed DCSiNB-I with $D_x=0$, 27.32 and 46.67 Å are calculated by the general utility lattice program (GULP)\textsuperscript{[41]}, which is shown in Figure 2 (d). For comparison, the DOS of straight Si beam is also computed. The DOS of the DCSiNB-I is close to that of the straight Si beam when the frequency is low (<3.5 THz) or high (<14 THz), while the peaks of DOS of the DCSiNB-I are much smaller than that of the straight Si beam when the frequency is between 3.5 and 14 THz, which can be caused by the symmetry breaking due to the shapes of the DCSiNB-I. In addition, the DOS of the deformed DCSiNB-I with different $D_x$ is almost the
same, which indicates that the distribution of modes in DCSiNB-I is less affected by the deformation. Therefore, the $\kappa$ of DCSiNB is little changed when it undergoes deformation.

Figure 3. (a) The structure of DCSiNB-II at initial state ($D_x=0$ Å) and under deformation ($D_x=40.22$ and 101.83 Å). The DCSiNB-II doubles the size of the DCSiNB-I in Figure 1 (b). The thickness of the DCSiNB-II is 21.72 Å. (b) Thermal conductivity of the DCSiNB-II. The $\kappa$ of the corresponding straight Si beam (black dashed line) is shown for comparison.

To investigate if the size of the DCSiNB can affect the thermal behavior under deformation, a thicker DCSiNB (denoted as DCSiNB-II in Figure 3 (a)) whose size doubles that of the DCSiNB-I in Figure 1 (b) are studied. The thickness of the DCSiNB-II is 21.72 Å. The force-displacement curve for the DCSiNB-II is shown in Figure S1 (a) in the Supplementary Material. Similar to the DCSiNB-I, the DCSiNB-II also has a plateau in the force-displacement curve, which implies that QZS feature is maintained in the thicker DCSiNB. The $\kappa$ of the deformed DCSiNB-II is shown in Figure 3 (b). The $\kappa$ of the corresponding straight Si beam with thickness of 21.72 Å and length of 47.8 Å is shown for comparison (black dashed lines). The temperature profiles and heat flux of the DCSiNB-II are shown in Figure S4 in the Supplementary Material. The $\kappa$ of DCSiNB-II at initial state is reduced 35.6% compared with that of the corresponding straight Si beam (12.1±0.66 W/m-K). However, the thermal conductivity of deformed DCSiNB-II with $D_x$ from 0 to 102 Å is almost unchanged, which is consistent with findings in the DCSiNB-I in Figure 2.
Figure 4. (a) Local stress ($\sigma_{xx}$) distribution in the DCSiNB-I at initial state ($D_x=0$ Å) and the deformed DCSiNB-I with $D_x=27.32$ and 46.67 Å. The value of the local stress is according the color bars. (b) Average value of local stress in section 1 to 3 (denoted as S1, S2 and S3). The dashed blue lines correspond to the stress in bulk Si with strain=$-0.5\%$,$^{[42]}$ bent Si nanowire$^{[32]}$ and Si nanowire with strain=$1\%$. The averaged local stress is ultralow compared with that in bulk Si and Si nanowire.

To further understand the deformation independent thermal conductivity in the deformed DCSiNB, the local stress are calculated by LAMMPS.$^{[39]}$ The distribution of the local stress in the deformed DCSiNB-I with $D_x=0$, 27.32 and 46.67 Å are shown in Figure 4 (a). The value of the local stress is according to the color bar. According to the distribution, the locations with larger curvature have relatively larger local stress, while other parts have small value of local stress under deformation. Moreover, the right end has large local stress. Therefore, most regions of the DCSiNB-I have small local stress, in addition, the relatively large stress is only localized in small regions of the DCSiNB. To clearly show the changes of the local stress under deformation, the average value of local stress ($\sigma_{xx}$, $\sigma_{yy}$ and $\sigma_{zz}$) in three sections (S1, S2 and S3 indicated in Figure 4 (a)) are calculated (Figure 4 (b)). Previous study found that the stress of bulk Si with strain=$-0.5\%$,$^{[42]}$ and Si nanowire with strain=$1\%$,$^{[5]}$ is larger than 1 GPa. The bent Si nanowire$^{[32]}$ has stress around 1.0 GPa in the region at half diameter. In the DCSiNB,
the average value of local stresses in these three sections are ultra-small (<151 MPa) under large deformation compared with that in bulk Si and Si nanowire with small strain (<1%). The strain effect on the \( \kappa \) of Si nanostructure in Ref.\textsuperscript{[24]} shows that small stress cannot cause visible changes in \( \kappa \). Therefore, the ultra-small stress in the DCSiNB under deformation leads to the little changed thermal conductivity.

4. Conclusion

In this work, the designed curved Si nanobeam is investigated by nonequilibrium molecular dynamics simulations. DCSiNBs have quasi-zero stiffness indicated by the plateau in its force-displacement curve. Interestingly, the deformed DCSiNBs have almost unchanged thermal conductivity when they undergo deformation and stress. Further analyses show that the DOS of DCSiNBs is little changed under deformation and the average value of local stress is ultra-small, which lead to the deformation independent thermal conductivity of the DCSiNB. Similar thermal transport behaviors are observed in two Si nanobeams with thickness of 10.86 Å (DCSiNB-I) and 21.72 Å (DCSiNB-II), respectively. The thermal conductivity of the DCSiNB-I and DCSiNB-II are reduced around 21.7% and 35.6% compared with that of the corresponding straight Si beam, respectively.

The results of this work are meaningful for the multifunctional applications of curved nanostructures with both unchanged thermal conductivity and quasi-zero stiffness feature under deformation, such as both stable thermal and stable mechanical properties.

5. Acknowledgements

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Reference

[1] X. Qian, J. Zhou, & G. Chen, Phonon-engineered extreme thermal conductivity materials. Nature Materials, 1 (2021).

[2] A.I. Hochbaum, R. Chen, R.D. Delgado, W. Liang, E.C. Garnett, M. Najarian, A. Majumdar, & P. Yang, Enhanced thermoelectric performance of rough silicon nanowires. Nature 451, 163 (2008).

[3] L. Yang, D. Huh, R. Ning, V. Rapp, Y. Zeng, Y. Liu, S. Ju, Y. Tao, Y. Jiang, & J. Beak, High thermoelectric figure of merit of porous Si nanowires from 300 to 700 K. Nature Communications 12, 1 (2021).

[4] I. Chowdhury, R. Prasher, K. Lofgreen, G. Chrysler, S. Narasimhan, R. Mahajan, D. Koester, R. Alley, & R. Venkatasubramanian, On-chip cooling by superlattice-based thin-film thermoelectrics. Nature Nanotechnology 4, 235 (2009).

[5] H. Zhang, J. Tersoff, S. Xu, H. Chen, Q. Zhang, K. Zhang, Y. Yang, C.-S. Lee, K.-N. Tu, & J. Li, Approaching the ideal elastic strain limit in silicon nanowires. Science Advances 2, e1501382 (2016).

[6] K. Biswas, J. He, I.D. Blum, C.-I. Wu, T.P. Hogan, D.N. Seidman, V.P. Dravid, & M.G. Kanatzidis, High-performance bulk thermoelectrics with all-scale hierarchical architectures. Nature 489, 414 (2012).

[7] S. Xiong, K. Sääskilahti, Y.A. Kosevich, H. Han, D. Donadio, & S. Volz, Blocking phonon transport by structural resonances in alloy-based nanophononic metamaterials leads to ultralow thermal conductivity. Physical Review Letters 117, 025503 (2016).

[8] J. Chen, Q. Sun, D. Bao, T. Liu, W.-D. Liu, C. Liu, J. Tang, D. Zhou, L. Yang, Z.-G. Chen, & Interfaces, Hierarchical structures advance thermoelectric properties of porous n-type β-Ag2Se. ACS Applied Materials 12, 51523 (2020).

[9] S. Wang, Y. Xiao, Y. Chen, S. Peng, D. Wang, T. Hong, Z. Yang, Y. Sun, X. Gao, & L.-D. Zhao, Hierarchical structures lead to high thermoelectric performance in Cu m+ n Pb 100 Sb m Te 100 Se 2m (CLAST). Energy Environmental Science 14, 451 (2021).

[10] L. Yang, N. Yang, & B. Li, Extreme low thermal conductivity in nanoscale 3D Si phononic crystal with spherical pores. Nano Letters 14, 1734 (2014).

[11] H. Honarvar, L. Yang, & M.I. Hussein, Thermal transport size effects in silicon
membranes featuring nanopillars as local resonators. Applied Physics Letters 108, 263101 (2016).

[12] A.R. Abramson, C.-L. Tien, & A. Majumdar, Interface and strain effects on the thermal conductivity of heterostructures: A molecular dynamics study. Journal of Heat Transfer 124, 963 (2002).

[13] Y. Kuang, L. Lindsay, S. Shi, X. Wang, & B. Huang, Thermal conductivity of graphene mediated by strain and size. International Journal of Heat and Mass Transfer 101, 772 (2016).

[14] Q. Wang, L. Han, L. Wu, T. Zhang, S. Li, & P. Lu, Strain effect on thermoelectric performance of InSe monolayer. Nanoscale Research Letters 14, 1 (2019).

[15] B. Ding, X. Li, W. Zhou, G. Zhang, & H. Gao, Anomalous strain effect on the thermal conductivity of low-buckled two-dimensional silicene. National Science Review 8, nwaa220 (2021).

[16] C. Portela & J. Ye, Architectures down to nano. Nature Materials 20, 1451 (2021).

[17] B. Tian, P. Xie, T.J. Kempa, D.C. Bell, & C.M. Lieber, Single-crystalline kinked semiconductor nanowire superstructures. Nature Nanotechnology 4, 824 (2009).

[18] Q. Zhang, Z. Cui, Z. Wei, S.Y. Chang, L. Yang, Y. Zhao, Y. Yang, Z. Guan, Y. Jiang, & J. Fowlkes, Defect facilitated phonon transport through kinks in boron carbide nanowires. Nano Letters 17, 3550 (2017).

[19] L.R. Meza, S. Das, & J.R. Greer, Strong, lightweight, and recoverable three-dimensional ceramic nanolattices. Science 345, 1322 (2014).

[20] J.-K. Yu, S. Mitrovic, D. Tham, J. Varghese, & J.R. Heath, Reduction of thermal conductivity in phononic nanomesh structures. Nature Nanotechnology 5, 718 (2010).

[21] Y. Zhao, D. Liu, J. Chen, L. Zhu, A. Belianinov, O.S. Ovchinnikova, R.R. Unocic, M.J. Burch, S. Kim, & H. Hao, Engineering the thermal conductivity along an individual silicon nanowire by selective helium ion irradiation. Nature Communications 8, 1 (2017).

[22] L. Yang, R. Prasher, & D. Li, From nanowires to super heat conductors. Journal of Applied Physics 130, 220901 (2021).

[23] Z. Yang, R. Feng, F. Su, D. Hu, X. Ma, & Nanostructures, Isotope and strain effects on thermal conductivity of silicon thin film. Physica E: Low-dimensional Systems 64, 204
[24] X. Li, K. Maute, M.L. Dunn, & R. Yang, Strain effects on the thermal conductivity of nanostructures. Physical Review B 81, 245318 (2010).

[25] M. Alam, M.P. Manoharan, M.A. Haque, C. Muratore, A. Voevodin, & Microengineering, Influence of strain on thermal conductivity of silicon nitride thin films. Journal of Micromechanics Microengineering 22, 045001 (2012).

[26] K.F. Murphy, B. Piccione, M.B. Zanjani, J.R. Lukes, & D.S. Gianola, Strain-and defect-mediated thermal conductivity in silicon nanowires. Nano Letters 14, 3785 (2014).

[27] D. Fan, H. Sigg, R. Spolenak, & Y. Ekinci, Strain and thermal conductivity in ultrathin suspended silicon nanowires. Physical Review B 96, 115307 (2017).

[28] J.-W. Jiang, N. Yang, B.-S. Wang, & T. Rabczuk, Modulation of thermal conductivity in kinked silicon nanowires: phonon interchanging and pinching effects. Nano Letters 13, 1670 (2013).

[29] Y. Zhao, L. Yang, C. Liu, Q. Zhang, Y. Chen, J. Yang, & D. Li, Kink effects on thermal transport in silicon nanowires. International Journal of Heat and Mass Transfer 137, 573 (2019).

[30] L. Yang, Q. Zhang, Z. Wei, Z. Cui, Y. Zhao, T.T. Xu, J. Yang, & D. Li, Kink as a new degree of freedom to tune the thermal conductivity of Si nanoribbons. Journal of Applied Physics 126, 155103 (2019).

[31] L.-C. Liu, M.-J. Huang, R. Yang, M.-S. Jeng, & C.-C. Yang, Curvature effect on the phonon thermal conductivity of dielectric nanowires. Journal of Applied Physics 105, 104313 (2009).

[32] X. Liu, H. Zhou, G. Zhang, & Y.-W. Zhang, The effects of curvature on the thermal conduction of bent silicon nanowire. Journal of Applied Physics 125, 082505 (2019).

[33] Q. Zhang, D. Guo, & G. Hu, Tailored Mechanical Metamaterials with Programmable Quasi-Zero-Stiffness Features for Full-Band Vibration Isolation. Advanced Functional Materials 31, 2101428 (2021).

[34] H.S. Bouna, B. Nbendjo, & P. Woaf, Isolation performance of a quasi-zero stiffness isolator in vibration isolation of a multi-span continuous beam bridge under pier base vibrating excitation. Nonlinear Dynamics 100, 1125 (2020).
[35] R. Ibrahim, Recent advances in nonlinear passive vibration isolators. Journal of sound and vibration 314, 371 (2008).

[36] P. Alabuzhev, Vibration protection and measuring systems with quasi-zero stiffness. (CRC Press, 1989).

[37] L. Wu, Y. Wang, Z. Zhai, Y. Yang, D. Krishnaraju, J. Lu, F. Wu, Q. Wang, & H. Jiang, Mechanical metamaterials for full-band mechanical wave shielding. Applied Materials Today 20, 100671 (2020).

[38] F.H. Stillinger & T.A. Weber, Computer simulation of local order in condensed phases of silicon. Physical Review B 31, 5262 (1985).

[39] A.P. Thompson, H.M. Aktulga, R. Berger, D.S. Bolintineanu, W.M. Brown, P.S. Crozier, P.J. in't Veld, A. Kohlmeyer, S.G. Moore, & T.D. Nguyen, LAMMPS-a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. Computer Physics Communications 271, 108171 (2022).

[40] J. Chen, G. Zhang, & B. Li, Molecular dynamics simulations of heat conduction in nanostructures: effect of heat bath. Journal of the Physical Society of Japan 79, 074604 (2010).

[41] J.D. Gale & A.L. Rohl, The general utility lattice program (GULP). Molecular Simulation 29, 291 (2003).

[42] V. Kuryliuk, O. Nepochatyi, P. Chantrenne, D. Lacroix, & M. Isaiev, Thermal conductivity of strained silicon: Molecular dynamics insight and kinetic theory approach. Journal of Applied Physics 126, 055109 (2019).
Deformation independent thermal conductivity of the designed Si nanobeam

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The force-displacement curve of the DCSiNB-I is calculated by displacing the right end of the DCSiNB-I in -x direction. Because the size of the DCSiNB in z direction is set as 1 CC of Si and the thickness is 2 CC of Si, so there are 4 atoms on top of the right end. The force on the right end of the DCSiNB-I in x direction (Figure S1 (a)) is the sum of the forces on these 4 atoms in x direction (Figure S1 (b)). Similarly, the force-constant curve of the DCSiNB-II in Figure 3 (a) is also calculated. As shown in Figure S1 (a), the force-displacement curve has a plateau for both the DCSiNB-I and the DCSiNB-II, which indicates the quasi-zero stiffness (QZS) feature of the DCSiNB. This phenomenon is similar to that of the macroscale curved beam with quasi-zero stiffness⁹. This result exhibits that curved nanostructure can realized QZS feature. In addition, the force of the atoms on top of the right end of DCSiNB-I is shown in Figure S1 (b). The trend of the force is different for different atoms, but the overall behavior of these atoms performs QZS feature. Local stress (σ_{xx}) on each atom on top of the right end of the DCSiNB-I is shown in Figure S1 (c). The trend of local stress is similar to the inverse trend of the force in Figure S1 (b). The average value of local stress (σ_{xx}) at each layer of the DCSiNB-I is presented in Figure S1 (d). Here, the atoms with the same coordinates x are set as in the
same layer. The atoms on top of the right end of DCSiNB-I is in layer 1, the atoms next to atoms in layer 1 are in layer 2, etc. As shown in Figure S1 (d), the average local stress is ultra-small even under large deformation.

![Figure S1](image)

Figure S1. (a) Force-displacement curve of the designed curved Si nanobeam (DCSiNB), DCSiNB-I (blue dashed line) and the DCSiNB-II (red dashed line), respectively. The direction of the force is in $x$ direction. There is a plateau in the force-displacement curve, which indicates quasi-zero stiffness (QZS) feature of the DCSiNB. (b) Force on each atom on top of the right end of the DCSiNB-I. The direction of the force is in $x$ direction. (c) Local stress ($\sigma_{xx}$) on each atom on top of the right end of the DCSiNB-I. (d) Average value of local stress ($\sigma_{xx}$) on each layer of the DCSiNB-I. The atoms with the same coordinates $x$ are set as in the same layer. The atoms on top of the right end of the DCSiNB-I is in layer 1, the atoms next to atoms in layer 1 are in layer 2, etc.
Figure S2. The force-displacement curve of DCSiNB-I with Nz = 2 CC of Si. The force-displacement curve of DCSiNB-I with Nz = 1 CC of Si is also presented for comparison. The direction of the force is in x direction.

The size of the DCSiNB in z direction in Figure 1 is set as 1 conventional cell (CC) of Si, which is noted as Nz=1 CC. Periodic boundary condition is used to simulate a curved nanobeam with larger size in z direction. To test whether 1 CC in z direction is large enough to predict converged force, a DCSiNB with Nz=2 CC is investigated. The force-displacement curve of DCSiNB-I with Nz=2 CC is shown in Figure S2. Because the DCSiNB-I with Nz=2 CC has 8 atoms on top of the right end, so its force is divided by 2 to be compared with that of DCSiNB-I with Nz=1 CC (solid blue line in Figure S2) which as 4 atoms. As shown in Figure S2, the force of DCSiNB-I with Nz=2 CC is the same as that of the DCSiNB-I with Nz=1 CC. Therefore, the 1 CC in z direction can predict converged force for the DCSiNB.
Figure S3. The force-displacement curve of DCSiNB-I under deformation. The right end of the DCSiNB-I is first displaced in \(-x\) direction from 0 to 55 Å (black dashed line), then it is reversely displaced in \(x\) direction from 55 to 0 Å (red dashed line). This curve indicates that the DCSiNB is elastically deformed.

To investigate if the DCSiNB can recover after it is deformed, the DCSiNB is reversely deformed, which is shown in Figure S3. After the right end of the DCSiNB-I is displaced in \(-x\) direction from 0 to 55 Å, it is reversely displaced in \(x\) direction from 55 to 0 Å to get the force-displacement curve for the reverse displacement (red dashed line). As shown in Figure S3, the force-displacement for the displacement and the inverse displacement is symmetrical. The initial state of the DCSiNB is recovered when its right end is back to the initial position. This result indicates that the deformation for the DCSiNB is elastic.
Figure S4. (a) Temperature profile of the DCSiNB-II at initial state (Dx=0 Å) and the corresponding straight Si beam along x direction. The black dashed line is the linear fit for the straight Si beam. (b) Heat flux for the deformed DCSiNB-II with displacement from 0 to 102 Å. The dashed line in (b) is for the corresponding straight Si beam.

The thermal conductivity of the DCSiNB-II is calculated by NEMD simulation method. The temperature profile for the DCSiNB-II at initial state (Dx=0 Å) and the corresponding straight Si beam along x direction are shown in Figure S4 (a). The black dashed line is the linear fit for the straight Si beam. Temperature jumps at the two ends are obvious for the straight Si beam, which are considered in the calculation of thermal conductivity. The heat flux of the DCSiNB-II under deformation is shown in Figure S4 (b). The heat flux for the straight Si beam is $4.58 \pm 0.25 \times 10^9$ W/m², which is represented by the black dashed lines. The reduction of heat fluxes of the DCSiNB-II at initial state (Dx=0 Å) is around 28.6%. However, the heat flux of the deformed DCSiNB-II with Dx from 0 to 102 Å are little changed, which implies that it has relatively stable thermal properties under deformation.

Figure S5. (a) Temperature distribution of the straight Si beam. (b) Temperature distribution of the deformed DCSiNB-I with Dx=0, 27.32, 42.43 Å. The value of temperature is according to
the color bar.

The temperature profile of DCSiNB in Figure 2 (a) and Figure S4 (a) is along x direction. To clearly show the local temperature in the DCSiNB-I, the temperature distribution is calculated and shown in Figure S5. For comparison, the temperature distribution of the corresponding straight Si beam is also shown in Figure S5 (a). The changes of temperature are along the curve lines in the deformed DCSiNB-I. The temperature on the surface of DCSiNB-I has larger value than that in the inside of DCSiNB-I, which indicates that the energy are likely localized on the surface of DCSiNB.