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SPECIAL TOPIC — Heat conduction and its related interdisciplinary areas

Strain modulated phonon transport in one-dimensional nonlinear lattice with on-site potential

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The one-dimensional (1D) nonlinear lattices with on-site potentials exhibit normal heat conduction and energy diffusion behaviors. The strain-modulated energy diffusion constants are studied for the 1D Frenkel–Kontorova (FK) lattices, which are typical lattices with on-site potentials. The 1D FK lattices show strain-modulated symmetric behaviors of local extrema in energy diffusion constants, similar to those previously observed in 1D Fermi–Pasta–Ulam (FPU) lattices that contain only interparticle potentials. However, the 1D FK lattices exhibit local minima in energy diffusion constants, which is in contrast to the behavior of the 1D FPU lattices. Although strain always enhances the phonon group velocity and suppresses the phonon relaxation time for both the 1D FK and FPU lattices, the suppression of the phonon relaxation time is much weaker for the 1D FK lattices compared to the 1D FPU lattices.

Keywords: heat conduction, nonlinear dynamics

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1. Introduction

The control of heat transport is of great importance for thermal management and thermoelectric devices.[1,2] Being one of the fundamental thermodynamic variables, pressure or strain is an efficient way to modulate heat transport on demand.[3] The underlying mechanism behind this modulation is that phonon properties can be modified by the applied compressive or tensile strain. Many theoretical and computational studies have explored the strain effects on phonon transport in low-dimensional materials due to their potential applications.[4–14] However, no conclusive results have been reached, partly because phonon structures are complex when empirical or first-principles-based potential models are used for real materials. Therefore, one-dimensional (1D) nonlinear lattice models with simple phonon structures provide a good testbed for investigating pressure- or strain-modulated phonon transport. Until recently, only a few studies have focused on the strain effects on heat transport in 1D nonlinear lattices.[15–17]

The most widely studied thermal property of 1D nonlinear lattices is the unusual size effect of heat conduction.[18–23] For 1D nonlinear lattices with conserved total momentum and unbounded total energy, such as the Fermi–Pasta–Ulam (FPU)-β lattice, heat conduction is anomalous, where the thermal conductivity κ diverges with the lattice length L following a power-law behavior $\kappa \propto L^{\beta}$ with $0 < \beta < 1$.[24–31] For 1D nonlinear lattices with conserved total momentum but bounded kinetic or potential energy, such as the coupled rotator lattice,[32–36] heat conduction is normal, similar to that in 1D nonlinear lattices with non-conserved total momentum, such as the Frenkel–Kontorova (FK) and ϕ^4 lattices.[37–39]

For typical 1D nonlinear lattices, two general properties exist in every lattice Hamiltonian: nonlinearity and symmetry. It is well known that nonlinearity is closely related to temperature, while symmetry is closely related to pressure. The temperature-dependent phonon transport in 1D nonlinear lattices has been extensively studied within the framework of effective phonon theory.[40–42] It is also of great interest to study pressure- or strain-modulated phonon transport in 1D nonlinear lattices. Previous studies have found that the symmetry of the potential term in the Hamiltonian is highly sensitive to strain modulation in phonon transport.[14,16,17] It has been shown that the introduction of slight asymmetry suppresses heat conduction in 1D nonlinear lattices with interactive potentials, such as the FPU lattices. Since 1D nonlinear lattices with on-site potentials exhibit different heat conduction behavior from that of the 1D FPU lattices, it is interesting to investigate how strain affects phonon transport in such lattices.

This article is organized as follows. In Section 2, the Hamiltonians of the considered symmetric and asymmetric 1D FK lattices are discussed. The numerical methods, in-

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cluding the equilibrium energy diffusion approach[43] and the resonance phonon approach,[44,45] are briefly introduced. In Section 3, the strain-modulated energy diffusion constants are calculated using the equilibrium energy diffusion approach for both symmetric and asymmetric 1D FK lattices. To uncover the underlying mechanism, the modifications of phonon group velocity and relaxation time under different strains are presented using the resonance phonon approach. The conclusions are summarized in Section 4.

2. The Hamiltonian and numerical methods

The well-known 1D FK lattice describes the motion of a chain of interacting particles subjected to an external on-site periodic potential.[46] Besides being a well-studied model in heat conduction,[47] the FK lattice is also widely used in condensed matter physics to model crystal dislocations, magnetic spirals, charge-density waves, adsorbed epitaxial monolayers, and related phenomena.[48,49] To study the effect of potential symmetry on strain-modulated phonon transport, we consider two types of 1D FK lattices with symmetric and asymmetric interaction potentials. The dimensionless Hamiltonian for the symmetric 1D FK lattice is

$$H = \sum_{i}^{N}\left[\frac{p_i^2}{2}+\frac{1}{2}(q_i-q_{i-1})^2+\frac{1}{4}(q_i-q_{i-1})^4 + \frac{1}{2\pi}(1-\cos 2\pi q_i)\right], \tag{1}$$

where q_i and p_i denote the displacement from the equilibrium position and the momentum of the ith atom, respectively. The lattice length is $Na = N$, since the lattice constant is set as $a = 1$ in the dimensionless form. The asymmetric 1D FK lattice has the following dimensionless Hamiltonian:

$$H = \sum_{i}^{N}\left[\frac{p_i^2}{2}+\frac{1}{2}(q_i-q_{i-1})^2+\frac{\alpha}{3}(q_i-q_{i-1})^3 + \frac{1}{4}(q_i-q_{i-1})^4+\frac{1}{2\pi}(1-\cos 2\pi q_i)\right], \tag{2}$$

where the parameter α represents the strength of the asymmetric interaction potential.

To apply strain, a modified periodic boundary condition $q_N - q_0 = N\delta$ is introduced.[16] The parameter δ is related to the average relative spacing between adjacent atoms as $\delta = \langle q_i - q_{i-1}\rangle$.[17] With this boundary condition, the actual lattice length L can be expressed as $L = N + N\delta$. The natural lattice length $L = N$ corresponds to $\delta = 0$. Under external pressure, the lattice can be stretched for $\delta > 0$ or compressed for $\delta < 0$.[16] Since the positive direction of strain is usually defined for compression, we define the strain variable as $Str = -\delta$.

It has been theoretically proven that energy diffusion and heat conduction exhibit a one-to-one correspondence. The mean square displacement (MSD) for energy diffusion, $\langle \Delta x^2(t)\rangle_{\mathrm{E}} \propto t^{\gamma}$, is connected to heat conduction $\kappa \propto L^{\beta}$ via the relation $\beta = \gamma - 1$.[50] This relation holds for typical 1D nonlinear atomic lattices, except for special lattices of charged particles that break time-reversal symmetry and lack sound waves.[51,52] Therefore, this relation enables the study of heat conduction in 1D nonlinear atomic lattices using the equilibrium energy diffusion method.[43] For normal heat conduction with $\beta = 0$, the corresponding energy diffusion is also normal, with $\gamma = 1$. The energy diffusion constant D_{E} can be obtained by fitting the linear time dependence of the MSD as $\langle \Delta x^2(t)\rangle_{\mathrm{E}} = 2D_{\mathrm{E}}t$. Using this method, the strain-modulated energy diffusion constants D_{E} for symmetric and asymmetric 1D FK lattices can be calculated.

In particular, for normal heat conduction with thermal conductivity κ, the diffusion constant D_{E} is related to κ as $D_{\mathrm{E}} = \kappa/c$, where c is the specific heat. Since the phonon thermal conductivity is proportional to the specific heat c, phonon group velocity v_k, and phonon relaxation time τ_k for a typical phonon mode k, i.e., $\kappa \propto c v_k^2 \tau_k$, the energy diffusion constant obtained from the equilibrium energy diffusion method follows $D_{\mathrm{E}} \propto v_k^2 \tau_k$. For each D_{E} derived under different strain values, the resonance phonon method enables the investigation of strain-modulated phonon group velocities and phonon relaxation times.[44,45] The resulting data provide deeper insight into the underlying mechanism of the strain effect on phonon transport in 1D FK lattices.

3. Results and discussion

For the symmetric 1D FK lattice, we derive the energy diffusion constants D_{E} under different strain values from the calculated energy correlation function based on the equilibrium diffusion method.[43] The strain-dependent energy diffusion constants D_{E} are plotted in Fig. 1 at temperature $T = 0.4$. The energy diffusion constants D_{E} exhibit an almost symmetric behavior with respect to strain modulation. The variations in phonon transport are nearly identical whether the lattice is compressed or stretched. Interestingly, this symmetric strain effect is similar to that observed in the previously studied 1D symmetric FPU-β lattice without on-site potentials.[17] It is well known that the internal pressure is always zero for symmetric lattice models, both with and without on-site potentials.[16] These results indicate that the influence of pressure on phonon transport is closely related to the symmetry of the lattice potential. In particular, for symmetric lattices, the symmetric dependence of phonon transport on strain may simply result from the symmetric potential adopted in the lattice Hamiltonian of Eq. (1).

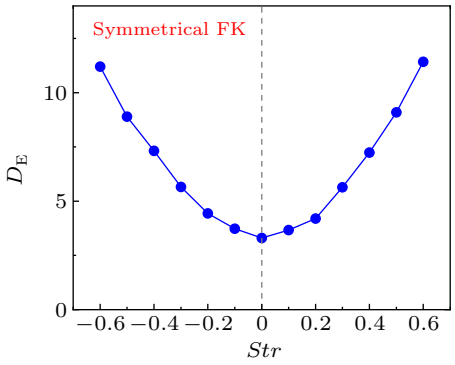


Fig. 1. The energy diffusion constant D_E as a function of Str for the 1D symmetrical FK lattice at temperature $T = 0.4$. The modulation of D_E is nearly symmetrical under positive and negative strains. The minimum D_E occurs at the strain-free condition, as strain always enhances phonon transport, whether under compression ($Str > 0$) or stretching ($Str < 0$).

Previous studies have found that a minor introduction of strain always tends to reduce the thermal conductivity in symmetric lattices.[14,16,17] This effect has been attributed to the strain-induced asymmetry in the lattice potential. However, this behavior is contrary to our findings, where a small strain consistently enhances the energy diffusion constant D_E in symmetric 1D FK lattices, as shown in Fig. 1. Specifically, the value of D_E increases from 3.3 at $Str = 0$ to 11.2 at $Str = \pm 0.6$.

To explain the difference between the symmetric 1D FK and FPU-β lattices, we calculate the renormalized phonon frequencies and phonon dispersion relations using the resonance phonon method.[44] The phonon dispersion relation provides information about the phonon group velocity, while the broadening of the renormalized phonon frequency reflects the phonon relaxation time.

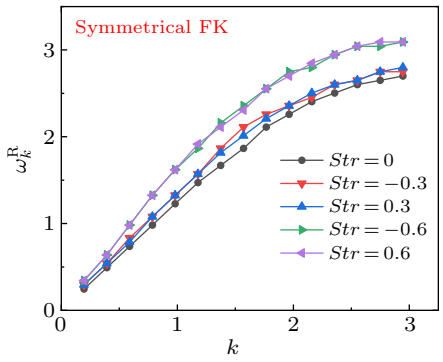


Fig. 2. The renormalized phonon frequency ω_k^R as a function of phonon wave number k (phonon dispersion relation) for the 1D symmetrical FK lattice under different strain values at temperature $T = 0.4$ and lattice length $N = 32$. The phonon group velocities, defined as $v_k = \mathrm{d}\omega_k^R/\mathrm{d}k$, are related to the slopes of the phonon dispersion relation. Nonzero strains always increase the phonon group velocities in the small wave number k region, which contributes most significantly to phonon transport.

In Fig. 2, the phonon dispersion relation ω_k^R is plotted for the symmetric 1D FK lattice at temperature $T = 0.4$ with a lattice size of $N = 32$. Since the phonon group velocity v_k is defined as the derivative of the phonon frequency, $\mathrm{d}\omega_k^R/\mathrm{d}k$, the slope of the dispersion curve ω_k^R directly represents v_k. Phonons with relatively small wave numbers k and large group velocities v_k contribute most to energy transport. As shown in the figure, strain — whether compressive or tensile — consistently enhances the phonon group velocity. For zero strain ($Str = 0$), the maximum phonon group velocity is fitted as $v_k = 1.24$. When the lattice is either compressed or stretched to $Str = \pm 0.6$, the fitted maximum group velocity increases to $v_k = 1.70$. Thus, for symmetric 1D FK lattices, the phonon group velocity is enhanced under both positive and negative strains, an effect similar to that observed in symmetric 1D FPU-β lattices.[17]

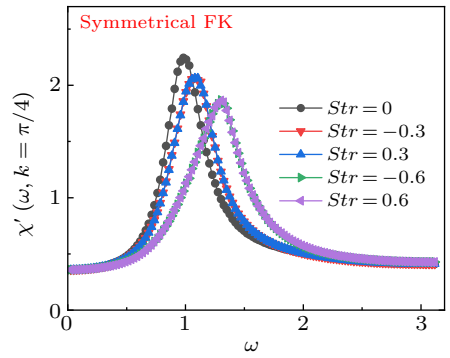


Fig. 3. The real part of the response function $\chi'(\omega, k = \pi/4)$ for the 1D symmetrical FK lattice under different strain values at temperature $T = 0.4$ and lattice length $N = 32$. The broadening of $\chi'(\omega, k)$ arises from phonon-phonon scattering. The curve of $\chi'(\omega, k)$ can be fitted by a Lorentzian peak function with a fitting parameter Γ_k, which represents the width of the curve. The phonon relaxation time τ_k is determined by the inverse of the scattering rate, $\tau_k = \Gamma_k^{-1}$.

In Fig. 3, the real parts of the response function $\chi'(\omega, k)$, calculated from the spatiotemporal correlation function of atomic momentum via the resonance phonon method, are shown. The phonon mode with $k = \pi/4$ is selected for different strain values $Str = 0, \pm 0.3$, and ± 0.6. A symmetric strain-modulation behavior is again observed, as the curves corresponding to the same absolute strain $|Str|$ nearly overlap. The response function $\chi'(\omega, k)$ can be fitted using the Lorentzian peak function

$$\chi'(\omega, k) = \frac{2}{\pi} \frac{\Gamma_k}{4(\omega - \omega_k^R)^2 + \Gamma_k^2}, \tag{3}$$

where the fitting parameter Γ_k represents the phonon scattering rate. The scattering rate Γ_k also determines the linewidth of $\chi'(\omega, k)$, and the phonon relaxation time τ_k is given by $\tau_k = \Gamma_k^{-1}$. With increasing absolute strain $|Str|$, the phonon relaxation time τ_k is consistently suppressed. This behavior is also similar to that observed in the symmetric 1D FPU-β lattice.[17] However, the suppression of τ_k in the FK lattice is much weaker than that in its FPU-β counterpart. For the zero-strain case $Str = 0$, the fitted linewidth is $\Gamma_k = 0.371$, while for $|Str| = 0.6$, it increases to $\Gamma_k = 0.534$. Thus, the suppression of the phonon relaxation time at $|Str| = 0.6$ is only about $0.371/0.534 \approx 0.70$. In contrast, the reduction of τ_k in the FPU-β lattice can be as low as ~ 0.20.[17]

Although strain enhances the phonon group velocity and suppresses the phonon relaxation time in both symmetric 1D FK and FPU-β lattices, their overall effects differ. Because the FK lattice exhibits a stronger enhancement in phonon group velocity and a much weaker suppression in relaxation time, strain ultimately increases its energy diffusion capability. The combined effect from $v_k^2\tau_k$ gives an enhancement factor of about 1.31 for $|Str| = 0.6$. However, the actual increase in the energy diffusion constant $D_{\rm E}$ is approximately $11.2/3.3 \approx 3.4$, suggesting that other underlying mechanisms may also contribute to this enhancement.

In the following, we investigate the strain-modulated energy diffusion in the asymmetric 1D FK lattices. The Hamiltonian in Eq. (2) is employed with the asymmetry parameter $\alpha = 1$. Because of the presence of the on-site potential, the exact value of the internal pressure at the natural length $L = N$ cannot be directly determined. Nevertheless, based on previous studies of the 1D FPU-$\alpha\beta$ lattice, the asymmetric 1D FK lattice with $\alpha = 1$ is also expected to exhibit a negative internal pressure.[17]

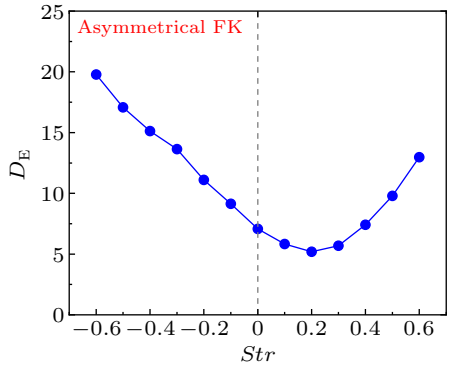


Fig. 4. The energy diffusion constant $D_{\rm E}$ as a function of strain for the 1D asymmetric FK lattice at temperature $T = 0.5$. The modulation of energy diffusion due to strain is asymmetrical. The minimum position of $D_{\rm E}$ occurs in the positive strain region, around $Str = 0.2$.

In Fig. 4, the strain-modulated energy diffusion constants $D_{\rm E}$ are plotted for the asymmetric 1D FK lattice with $\alpha = 1$. A clear asymmetrical dependence between $D_{\rm E}$ and Str is observed. In the positive strain direction, where the lattice is compressed, the energy diffusion constant first decreases and then increases. In contrast, $D_{\rm E}$ increases monotonically in the negative strain direction when the lattice is stretched. The minimum value of $D_{\rm E}$ occurs under positive strain, i.e., when the lattice is compressed. This rightward shift of the minimum may arise from the presence of negative internal pressure, similar to that observed in the asymmetric 1D FPU-$\alpha\beta$ lattice.[17] It is also possible that the total pressure becomes approximately zero at an external strain of $Str = 0.2$ because of the compensating effect of the negative internal pressure.

In Fig. 5, the strain-modulated phonon dispersion relations $\omega_k^{\rm R}$ are plotted for the asymmetric 1D FK lattices at temperature $T = 0.5$ and lattice length $N = 32$. It can be seen that the phonon group velocity at small k values decreases under positive strain ($Str = 0.2$), whereas for negative strain values ($Str = -0.2$, -0.4, and -0.6), the maximum phonon group velocity increases progressively with increasing negative strain. For the strain-free case ($Str = 0$), the largest phonon group velocity can be fitted as $v_k = 1.25$. Under negative strain ($Str = -0.6$), the fitted maximum phonon group velocity reaches approximately $v_k = 1.86$. The enhancement from the v_k^2 term at $Str = -0.6$ is about 2.21 compared with the strain-free condition.

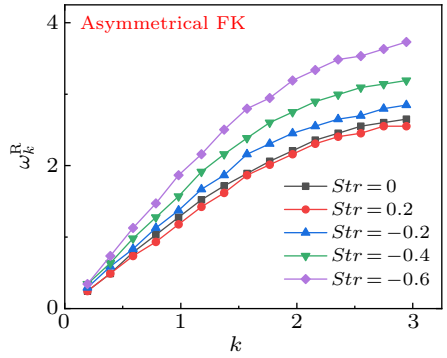


Fig. 5. The renormalized phonon frequency $\omega_k^{\rm R}$ as a function of phonon wave number k for the 1D asymmetric FK lattice under different strain values at temperature $T = 0.5$ and lattice length $N = 32$. For positive strain with $Str = 0.2$, the phonon group velocity is reduced compared to the strain-free case. For negative strain values ($Str < 0$), the phonon group velocity increases as $|Str|$ increases.

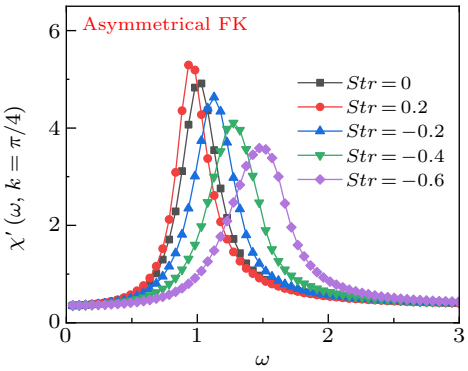


Fig. 6. The real part of the response function $\chi'(\omega, k = \pi/4)$ for the 1D asymmetric FK lattice under different strain values at temperature $T = 0.5$ and lattice length $N = 32$. The phonon scattering rate, or the width of the curve Γ_k, decreases in the positive strain direction up to $Str = 0.2$ and increases in the negative strain direction ($Str < 0$). The phonon relaxation time τ_k is related to Γ_k as $\tau_k = \Gamma_k^{-1}$.

In Fig. 6, the real parts of the response function $\chi'(\omega, k = \pi/4)$ are plotted for the asymmetrical 1D FK lattices under different strain values, $Str = 0$, 0.2, -0.2, -0.4, and -0.6. The curves of $\chi'(\omega, k = \pi/4)$ can be well fitted by Lorentzian peak functions. The width of the peak, corresponding to the phonon scattering rate Γ_k, decreases under positive strain ($Str = 0.2$). In contrast, in the negative strain region ($Str < 0$), Γ_k increases monotonically. The fitted value for the strain-free case is $\Gamma_k = 0.313$, while for $Str = -0.6$, it increases to $\Gamma_k = 0.473$. Consequently, the phonon relaxation time τ_k is suppressed by

a factor of approximately $0.313/0.473 = 0.66$ when the strain changes from $Str = 0$ to $Str = -0.6$.

For the negative strain $Str = -0.6$, the enhancement from the phonon group velocity term v_k^2 is about 2.21, whereas the suppression from the relaxation time term τ_k is about 0.66. Therefore, the combined effect of $v_k^2\tau_k$ yields an overall enhancement of roughly 1.46 compared with the strain-free case. However, the actual enhancement of the energy diffusion constant $D_{\rm E}$ obtained from Fig. 4 is about $19.8/7.1 = 2.8$. This discrepancy between the calculated $D_{\rm E}$ and the estimated $v_k^2\tau_k$ suggests that additional mechanisms may contribute to the enhancement, which merits further investigation in the future.

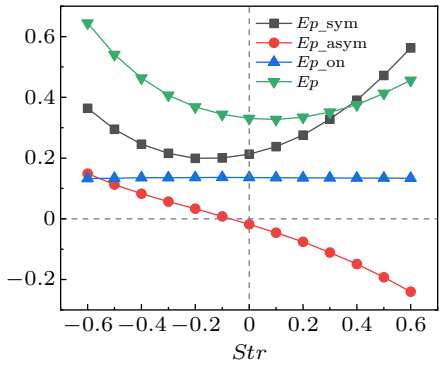


Fig. 7. The average potential energy Ep and its three components, Ep_asym, Ep_sym, and Ep_on, as a function of strain for the 1D asymmetric FK lattice at temperature $T = 0.5$. The strain value corresponding to the minimum average potential Ep is around $Str = 0.1$, which is slightly less than the value of $Str = 0.2$, where the minimum energy diffusion constant $D_{\rm E}$ occurs.

In order to provide further insight into the minimum position of phonon transport under strain in the 1D asymmetric FK lattice, the average potential and its components for each atom may be informative. The total potential energy Ep is defined as the time average of the potential energy

$$Ep = \left\langle \frac{1}{2}(q_i - q_{i-1})^2 + \frac{\alpha}{3}(q_i - q_{i-1})^3 + \frac{1}{4}(q_i - q_{i-1})^4 + \frac{1}{2\pi}(1 - \cos 2\pi q_i) \right\rangle, \quad (4)$$

which is independent of the index i in thermal equilibrium. Its three components, Ep_asym, Ep_sym, and Ep_on, are defined as

$$\begin{aligned} Ep_\text{asym} &= \left\langle \frac{\alpha}{3}(q_i - q_{i-1})^3 \right\rangle, \\ Ep_\text{sym} &= \left\langle \frac{1}{2}(q_i - q_{i-1})^2 + \frac{1}{4}(q_i - q_{i-1})^4 \right\rangle, \\ Ep_\text{on} &= \left\langle \frac{1}{2\pi}(1 - \cos 2\pi q_i) \right\rangle, \end{aligned} \quad (5)$$

representing the average asymmetrical interatomic potential, symmetrical interatomic potential, and on-site potential, respectively. In Fig. 7, the average potential Ep and its components Ep_asym, Ep_sym, and Ep_on are plotted as functions of strain for the 1D asymmetric FK lattice. It can be seen that the minimum position of the average potential Ep shifts toward positive strain. However, the strain corresponding to the minimum Ep is around 0.1, which differs from $Str = 0.2$, where the minimum energy diffusion constant $D_{\rm E}$ occurs.

In the 1D asymmetric FK lattice described by the Hamiltonian in Eq. (2), the parameter α in the third-order interatomic potential represents the asymmetry strength. We can also study the effect of varying α on the strain-modulated phonon transport. In Fig. 8, the energy diffusion constants $D_{\rm E}$ are plotted for the 1D asymmetric FK lattices with four different asymmetry strengths: $\alpha = -1$, 0.5, 1, and 1.5. For $\alpha = -1$ and $\alpha = 1$, the strain-dependent $D_{\rm E}$ exhibits the same odd symmetry, $D_{\rm E}(-\alpha, -Str) = D_{\rm E}(\alpha, Str)$, as observed previously in 1D FPU-$\alpha\beta$ lattices.[17] The minimum positions of $D_{\rm E}$ occur at approximately $Str = 0.1$, 0.2, and 0.4 for $\alpha = 0.5$, 1, and 1.5, respectively. For positive α, it is clear that the minimum position of $D_{\rm E}$ shifts toward positive strain as the asymmetry strength α increases.

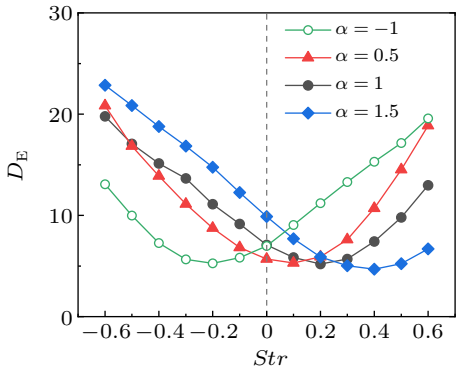


Fig. 8. The energy diffusion constant $D_{\rm E}$ as a function of strain for the 1D asymmetric FK lattice at temperature $T = 0.5$, with four different asymmetry parameters $\alpha = -1$, 0.5, 1, and 1.5. From the curves with $\alpha = -1$ and 1, it can be seen that $D_{\rm E}$ exhibits the same odd symmetry, $D_{\rm E}(-\alpha, -Str) = D_{\rm E}(\alpha, Str)$, as in the previously studied 1D FPU-$\alpha\beta$ lattices.[17] For positive α values of 0.5, 1, and 1.5, the minimum position of $D_{\rm E}$ shifts toward positive strain as the asymmetry strength α increases.

4. Conclusion

In conclusion, we have systematically studied strain-modulated phonon transport using the energy diffusion method for both symmetrical and asymmetrical 1D FK lattices with on-site potentials. For symmetrical 1D FK lattices, the energy diffusion constants exhibit a symmetrical dependence on strain, similar to that observed in previously studied symmetrical 1D FPU-β lattices. However, the energy diffusion constant attains its minimum at the strain-free condition, in contrast to the 1D FPU-β case. Although the phonon group velocity is enhanced and the phonon relaxation time is suppressed by the magnitude of strain, as in the FPU-β lattices, the suppression of the phonon relaxation time is much weaker in the FK lattices studied here. For asymmetrical 1D FK lattices, a similar shift of the extreme values of energy diffusion

constants is observed, analogous to the behavior in asymmetrical 1D FPU-$\alpha\beta$ lattices. Our results indicate that strain-modulated phonon transport is closely related to the symmetry properties of the lattice potentials, regardless of the presence of an on-site potential.

Acknowledgments

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