The effective length of the atomic or molecular SPL increases by random intersections with other SPLs in the rough surface or edge layer.

The proposed phonon scattering mechanism gives finite and frequency-independent mean free path \( l_{ph} \) of the propagating along Q1DPW longitudinal acoustic phonons in a wide frequency range, including low frequencies [18]. The value of phonon mean free path due to the dynamical-roughness-induced momentum-nonconserving scattering is given by the lattice spacing in the Q1DPW \( a \) and coupling parameter between a SPL and Q1DPW \( g \): \( l_{ph} = a/g \). Coupling parameter \( g \) is determined by the ratio of the cross-section area of the rough layer \((\sim \pi D \delta)\) with the average root-mean-square roughness height \( \delta \) and cross-section area of NW with diameter \( D: g \sim \delta/D \) [18]. For atomically-thick rough surface layer with \( \delta > a \), acoustic phonon mean free path \( l_{ph} \sim D(a/\delta) \) can become shorter than NW diameter [18]. Therefore this channel of surface phonon scattering substantially reduces mean free path of “long longitudinal waves” which give dominant contribution to phonon TC of quasi-1D systems, see Refs. [10, 11, 16]. This in turn causes a substantial reduction of phonon TC in NWs and NRs with dynamically rough surfaces or edges, which explains the significant TC reduction, down to the level of TC of amorphous Si, observed in single-crystalline Si NWs with rough surfaces [3]. The predicted reduction factor \( a/\delta \) is quantitatively consistent with the ob-
served reduction of TC of Si NWs with rough surface layers with controlled thicknesses \( \delta > a \) [3] with respect to TC of Si NWs with the same diameters and smooth surfaces (with \( \delta \sim a \)) [18].

This mechanism of momentum-nonconserving acoustic phonon scattering gives finite and length-independent coefficient of TC of Q1DPWs with atomically rough surfaces or edges with \( \delta > a \), in contrast to the divergent with the system length coefficient of TC of anharmonic Q1DPWs with atomically smooth surfaces or edges with \( \delta \ll a \), when the momentum-nonconserving channel of acoustic phonon scattering is closed and mean free path of long-wave phonons substantially increases, \( l_{ph} \sim \omega^{-2} \), and becomes \( l_{ph} \gg D \). The considered mechanism of acoustic phonon scattering by vibration of atomic or molecular chains in dynamically rough surfaces and edges of NWs and NRs is qualitatively different from usually considered acoustic wave scattering by static (geometric) roughness on stress-free surfaces of solids [5, 14].

**Analytical model of phonon transport in quasi-1D phonon waveguides with side phonon leads.** We consider 1D lattice with period \( a \) of coupled oscillators, with coupling constant \( c \) and mass \( m \), in which each oscillator is weakly coupled to SPL (“lateral” atomic chain with weakly-anharmonic coupling), with (linear) interatomic coupling \( c_i = \zeta_0 c \) and atomic mass \( m_i = \gamma m \ll m \). Distribution of such SPLs along the Q1DPW models its dynamical surface roughness [18].

The most important assumption of this model is that acoustic phonon, propagating along the Q1DPW, excites acoustic waves in SPLs which propagate along the leads only outwards the Q1DPW and do not return back to the waveguide in the form of coherent waves. With this assumption, we obtain dispersion equation for the dimensionless complex wave number \( k_{\parallel} a \) of the damped acoustic phonons, propagating along the Q1DPW [18]:

\[
k_{\parallel} a^2 = \omega^2 \frac{m}{c} + i \omega g \sqrt{\frac{m}{c}}.
\] (1)

This equation predicts that phonons with frequencies \( \omega \gg \omega^* \equiv g \sqrt{c/\gamma m} \) propagate quasi-ballistically, when

\[
k_{\parallel} a = \omega \sqrt{\frac{m}{c}} + i \frac{g}{2},
\] (2)

while low-frequency phonons, with \( \omega \ll \omega^* \), propagate diffusively, when \( \omega = -i D_{ph} k_{\parallel}^2 \), with the diffusion coefficient \( D_{ph} = a^2 \sqrt{c/m}/g = V_{ph} l_{ph} \), where \( V_{ph} = a \sqrt{c/m} \) and \( l_{ph} = a/g \) are velocity and energy mean free path of long-wave acoustic phonons, cf. Eq. (2). Both quasi-ballistic and diffusive acoustic phonons contribute to phonon TC coefficient \( \kappa_{ph} \) of Q1DPW as \( \kappa_{ph} \sim C_{ph} D_{ph} \sim C_{ph} V_{ph} a/g \), where \( C_{ph} \) is the contribution of longitudinal phonons to the specific heat of NW or NR. This predicts, in agreement with the observations [3, 4] and our MD simulations, the significant reduction of phonon mean free path and TC caused by phonon scattering by dynamical surface roughness in NWs and NRs (with \( \gamma \sim \delta/D \) and \( \delta \gg a \)).

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**Figure 1:** (a) Model of 2D atomic ribbon with rough edges which consists of \( M = 12 \) chains with ideal core of \( M_0 = 4 \) chains and two rough edges of \( M_1 = 4 \) chains with \( p = 0.3 \) randomly deleted atoms. (b) Model of 3D nanowire with rough surface layers of 2 atom thickness. (c) Ideal 3D core.

**MD simulations of TC of 2D nanoribbons.** We consider the atomic structure consisting of \( M \) parallel chains of atoms placed in one plane. We consider the Hamiltonian of the scalar model of the ribbon lattice in which only the longitudinal displacements of atoms are taken into account and displacement of the \( (m, n) \)th atom from its equilibrium position. The Hamiltonian, which accounts for interaction between only the nearest-neighbor atoms (with unit mass):

\[
H = \sum_{m=1}^{M} \sum_{n=1}^{N} \frac{1}{2} \hat{u}_{mn}^2 + \sum_{m=1}^{M} \sum_{n=1}^{N-1} V_{mn}(u_{m,n+1} - u_{m,n})
\]

\[
+ \sum_{m=1}^{M-1} \sum_{n=1}^{N} U_{mn}(u_{m+1,n} - u_{m,n}),
\] (3)

where \( N \) is number of atoms in each chain, \( V_{mn} \) and \( U_{mn} \) are potentials of the intra- and interchain interaction between \( (m, n) \) and \( (m, n + 1) \) atoms, and between \( (m, n) \) and \( (m + 1, n) \) atoms, respectively. For the purpose of calculating the heat flux along the NR, we can define the corresponding total energy of the \( n \)th cross-section \( e_n \) and local energy flux \( j_n \) in the ribbon, which satisfy the continuity condition \( \dot{e}_n = j_{n-1} - j_n \), see, e.g., Ref. [19].

We consider a NR built of \( M = M_0 + 2M_1 \) chains. To model two dynamically rough edges with widths \( M_1 \), we randomly delete some atoms in the chains \( m = 1, ..., M_1 \) and \( m = M_1 + M_0 + 1, ..., M_1 + M_0 + M_1 \). Let \( 0 \leq p \leq 1 \) be the probability of atom removal. In result of the random atom removal from the edge layers, some atoms in the edges will become completely isolated and should be deleted as well. Model NR with two rough edges with \( p = 0.3 \) randomly deleted atoms is shown in Fig. 1(a).

Assuming for the certainty that \( U(\rho) = \frac{1}{2} V(\rho) \), where \( V(\rho) \equiv V_{mn}(\rho) \) and \( U(\rho) \equiv U_{mn}(\rho) \), we consider \( V(\rho) = \rho^2/2, V(\rho) = \rho^2/2 + \rho^4/4, V(\rho) = \exp(-\rho) + \rho - 1, \), \( V(\rho) = (\exp(-\rho) - 1)^2/2 \) and \( V(\rho) = 1 - \cos(\rho) \) as, respectively, the harmonic, Fermi-Past-Ulam (FPU), Toda, Morse
and rotational potentials. It is worth mentioning that the ribbons with the harmonic, FPU, Toda or Morse interatomic potentials and ideal atomically smooth edges have infinite coefficients of TC in the limit of \( N \to \infty \). In purely harmonic systems, acoustic phonons do not interact and there is no energy scattering in phonon thermal transport. Infinite TC coefficients in ribbons with the anharmonic FPU, Toda or Morse interatomic potentials are related with the quasi-ballistic transport of the long-wave acoustic phonons with long mean free paths \( l_{ph} \propto \omega^{-2} \). Ideal ribbons with the rotational potential have finite TC in the limit of \( N \to \infty \) and finite temperatures [20, 21].

The ribbon TC is found in two independent ways. The first method relies on direct modeling of heat transport along the ribbon. For this purpose, we consider a ribbon with total length \( N + 2N_0 \) \((N_0 = 40\) is the length of ribbon ends), which ends are placed in Langevin thermostats with different temperatures of the left, \( T_+ = 1.1T \), and right, \( T_- = 0.9T \), ends, where \( T \) is average temperature). In the middle part of the ribbon with length \( N \) the stationary heat flux \( J_n = J \) and linear temperature gradient of ribbon temperature \( T_n \) are established (where \( J_n \) is determined by the time-average of the local heat flux \( \langle j_n \rangle \) in the stationary conditions). Thus the TC coefficient \( \kappa(N) \) of the finite-length ribbon can be reliably determined as

\[
\kappa(N) = \frac{J(N-1)}{(T_{N_0+1} - T_{N_0+N})(M_0 + 2M_1q)},
\]

where \( M_0 \) is the width of central ideal strip, \( 2M_1q \) is total width of rough edges with filling fraction \( q = 1 - p < 1 \). TC coefficient \( \kappa \) is determined from \( \kappa(N) \) as the limit of \( N \to \infty \). The ribbon temperature profile \( T_n \) depends on a particular realization of the edge roughness and therefore it is necessary to perform averaging over its independent realizations. In our simulations, we averaged over 120 independent realizations of the edge roughness.

We modeled heat transport in rough-edge NRs with central part length of \( N = 20, 40, 80, 160, 320, 640 \). Dependence of TC coefficients on the length of NR with rough edges, with \( p = 0.3 \) randomly deleted atoms, is shown in Fig. 2(a) for different interatomic potentials. As one can see in this figure, the rough-edge ribbon has finite coefficient of TC in the limit of infinite length for all the considered nonlinear interatomic potentials. In contrast to that, TC coefficient \( \kappa(N) \) of the rough-edge ribbon with purely harmonic lattice continuously decreases for \( N \to \infty \), see Fig. 2(b), and the limiting value of TC coefficient of such NR is zero, \( \kappa(\infty) = 0 \). Figure 2(b) also shows that for the given width of the ideal ribbon core \( M_0 \), TC coefficient of the NR decreases with the increase of the rough edges width \( M_1 \). Therefore the infinite-length ribbon core \( M_0 \) with purely harmonic lattice and dynamically rough edges can be considered as an ideal thermal insulator.

We relate the reason for such strong difference between TC coefficients of rough-edge NRs with harmonic and anharmonic interatomic potentials with the properties of SPLs in corresponding systems. In the anharmonic systems, long acoustic waves, excited in SPLs, do not return back and the effective “internal radiative losses” result in finite phonon mean free path and phonon TC in the Q1DPW, see Eqs. (1) and (2). In purely harmonic systems, the long acoustic waves, excited in SPLs, return back into the Q1DPW and strongly suppress the transmission of low-frequency acoustic phonons through the Q1DPW because of destructive interference with the phonons propagating along the waveguide core (the phonon Fano resonance, see Ref. [18] for a brief review). This produces the effective stop band (or Anderson-Fano localization) for low-frequency acoustic phonons in the Q1DPW with harmonic lattice and dynamically rough edges [18], and, correspondingly, the decrease of TC coefficient of the NR in the limit of \( N \to \infty \). Indeed, we observe only the localized vibration eigenstates in harmonic phonon spectrum of such system (not shown).

In the approach based on Green-Kubo method, TC is de-

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In the approach based on Green-Kubo method, TC is de-

![Figure 2: (a) Dependence of TC coefficient \( \kappa \) on length \( N \) of 2D ribbons with smooth and rough edges for the Toda (curves 1 and 4, temperature \( T = 1 \)), Morse (curves 2 and 5, temperature \( T = 0.1 \)) and FPU (curves 3 and 6, \( T = 10 \)) interatomic potentials. (b) Dependence of TC coefficient \( \kappa \) on length \( N \) of 2D ribbons with purely harmonic lattices and rough edge widths \( M_1 = 1 \) and \( M_1 = 4 \) (curves 7 and 8) with \( p = 0.3 \) randomly deleted atoms. Ideal core width is \( M_0 = 2 \), temperature \( T = 1 \).](image)
fined as integral of the autocorrelation of heat fluxes:

$$\kappa(N) = \lim_{t \to \infty} \frac{1}{NT^2(M_0 + 2M_1q)} \int_0^t \langle J(\tau)J(\tau-t) \rangle d\tau,$$  \hspace{1cm} (5)

where $J(t) = \sum_n j_n(t)$ is the average heat flux in the NR. Values of $\kappa(N)$ obtained with the use of two different approaches, Eqs. (4) and (5), coincide with good accuracy.

We also perform MD simulations of the temperature dependence of TC of rough-edge NRs with the FPU, Toda and rotational interatomic potentials (not shown). All the obtained dependencies confirm the finite coefficients of TC of the NRs in the low temperature limit $T \to 0$ when the coefficients of classical TC of corresponding NRs with atomically smooth edges diverge.

**MD simulations of TC of 3D nanowires.** We consider 3D model system made of $M \times K$ parallel molecular chains as it is shown in Figs. 1(b) and 1(c). The Hamiltonian of the system we take as a 3D generalization of the Hamiltonian (3) of 2D ribbon scalar model. In Fig. 3 we show the length dependence of nanowire TC coefficient for the Toda and harmonic interatomic potentials. It demonstrates that similar to the case of 2D nanoribbon, the dynamical roughness of the surface layer changes the increasing (divergent) with the length TC of 3D nanowire to the finite or decreasing with the nanowire length of nanowire with, respectively, the anharmonic or harmonic interatomic potential.

In summary, we present analytical model and molecular dynamics simulations of phonon heat transport in nanowires and nanoribbons with anharmonic lattices and dynamically rough surfaces and edges. In agreement with recent experiments on heat transport in single-crystalline silicon nanowires with rough surfaces, our model and simulations predict finite and length-independent phonon thermal conductivity in such quasi-one-dimensional systems, in contrast to anomalous phonon thermal conductivity of corresponding momentum-conserving systems with atomically smooth surfaces, divergent with the system length. We also present the thermal-insulator-like heat transport in long-length nanowires and nanoribbons with purely harmonic lattices and dynamically rough surfaces, caused by the Anderson-Fano phonon localization.

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