

WITHDRAWN: Effects of different factors on the heat conduction properties of two-dimensional carbon-based nanostructured materials

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Abstract

Non-equilibrium molecular dynamics simulations were carried out to study the properties of nanoscale thermal transport in graphene. The effects of crystal length and edge states on the thermal conductivity of graphene were investigated. The thermal conductivity of carbon-based nanostructured materials was determined to understand the characteristics of thermal transport in the nanostructured materials. The objective is to gain insight into the fundamental characteristics of thermal transport in graphene. Particular emphasis is placed on the dependence of crystal length and edge states on the thermal conductivity of graphene, with an attempt to improve the heat conduction properties for carbon-based nanostructured materials. The results indicated that phonons are derived from the crystal lattice. The crystal length is the primary factor affecting the thermal conductivity of graphene. The edge termination state has little effect on the thermal conductivity, since there is little difference in thermal conductivity between two-dimensional zigzag-edged and armchair-edged crystals. The difference in thermal conductivity is insignificant between zigzag-edged and armchair-edged crystals. However, the thermal conductivity of the two-dimensional crystal depends strongly upon the crystal length. There is a significant effect of crystal length on the thermal conductivity. Phonon-boundary scattering instead of phonon-phonon Umklapp scattering is the dominant scattering mechanism. Excess small crystals can block phonons, causing a decrease in the thermal conductivity.

1. Introduction

Graphene is a two-dimensional form of crystalline carbon, either a single layer of carbon atoms forming a hexagonal lattice or several coupled layers of this honeycomb structure [1, 2]. The word graphene, when used without specifying the form, for example, bilayer graphene and multilayer graphene, usually refers to single-layer graphene. Graphene is a parent form of all graphitic structures of carbon [3, 4]: graphite, which is a three-dimensional crystal consisting of relatively weakly coupled graphene layers; carbon nanotubes, which may be represented as scrolls of graphene; and buckyballs, spherical molecules made from graphene with some hexagonal rings replaced by pentagonal rings.

The theoretical study of graphene was started in 1947 by physicist Philip Russell Wallace as a first step to understanding the electronic structure of graphite [5]. The term graphene was introduced by chemists Hanns-Peter Boehm, Ralph Setton, and Eberhard Stumpp in 1985 as a combination of the word graphite, referring to carbon in its ordered crystalline form, and the suffix, referring to polycyclic aromatic hydrocarbons in which the carbon atoms form hexagonal, or six-sided, ring structures [6]. In 2004 University of Manchester physicists Konstantin Novoselov and Andre Geim and colleagues isolated single-layer graphene using an extremely simple method of exfoliation from graphite [7]. Their scotch-tape method used adhesive tape to remove the top layers from a sample of graphite and then apply the layers to a substrate material. When the tape was removed, some graphene remained on the substrate in single-layer form. In fact, derivation of graphene is not a difficult task by itself; each time someone draws with a pencil on paper, the pencil trace contains a small fraction of single-layer and multilayer graphene. The achievement of the Manchester group was not only to isolate graphene flakes but also to study their

physical properties. In particular, they demonstrated that electrons in graphene have a very high mobility, which means that graphene could possibly be used in electronic applications. In 2010 Geim and Novoselov were awarded the Nobel Prize for Physics for their work [8]. In these first experiments, the substrate for graphene was silicon naturally covered by a thin transparent layer of silicon dioxide. It turned out that single-layer graphene created an optical contrast with the silicon dioxide that was strong enough to make the graphene visible under a standard optical microscope. This visibility has two causes. First, electrons in graphene interact very strongly with photons in the visible light frequencies, absorbing about 2.3 percent of the light's intensity per atomic layer. Second, the optical contrast is strongly enhanced by interference phenomena in the silicon dioxide layer; these are the same phenomena that create rainbow colors in thin films such as soap film or oil on water.

The basic electronic structure of graphene and, as a consequence, its electric properties are very peculiar [9, 10]. By applying a gate voltage or using chemical doping by adsorbed atoms and molecules, one can create either electron or hole, a region where an electron is missing that acts as a positive electric charge, conductivity in graphene that is similar to the conductivity created in semiconductors [9, 10]. However, in most semiconductors there are certain energy levels where electrons and holes do not have allowed quantum states, and, because electrons and holes cannot occupy these levels, for certain gate voltages and types of chemical doping, the semiconductor acts as an insulator. Graphene, on the other hand, does not have an insulator state, and conductivity remains finite at any doping, including zero doping [11, 12]. Existence of this minimal conductivity for the undoped case is a striking difference between graphene and conventional semiconductors [11, 12]. Electron and hole states in graphene relevant for charge-carrier transport are similar to the states of ultra-relativistic quantum particles, that is, quantum particles moving at the speed of light, the ultimate velocity in nature, according to the theory of relativity.

The honeycomb lattice of graphene actually consists of two sublattices, designated A and B, such that each atom in sublattice A is surrounded by three atoms of sublattice B and vice versa [13]. This simple geometrical arrangement leads to the appearance that the electrons and holes in graphene have an unusual degree of internal freedom, usually called pseudospin [14]. In fact, making the analogy more complete, pseudospin mimics the spin, or internal angular momentum, of subatomic particles [15, 16]. Within this analogy, electrons and holes in graphene play the same role as particles and antiparticles, for example, electrons and positrons, in quantum electrodynamics [15, 16]. At the same time, however, the velocity of the electrons and holes is only about one three-hundredth the speed of light. This makes graphene a test bed for high-energy physics: some quantum relativistic effects that are hardly reachable in experiments with subatomic particles using particle accelerators have clear analogs in the physics of electrons and holes in graphene, which can be measured and studied more easily because of their lower velocity [17]. An example is the Klein paradox, in which ultra-relativistic quantum particles, contrary to intuition, penetrate easily through very high and broad energy barriers [18]. Therefore, graphene provides a bridge between materials science and some areas of fundamental physics, such as relativistic quantum mechanics.

There is another reason why graphene is of special interest to fundamental science: it is the first and simplest example of a two-dimensional crystal, that is, a solid material that contains just a single layer of atoms arranged in an ordered pattern [19]. Two-dimensional systems are of huge interest not only for physics and chemistry but also for other natural sciences [20]. In many respects, two-dimensional systems are fundamentally different from three-dimensional systems [21]. In particular, due to very strong thermal fluctuations of atomic positions that remain correlated at large distances, long-range crystalline order cannot exist in two dimensions [22]. Instead, only short-range order exists, and it does so only on some finite scale of characteristic length, a caveat that should be noted when graphene is called a two-dimensional crystal [23]. For this reason, two-dimensional systems are inherently flexural, manifesting strong bending fluctuations, so that they cannot be flat and are always rippled or corrugated [24]. Graphene, because of its relative simplicity, can be considered as a model system for studying two-dimensional physics and chemistry in general [25, 26]. Other two-dimensional crystals besides graphene can be derived by exfoliation from other multilayer crystals, for example, hexagonal boron nitride, molybdenum disulfide, or tungsten disulfide, or by chemical modification of graphene, for example, graphane, hydrogenated graphene, or fluorinated graphene.

Modern electronics, for example, integrated circuits in computer chips, are basically two-dimensional in that they use mainly the surface of semiconducting materials. Therefore, graphene and other two-dimensional materials are considered very promising for many such applications [27, 28]. Using graphene, for example, it should be possible to make transistors and other electronic devices that are much thinner than devices made of traditional materials. Many other applications have been proposed. For example, graphene, being electrically conducting, transparent, strong, and flexible, may be a prospective material for use in touch screens [29]. Graphene also has very high thermal conductivity [30] and, therefore, could be used to remove heat from electronic circuits.

The field of graphene science and technology is relatively new, having emerged since Geim and Novoselov's work in 2004 [7, 8]. In the decades that followed, it remained difficult to determine which applications would prove to be the most popular [31]. Progress depends not only on the basic science but also on the development of new ways to produce graphene on an industrial scale. Obtaining graphene by exfoliation is too expensive for mass production [32]. Methods proposed include the formation of graphene layers by burning silicon carbide or by chemical vapor deposition of carbon on the surface of some metals such as copper or nickel [33, 34]. These methods would allow the production of samples of graphene that were macroscopically large in two dimensions, up to tens of centimeters, but still atomically thin [35, 36]. While graphene exhibits extremely high thermal conductivity, the effects of crystal length and edge states on the heat conduction properties of the two-dimensional crystal are poorly understood.

This study relates to the heat conduction properties of graphene. The effects of crystal length and edge states on the heat conduction properties of graphene were investigated by using the nonequilibrium molecular dynamics method. Computational simulations were performed using molecular dynamics to investigate the heat transport properties of graphene. The intrinsic thermal conductivity of graphene was

determined to understand the characteristics of thermal transport in the nanostructured materials. The mechanism of phonon transport in graphene was discussed. The physical factors limiting heat conduction in graphene with atomically-disordered edges were provided. The objective is to gain insight into the fundamental characteristics of thermal transport in graphene. Particular emphasis is placed on the dependence of crystal length and edge states on the thermal conductivity of graphene, with an attempt to improve the heat conduction properties for carbon-based nanostructured materials.

2. Numerical Methods

The heat transport characteristics of graphene ribbons are investigated using molecular dynamics. The two-dimensional crystal modeled in this study with substantially smooth edges is depicted schematically in Fig. 1. The design of the molecular-dynamics simulation should account for the available computational power. The number of particles, simulation size, timestep, and total time duration must be selected so that the computation can finish within a reasonable time period. The length of the two-dimensional crystal is typically significantly greater than its width, but of course, there are exceptions. Unless otherwise stated, the two-dimensional crystal is 5.4 nm in width, 0.335 nm in thickness, and 70 nm in length. Molecular dynamics is a computer simulation method for analyzing the physical movements of atoms and molecules. The atoms and molecules are allowed to interact for a fixed period of time, giving a view of the dynamic "evolution" of the system. The trajectories of atoms and molecules are determined by numerically solving Newton's equations of motion for the system of interacting particles, where forces between the particles and their potential energies are computed using interatomic potentials. In physics, molecular dynamics is used to examine the dynamics of atomic-level phenomena that cannot be observed directly, such as thin-film growth and ion-sub-plantation, and also to examine the physical properties of nanotechnological devices that have not or cannot yet be created. Limits of the method are related to the parameter sets used, and to the underlying molecular mechanics force fields. The environment-dependence of van der Waals forces is ignorable in standard simulations, but can be included by developing polarizable force fields.

A specific heat flux imposed through the two-dimensional crystal with substantially smooth edges is depicted schematically in Fig. 2. The two-dimensional crystal is monolayer and therefore can be considered as a single layer of carbon atoms with each atom bound to three neighbors in a honeycomb structure. The substantially flat monolayer of carbon atoms is usually referred to as the basal plane of the two-dimensional crystal. The two-dimensional crystal includes an edge irregularity, such as a zig-zag configuration edge or an armchair-configuration edge. The transverse edges at both ends of the two-dimensional crystal are rough. The longitudinal edges at both sides of the two-dimensional crystal are also substantially smooth. Because the molecular system consists of a vast number of particles, it is impossible to determine the properties of such a complex system analytically. Molecular dynamics simulation circumvents this problem by using numerical methods. However, long molecular dynamics simulations generate cumulative errors in numerical integration that can be minimized with proper selection of algorithms and parameters, but not eliminated entirely. Ab initio quantum mechanical and chemical methods are used to compute the potential energy of a system on the fly, as needed for

conformations in a trajectory. This computation is usually made in the close neighborhood of the reaction coordinate. Although various approximations are used, these are based on theoretical considerations, not on empirical fitting. Ab initio computations produce a vast amount of information that is not available from empirical methods, such as density of electronic states or other electronic properties. A significant advantage of using ab initio methods is the ability to study reactions that involve breaking or formation of covalent bonds, which correspond to multiple electronic states. Moreover, ab initio methods also allow recovering effects beyond the Born-Oppenheimer approximation using approaches like mixed quantum-classical dynamics. A temperature-related phenomenon arises due to the small number of atoms that are used in molecular dynamics simulations. But temperature is a statistical quantity. If there is a large enough number of atoms, statistical temperature can be estimated from the instantaneous temperature.

The structure of the two-dimensional crystal is divided into specific regions by defining hot and cold slabs. Heat is continually being transferred from the hot slab to the cold slabs so as to equalize the temperature within the two-dimensional crystal. The temperature gradient can be determined in the direction of heat flow, since the total energy is conserved in the heat conduction process. Accordingly, the thermal conductivity can be determined from the temperature gradient obtained and the heat flux imposed. The basic rate equation of the heat conduction process within the two-dimensional crystal, known as Fourier's law of heat conduction. The law of heat conduction, also known as Fourier's law, states that the rate of heat transfer through a material is proportional to the negative gradient in the temperature and to the area, at right angles to that gradient, through which the heat flows. The local heat flux density is equal to the product of thermal conductivity and the negative local temperature gradient. The heat flux density is the amount of energy that flows through a unit area per unit time. The ratio of heat flux to the slope of the temperature profile is proportional to the thermal conductivity of the two-dimensional crystal.

Atomistic simulations are performed using a classical molecular dynamic code LAMMPS [37]. Since the system doesn't satisfy equilibrium conditions, reverse non-equilibrium molecular dynamics are used. The Müller-Plathe algorithm [38] is used to exchange kinetic energy between two atoms in different regions of the two-dimensional crystal. This induces a temperature gradient in the system, thereby enabling the thermal conductivity of the two-dimensional crystal to be computed. The atomistic interactions in the two-dimensional crystal are treated with the AIREBO potential in its second-generation form [39]. This potential function can be used to describe the intermolecular interactions in condensed-phase hydrocarbon systems [40]. In the microcanonical ensemble, the system is isolated from changes in moles, volume, and energy. It corresponds to an adiabatic process with no heat exchange. A microcanonical molecular dynamics trajectory can be considered as an exchange of potential and kinetic energy, with total energy being conserved. The potential energy function of the system is a function of the particle coordinates. It is referred to simply as the potential in physics, or the force field in chemistry. For every time step, each particle's position and velocity may be integrated with a symplectic integrator method such as Verlet integration. The time evolution of each particle's position and velocity is called a trajectory. Given the initial positions and velocities, all future positions and velocities can be determined.

The simulations should be long enough to be relevant to the time scales of the natural processes being studied. To make statistically valid conclusions from the simulations, the time span simulated should match the kinetics of the natural process. Molecular dynamics simulations are carried out in a microcanonical ensemble on the relaxed structure, with the velocity-Verlet integrator and a time step of 0.5 fs. After the system reaches a steady state finally, it will continue to carry out molecular dynamics simulations up to 2 ns to ensure reliable statistics for the heat transfer process. Parallel algorithms allow the load to be distributed among central processing units. The spatial and force decomposition algorithms are used. During the molecular-dynamics simulations, the most central processing unit intensive task is the evaluation of the potential as a function of the particles' internal coordinates. Within that energy evaluation, the most expensive one is the non-bonded or non-covalent part. All pair-wise electrostatic and van der Waals interactions must be accounted for explicitly. This computational cost is reduced by employing electrostatics methods. Another factor that impacts total central processing unit time needed by a simulation is the size of the integration timestep. This is the time length between evaluations of the potential. This is the time length between evaluations of the potential. The timestep must be chosen small enough to avoid discretization errors, namely smaller than the period related to fastest vibrational frequency in the system.

3. Results And Discussion

Steady-state temperature profiles obtained for the two-dimensional crystal with substantially smooth edges are presented in Fig. 3. The two-dimensional crystal has transverse edges that have an armchair configuration. The longitudinal edges of the two-dimensional crystal have a perfect zigzag configuration. The length of the two-dimensional crystal is assumed to be 70 nm. Thermal conduction is defined as the transport of energy due to random molecular motion across a temperature gradient. It is distinguished from energy transport by convection and molecular work in that it does not involve macroscopic flows or work-performing internal stresses. Energy flow due to thermal conduction is classified as heat. According to the second law of thermodynamics, heat flows from high to low temperature. Hence, it is reasonable to postulate that energy flow due to thermal conduction is proportional to the gradient of the temperature field. The constant of proportionality is the thermal conductivity. This is called Fourier's law of heat conduction. Despite its name, it is not a law but a definition of thermal conductivity in terms of the independent physical quantities, namely the energy flow vector and the temperature field. As such, its usefulness depends on the ability to determine the thermal conductivity for a given material under given conditions. The constant thermal conductivity itself usually depends on the temperature field and thereby implicitly on space and time. An explicit space and time dependence could also occur if the material is inhomogeneous or changing with time. The temperature has a nonlinear dependence on the distance from the given reference point in the direction of heat flow. More specifically, in the vicinity of the hot and cold regions, there exists a nonlinear dependence of the temperature with respect to the distance. This nonlinear dependence is caused by the finite-size effect arising from the two-dimensional crystal, given the fact that the characteristic length scale of the two-dimensional crystal is much smaller than the mean free path of phonons in graphene. In the regions between the hot slab and the cold slabs, the temperature

has a more or less linear dependence on the distance, and therefore the thermal conductivity of the two-dimensional crystal can be determined by the temperature gradient. In graphene, thermal conduction is anisotropic, namely the heat flux is not always parallel to the temperature gradient [41, 42]. Graphene exhibits different thermal conductivities along different crystal axes. Graphene is a notable example of variable thermal conductivity based on orientation and temperature. To account for such behavior, a tensorial form of Fourier's law must be used. An implicit assumption in the description of the thermal conductivity tensor is the presence of local thermodynamic equilibrium, which allows one to define a temperature field. When anisotropy is present, the direction of heat flow may differ from the direction of the thermal gradient.

In engineering practice, it is common to work in terms of quantities which are derivative to thermal conductivity and implicitly take into account design-specific features, for example, component dimensions [43, 44]. The thermal properties of the two-dimensional crystal with different lengths are investigated to determine the structure factors limiting the heat transfer process. The thermal conductivity of the two-dimensional crystal can conveniently be determined by the temperature gradient in the direction of heat flow. The effect of crystal length on the thermal conductivity of the two-dimensional crystal with different transverse edge states is illustrated in Fig. 4, in which the results obtained for both zigzag edges and armchair edges are presented. The transverse edges of the two-dimensional crystal are substantially smooth. The thermal conductivity of the two-dimensional crystal does not change significantly as the transverse edge state is varied from zigzag edges to armchair edges. The edge termination state has little effect on the thermal conductivity, since there is little difference in thermal conductivity between two-dimensional zigzag-edged and armchair-edged crystals. However, the thermal conductivity of the two-dimensional crystal depends strongly upon the crystal length. More specifically, the thermal conductivity of the two-dimensional crystal increases with increasing crystal length due to the reduced probability of phonon scattering from grain boundaries. Phonons can scatter through several mechanisms as they travel through the material. These scattering mechanisms are: Umklapp phonon-phonon scattering, phonon-impurity scattering, phonon-electron scattering, and phonon-boundary scattering. Each scattering mechanism can be characterized by a relaxation rate, which is the inverse of the corresponding relaxation time. All scattering processes can be taken into account using Matthiessen's rule. Thermal transport in graphene is usually considered to be governed by the three-phonon scattering process, and the role of four-phonon and higher-order scattering processes is believed to be negligible. Therefore, the larger the carrier density, heat capacity and speed, and the less significant the scattering, the higher is the thermal conductivity. This is because the mean free path of phonons in graphene is very large compared to the dimensions of the two-dimensional crystal. As a result, the length of the two-dimensional crystal is vital in determining the thermal conductivity. Consequently, the length of the two-dimensional crystal is an important factor affecting the thermal properties, and must be taken into account so as to provide more accurate predictions about the thermal conductivity.

The effect of crystal length on the thermal conductivity of the two-dimensional crystal with zigzag edges is illustrated in Fig. 5. Gases generally have low thermal conductivity, and pure metals have high thermal conductivity. The two-dimensional crystal has extremely high thermal conductivity. The thermal

conductivity of the two-dimensional crystal with zigzag edges spans at least one order of magnitude. The thermal conductivity of the two-dimensional crystal with zigzag edges at room temperature is several times higher than that of a highly conductive metal. Heat transfer occurs at a lower rate in materials of low thermal conductivity than in materials of high thermal conductivity. On a microscopic scale, heat conduction occurs as hot, rapidly moving or vibrating atoms and molecules interact with neighboring atoms and molecules, transferring some of their energy to these neighboring particles. In other words, heat is transferred by conduction when adjacent atoms vibrate against one another. Conduction is the most significant means of heat transfer within the two-dimensional crystal. Phonon, quantized lattice vibration wave, is a central thermal energy carrier contributing to heat capacity and conductive heat transfer in condensed phase, and plays a very important role in thermal energy conversion. The transport properties of phonons are represented by the phonon conductivity tensor for bulk materials and the phonon boundary resistance for solid interfaces. The phonon specific heat capacity includes the quantum effect. Heat transfer physics describes and predicts the phonon specific heat capacity, phonon conductivity tensor, and phonon boundary resistance, based on atomic-level properties [45, 46]. Optical phonons have higher frequencies, but make smaller contribution to conduction heat transfer, because of their smaller group velocity and occupancy. When the two-dimensional crystal is 20 nm in length, the thermal conductivity at room temperature is comparable to that of a highly conductive metal. The thermal conductivity at room temperature increases with increasing the length of the two-dimensional crystal. Phonons are the remarkably particle-like vibrational modes of a crystal. Their behavior, and the way in which they are modeled, bears a startling similarity to that of particles as described by quantum field theory. The relation of quantum particles to the underlying quantum fields is often taken to be a paradigm case of emergence, claims that phonons are emergent therefore carry considerable weight.

The effect of crystal length on the thermal conductivity of the two-dimensional crystal with armchair edges is illustrated in Fig. 6. The thermal conductivity of the two-dimensional crystal with armchair edges spans at least one order of magnitude. The thermal conductivity of the two-dimensional crystal with armchair edges at room temperature is several times higher than that of a highly conductive metal. There is a significant effect of crystal length on the thermal conductivity. This indicates that phonon-boundary scattering instead of phonon-phonon Umklapp scattering should be the dominant scattering mechanism. Excess small crystals can block phonons, causing a decrease in the thermal conductivity. In crystalline materials, Umklapp scattering is a scattering process that results in a wave vector which falls outside the first Brillouin region. If a material is periodic, it has a Brillouin region, and any point outside the first Brillouin region can also be expressed as a point inside the region. So, the wave vector is then mathematically transformed to a point inside the first Brillouin region. This transformation allows for scattering processes which would otherwise violate the conservation of momentum: two wave vectors pointing to the right can combine to create a wave vector that points to the left. This non-conservation is why crystal momentum is not a true momentum. Umklapp scattering is one process limiting the thermal conductivity of the two-dimensional crystal, the others being phonon scattering on crystal defects and at the surface of graphene. Umklapp scattering is the dominant process for thermal resistivity at high temperatures for low defect crystals. Boundary scattering is particularly important for low-dimensional

nanostructures. In nanostructures, phonons usually dominate and the phonon properties of the structure become of a particular importance for thermal conductivity. These phonon properties include: phonon group velocity, phonon scattering mechanisms, heat capacity, Grüneisen parameter. Unlike bulk materials, nanoscale devices have thermal properties which are complicated by boundary effects due to small size. In some cases, phonon-boundary scattering effects dominate the thermal conduction processes, reducing thermal conductivity. Depending on the nanostructure size, the phonon mean free path values may be comparable or larger than the two-dimensional crystal. When the two-dimensional crystal is larger than the mean free path of phonons, Umklapp scattering process limits thermal conductivity, namely in the regime of diffusive thermal conductivity. When the two-dimensional crystal is comparable to or smaller than the mean free path of phonons, the continuous energy model used for bulk materials no longer applies and nonlocal and nonequilibrium aspects to heat transfer also need to be considered [47, 48]. In this case phonons in defect-less structure could propagate without scattering and thermal conductivity becomes ballistic. Thermal conductivity in the two-dimensional crystal can be computed based on complete phonon dispersions instead of the linearized dispersion relations commonly used to compute thermal conductivity in bulk materials.

4. Conclusions

This study relates to the heat conduction properties of carbon-based nanostructured materials. Computational simulations were performed using molecular dynamics to investigate the heat transport properties of graphene. The intrinsic thermal conductivity of graphene was determined to understand the characteristics of thermal transport in the nanostructured materials. The effects of crystal length and edge states on the heat conduction properties of graphene were investigated. The mechanism of phonon transport in graphene was discussed. The physical factors limiting heat conduction in graphene with atomically-disordered edges were provided.

The results indicated that the thermal properties of graphene are directly related to its unique structure. Phonons are derived from the crystal lattice. The crystal length is the primary factor affecting the thermal conductivity of graphene. Graphene generally has very high thermal conductivity, but the presence of impurities reduces the degree of the mean free path of phonons, thereby degrading the thermal performance. The edge termination state has little effect on the thermal conductivity, since there is little difference in thermal conductivity between two-dimensional zigzag-edged and armchair-edged crystals. The difference in thermal conductivity is insignificant between zigzag-edged and armchair-edged crystals. However, the thermal conductivity of the two-dimensional crystal depends strongly upon the crystal length. There is a significant effect of crystal length on the thermal conductivity. All scattering processes can be taken into account using Matthiessen's rule. Phonon-boundary scattering instead of phonon-phonon Umklapp scattering is the dominant scattering mechanism. Phonon scattering by grain boundaries reduces the efficiency of thermal transport in graphene. Boundary scattering is particularly important for low-dimensional nanostructures. Excess small crystals can block phonons, causing a decrease in the thermal conductivity.

Declarations

Declaration of competing interest

The authors declare that there is no conflict of interest.

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Figures

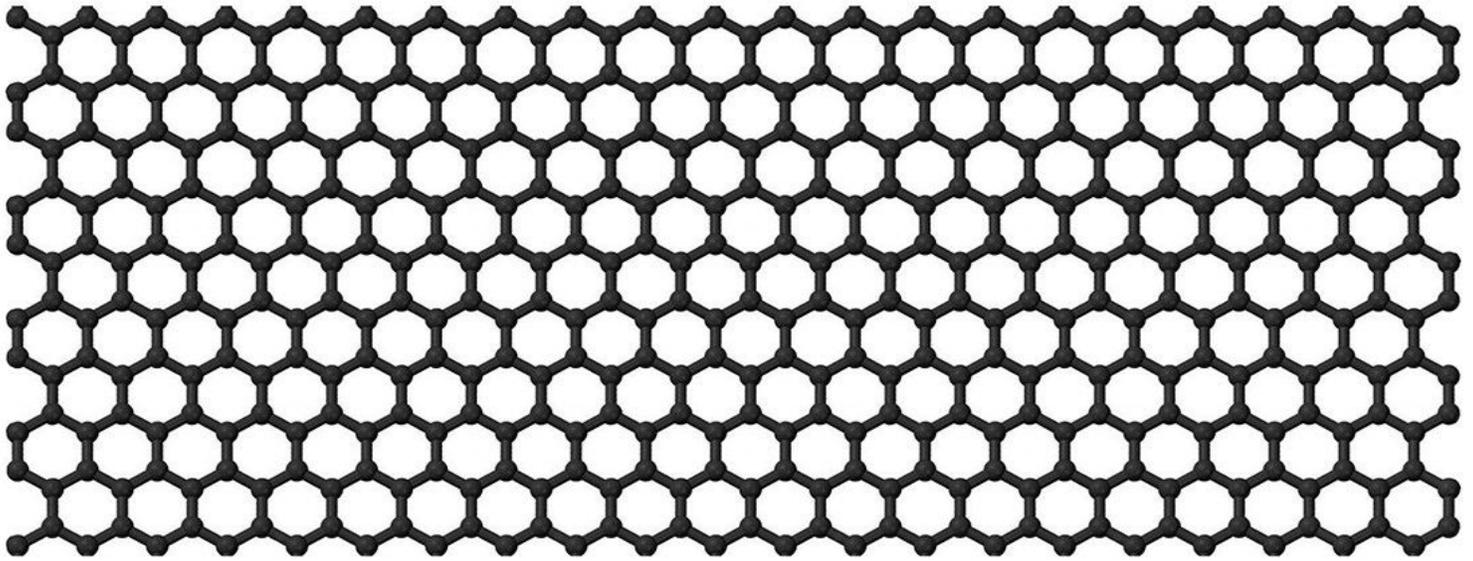


Figure 1

Schematic illustration of one individual graphene ribbon with substantially smooth edges. The two-dimensional crystal is 5.4 nm in width, 0.335 nm in thickness, and 70 nm in length.

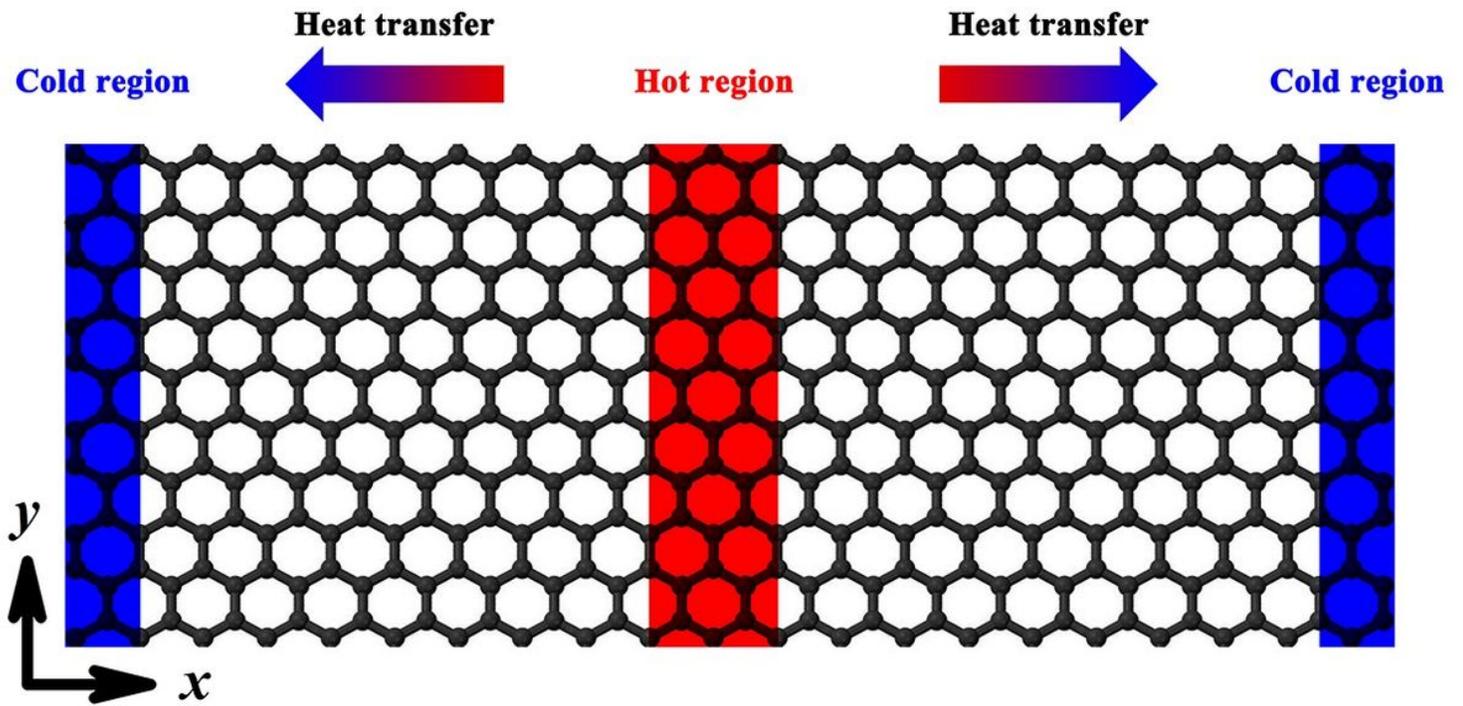


Figure 2

Schematic illustration of a specific heat flux imposed through the two-dimensional crystal using the Müller-Plathe algorithm. It is assumed and indicated that the red region has a higher value of temperature than the blue regions and that the property being transported in the two-dimensional crystal therefore flows from the red region to the blue regions. The arrows indicate the direction of heat transfer between the hot and cold regions. Linear momentum of the atoms is transferred to maintain a constant heat flux between the red region and the blue regions and a constant temperature gradient across the two-dimensional crystal.

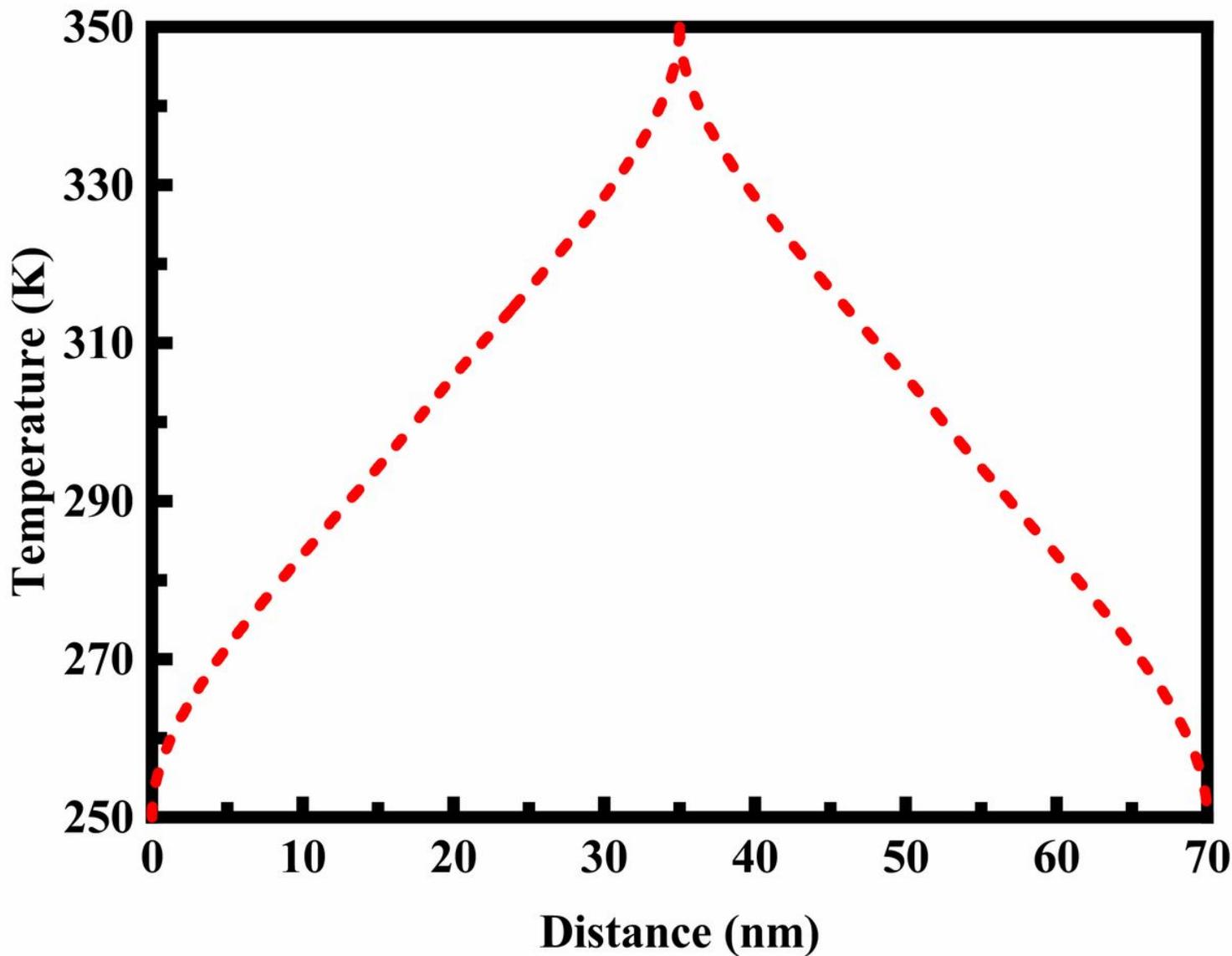


Figure 3

Steady-state temperature profiles obtained for the two-dimensional crystal with substantially smooth edges. The length of the two-dimensional crystal is 70 nm. The two-dimensional crystal has transverse edges that have an armchair configuration.

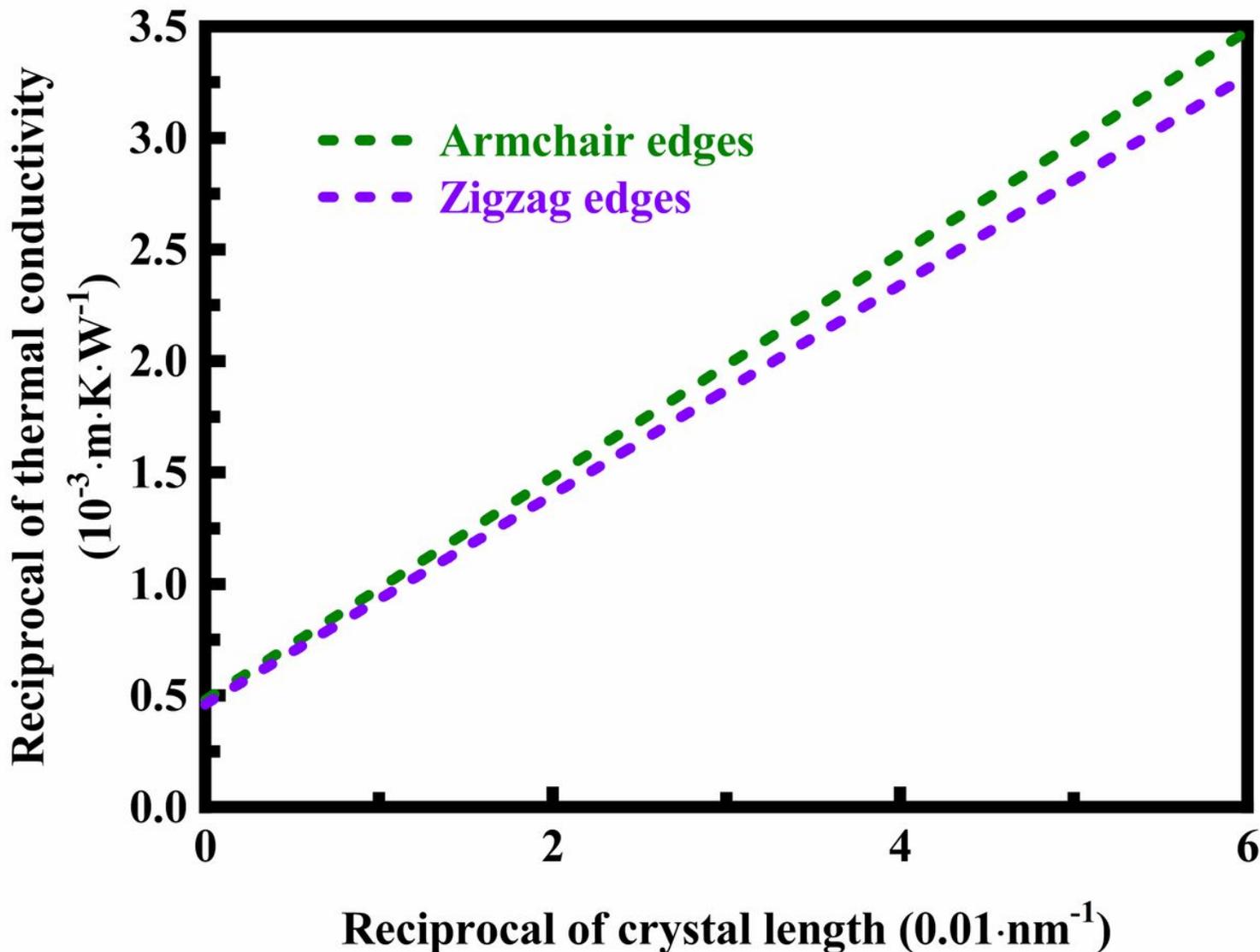


Figure 4

Effect of crystal length on the thermal conductivity of the two-dimensional crystal with different transverse edge states. The transverse edges of the two-dimensional crystal are substantially smooth.

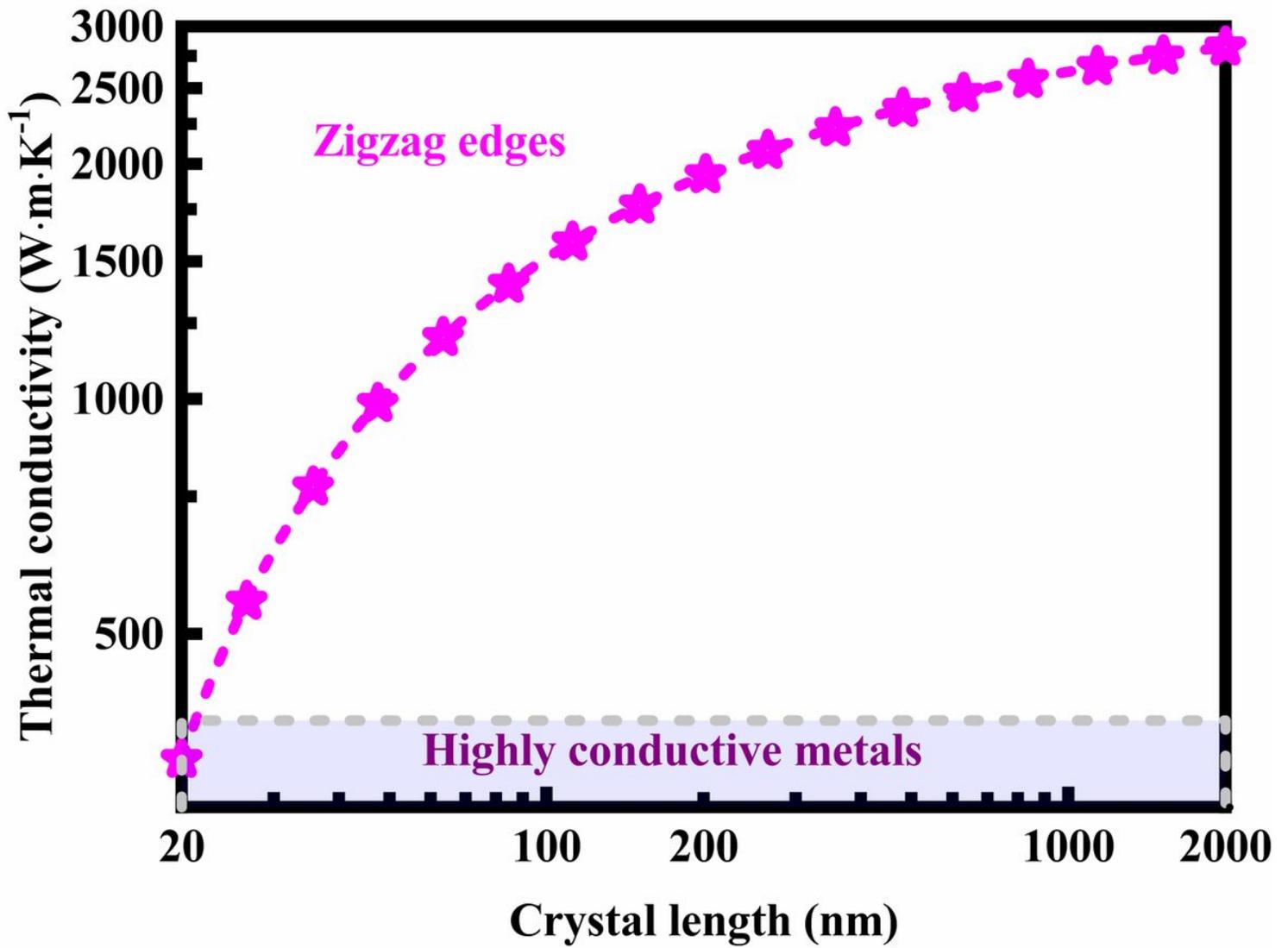


Figure 5

Effect of crystal length on the thermal conductivity of the two-dimensional crystal with zigzag edges. The transverse edges of the two-dimensional crystal are substantially smooth.

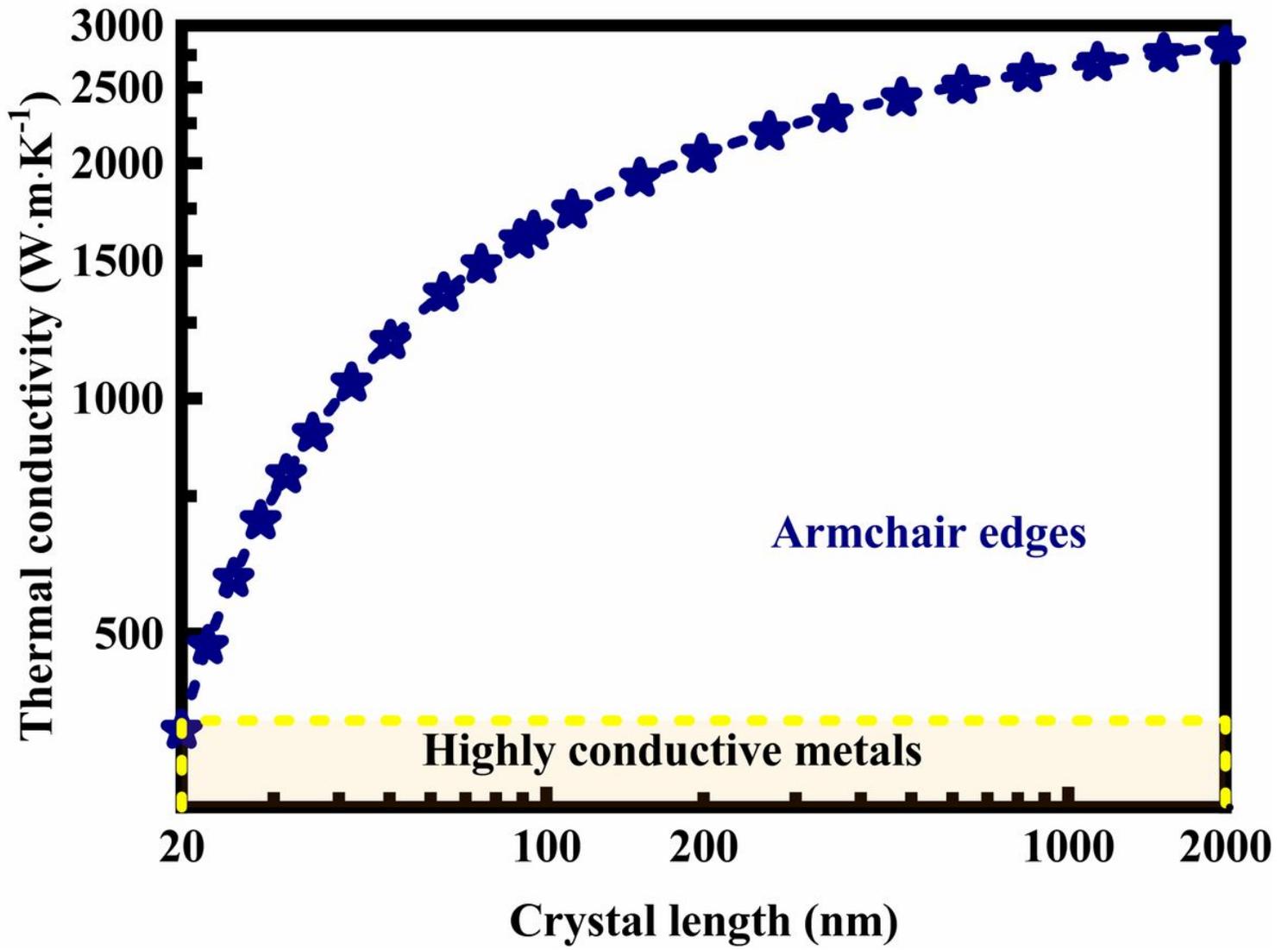


Figure 6

Effect of crystal length on the thermal conductivity of the two-dimensional crystal with armchair edges. The transverse edges of the two-dimensional crystal are substantially smooth.