A thermal diode using phonon rectification

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Abstract. A diode is an element blocking flow in one direction, but letting it pass in the other. The most prominent realization of a diode is an electrical rectifier. In this paper, we demonstrate a thermal diode based on standard silicon processing technology using rectification of phonon transport. We use a recently developed detection method to directly visualize the heat flow through such a device fabricated in a thin silicon membrane. The diode consists of an array of differently shaped holes milled into the membrane by focused ion beam processing. In our experiment, we achieve a rectification ratio of the heat current of 1.7 at a temperature of 150 K.

A majority of minimized integrated circuits merely use electrical functionality and are based on silicon (Si) technology. As the counterpart of the electrical properties at the nano- and microscale, other transport mechanisms become more and more the focus of attention [1, 2]. Most transport phenomena are accompanied by heat flow, however, thereby making the study of thermal transport on the microscale all the more interesting. To understand the underlying effects better, the basic elements have to be developed and characterized—the most common one being a diode. In this paper, we study the rectification of heat flow carried by phonons in a thin Si membrane [3, 4], while leaving the electrical transport unaffected. We directly visualize the heat flow through such a device [5]. The diode consists of an array of triangular- and rhombic-shaped holes fabricated into the membrane by standard focused ion beam (FIB) techniques, rectifying phonons depending on the direction of heat flow. In the presented experiment, we achieve a rectification ratio of the heat current of 1.7 ± 0.2 at a measurement temperature of 150 K. Starting from this rectification, we suggest a thermal diode to serve as the building block in full analogy to electrical circuits such as memory [6], gates [7] and transistors [8]. Furthermore, diodes based on phonon rectification should lend themselves as passive devices

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to control heat flow in addition to actively driven thermoelectric designs. They could further improve the figure of merit in energy conversion setups [9].

So far, a small number of works have been reported on the experimental observation of phonon rectification. Since the phonon distribution is difficult to measure directly, one usually takes anisotropies of the heat flow as a measure for phonon rectification. Carbon nanotubes with an asymmetric mass distribution changing the temperature dependence of the resonant frequencies showed a rectification effect of 2% at 300 K [10–12]. Furthermore, a gallium-arsenide-based quantum dot asymmetrically coupled to its leads showed a rectification ratio of 10.5% below 100 mK [13]. The effect was also visible in bulk material below 100 K. Two cobalt oxides with different temperature-dependent thermal conductivities, and bonded to each other, rectified the heat current by a factor of 1.43 [14, 15]. Rectification of an acoustic energy flux in the frequency range around 1 MHz with a ratio as high as 10^4 was possible by up-converting the phonons in a nonlinear medium solely enabling the second harmonic to pass [16].

As mentioned above, heat can be transported via charge carriers, too. In narrow-bandgap semiconductors, the contribution of the phonons can be designed to be negligible compared to the carrier contribution. In principle, an electrical diode should also act as a thermal diode under those circumstances. A thermoelectric structure in $Hg_{0.86}Cd_{0.14}Te$ converting electrical into thermal energy shows current flow asymmetries [17] and could be used to control phonon flow electrically. However, for applications in passive devices, the capability of controlling the heat flow without the accompanying electrical current is required. Control of the phonon flow while leaving the electron flow unaffected is possible in a system in which the phonon mean free path is much longer than the electron mean free path, such that the phonon transport is ballistic while the electron transport is diffusive on a particular lengthscale. By adequately patterning the system on this lengthscale, asymmetries in the phonon flow are caused. In addition, a system in which the contribution of the electrons to the heat flow is smaller than that of the phonons is favorable, i.e. an undoped Si membrane.

In this paper, we present a new technique of phonon-based thermal rectification on 340 nm thin Si membranes. We visualize the heat flow through the device by detecting the temperature distribution directly. The measurement concept is based on utilizing the temperature-dependent optical transmissivity of Si membranes [5]. Here we use a microscopy setup in transmission geometry to image the membrane (see the appendix) and a focused laser beam to induce a temperature gradient.

Taking into account the radial symmetric geometry of the heat flow induced by the laser focus in the two-dimensional membrane, Fourier's law can be solved to obtain an expression for the temperature distribution $T(r)$ at a distance r from the heating laser spot

$$T(r) = \frac{-J}{2\pi\kappa d} \ln\frac{r}{r_0} + T_0,$$

where J is the total amount of heat flow, κ the thermal conductivity, d the membrane thickness and r_0, T_0 are constants that define the starting values. The temperature profile shows a logarithmic dependence on the distance from the heating laser and is isotropic for all directions, despite the anisotropy of the (100) surface used [18, 19]. If κ and d are constants over the whole membrane, a change in the slope of $T(r)$ indicates a change in the heat flow. $T(r)$ can therefore be used as a quantitative measure for J.

In order to build a diode, the symmetry of the heat flow has to be broken by preferably directing the phonon motion into one direction. We therefore pattern holes into the Si membrane
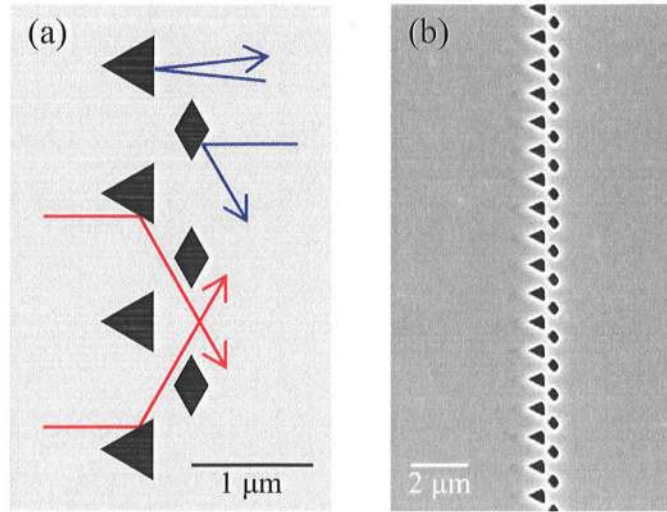
Figure 1. (a) Design of the triangular and rhombic hole array. The red arrows indicate the way of the phonons that can pass the array, whereas the blue arrows denote those being reflected. (b) Scanning electron microscope (SEM) image of the structure after milling. The image is slightly dilated due to the tilt of the SEM with respect to the FIB column.

by means of FIB milling. Figure 1 shows a set of triangular and rhombic holes cut through the membrane. The edges of the holes serve as walls for specular reflection for the phonons.

In general, in bulk systems at room temperature or above, the phonon transport is diffusive because the phonon scattering length or mean free path is smaller than any relevant lengthscale (30 nm for Si at 300 K). This means that the motion direction of the phonons is randomized by scattering on distances corresponding to this value. At low temperatures the phonon mean free path may increase up to several mm [20]. The phonons travel ballistically between scattering events taking place at surfaces only. If the surfaces are flat [21], the reflection occurs in a specular manner like light being reflected at conventional mirrors. By patterning the shape of the membrane, e.g. by milling holes into it, it is thus possible to build phonon waveguides and to direct the heat flow.

In the following, we first consider *ballistic* phonons traveling along the membrane plane and undergoing solely specular reflection at the edges of the holes. Such a phonon, arriving from the *left* in figure 1(a) perpendicular to the hole array and hitting one of the triangles in the first row, will be reflected there and will travel through the second row of holes. The distance and shape of the rhombic holes are designed exactly to let these phonons pass the complete array without further scattering. A phonon impinging directly on a rhombic hole is reflected at least three times before it can leave the structure. Its probability of scattering increases accordingly, so it has a reduced probability to leave the structure with a well-defined direction. This phonon will rather contribute to the diffuse background and will therefore be neglected in the following consideration.

A ballistic phonon arriving from the *right* side in figure 1(a) will be back-reflected regardless of whether it hits a triangle or a rhomboid first. The asymmetric design leads to a
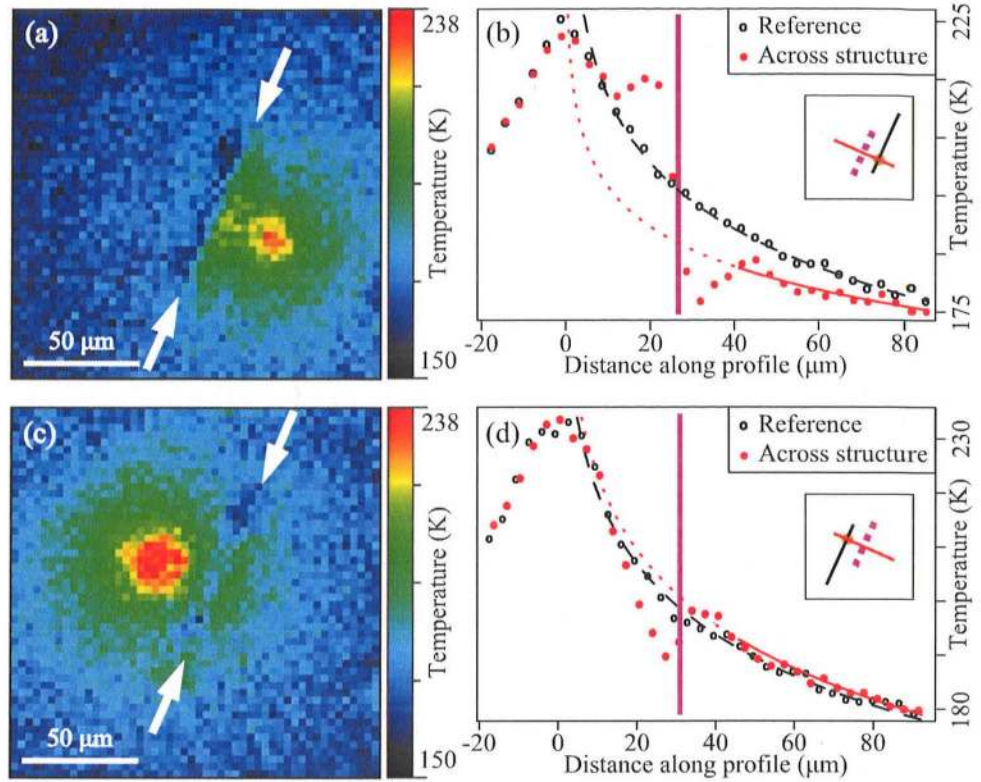
Figure 2. (a, b) Blocking direction of the diode. Panel (b) shows temperature profiles across the diode structure in (a) and parallel to the reference. The change in J indicates that less heat is flowing in this direction compared to the reference. The white arrows as well as the magenta-colored lines are a guide to the eye to indicate the position of the structure. Panels (c, d) are alike, but describe the situation for the non-blocking direction of the diode. J is the same for the normal and reference directions. Control measurements at 300 K do not show any rectification, see figure 3.

rectification of part of the phonons and will therefore influence the predominant direction of heat flow.

In a realistic experiment, however, there is a certain distribution of directions of incoming phonons given by the phonon mean free path and the geometry of the source of the phonon flow which limits the rectification. A simple ray-tracing simulation reveals that the design of the hole array favors transmission at low angles of incidence for the transfer direction, whereas in the blocking direction these low-angle phonons are reflected.

The measurements show that rectification is feasible indeed. Their results are visualized in figure 2 and discussed below.

Figures 2(a) and (c) show the temperature distribution obtained at 150 K substrate temperature. This temperature has been chosen as a compromise between the high sensitivity of the temperature measurement and a sufficiently long phonon mean free path for ensuring the presence of ballistic phonons (140 nm at $T = 150$ K [20]). At this temperature, not only

is the mean free path longer than that at room temperature, but also the wavelength of the phonons increases as compared to room temperature [22, 23]. The first fact ensures that parts of the phonons pass through the diode structure without being scattered; the latter reduces non-specular reflection at the boundaries. In figure 2(a), phonons are created by laser heating with a point focus at the side of the rhombic holes, whereas in figure 2(c) the heat is induced at the opposite site. The distance between the laser focus and the diode is $30\,\mu$m, resulting in an angular distribution of the phonon directions given by Lambert's law, but still providing a preferred impact direction perpendicular to the array axis. The temperature rise in the laser focus is in both cases about 70 K. According to the description above, figure 2(a) corresponds to the blocking direction and figure 2(c) to the transfer direction, respectively. The rectification effect due to the asymmetric hole array is clearly visible by comparing figures 2(a) and (c). While in the limits of the experimental resolution the heat passes through the structure apparently unhindered in figure 2(c), it is partially reflected in figure 2(a).

In order to analyze the data set more quantitatively, temperature profiles are taken perpendicular and parallel to the diode structure (figures 2(b) and (d)). The open circles give the direction parallel to the hole array as reference, whereas the closed circles visualize the heat flow across the structure. The position of the structure is marked by the vertical bar in both graphs. The dashed line gives a fit to the reference data according to the theory stated above, and the solid and dotted line describe the data across the structure, respectively. As FIB milling induces gallium defects in the membrane [24, 25], we exclude data within $20\,\mu$m on both sides of the array for our fits. The solid line represents the amount of data used for the fit, whereas the dotted line is an extrapolation towards the center.

In the transfer direction (figure 2(d)), both profiles overlap within their error bars, proving that the phonons flow through the structure almost unhindered. The fits show the same behavior of the logarithmic function, thus corresponding to the same value of J. Even though the hole array appears to provide a reduced κ, owing to the missing material, the temperature jump across the structure is < 1 K because of its small width.

In contrast to this behavior, figure 2(b) represents the temperature distribution in the blocking direction, with the same pictograms as before. The rectification is visible by comparing the profiles on the right-hand side of the graph to those in figure 2(d). The slope of the logarithmic function decreases, indicating that phonons are partly reflected and therefore less heat is flowing through the diode.

From the fits we calculate the heat currents J_{trans} and J_{blocking} in the transfer and blocking directions, respectively. The ratio $J_{\text{trans}}/J_{\text{blocking}}$ gives the rectification ratio of the diode, in our case 1.7 ± 0.2. This value could be enhanced by optimizing the geometry, e.g. to prevent multiple reflections as described above or by lowering the temperature for enhancing the phonon mean free path. The latter would, however, reduce our detection sensitivity.

Control measurements obtained at 300 K do not show any rectification as expected, see figure 3. The annotation is equivalent to that in figure 2. As is obvious from the temperature distributions in figures 3(a) and (c), as well as from the profiles in figures 3(b) and (d), there is no difference between the two directions. Heat can flow from one side to the other without being impeded by the FIB structure. At 300 K the mean free path of the phonons is much smaller than the typical dimension of the hole array and scattering at the edges is diffusive.

At a first glance the diode structure seems to embody Maxwell's demon [26]. The 'conceivable being' separates phonons, since one side of the diode heats up more than the other. Even though the experiment is performed under quasi-equilibrium conditions, heat is constantly
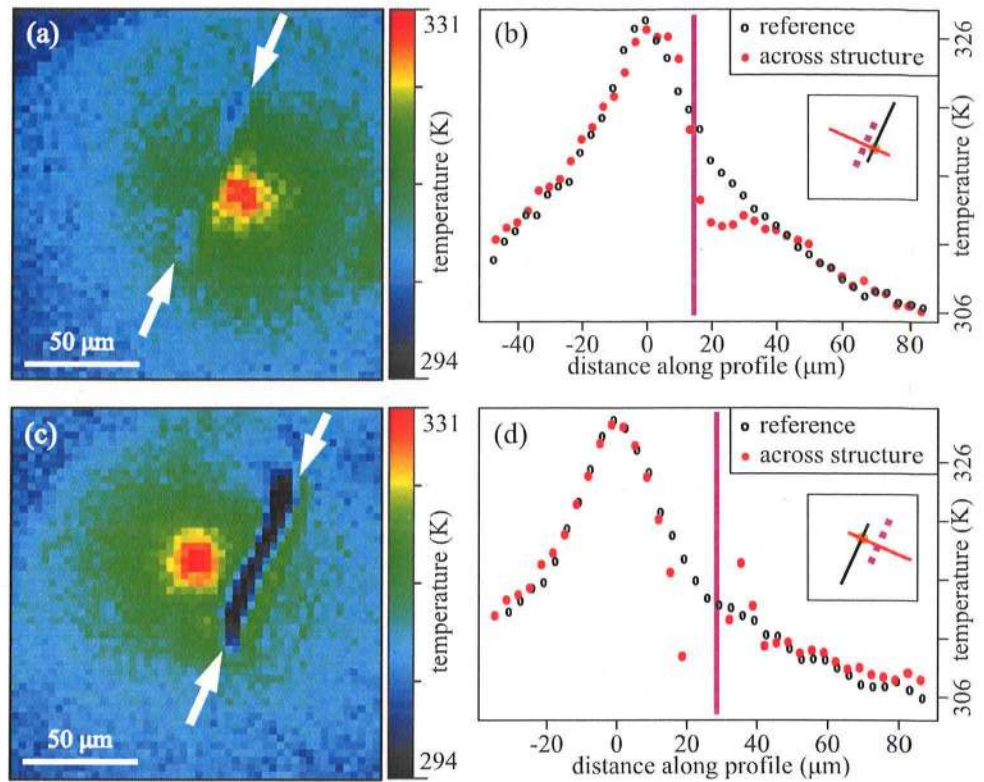
Figure 3. Annotation is the same as in figure 2. (a, b) Blocking direction of the diode and (c, d) non-blocking direction. Panels (b, d) show the temperature profiles across the diode structure and parallel to the reference. The white arrows as well as the magenta-colored lines are a guide to the eye to indicate the position of the structure. There is no detectable difference in the shape of the profiles, which implies that there is no rectification effect at 300 K.

flowing from the focus center to the Si wafer surrounding the membrane. We therefore have to include the laser source and the wafer into this consideration. Furthermore, the rectification effect vanishes for a completely isotropic distribution of incoming phonon directions. Hence, the experiment does not violate the second law of thermodynamics, but rather the phonons are guided inside the membrane.

The data clearly demonstrate the thermal rectification effect obtained by nanostructuring a thin membrane, which is based on standard Si processing techniques. It can be implemented in any device based on Si as well. The new aspect in our device is that the heat flow is carried mainly by phonons, leaving the electronic degree of freedom completely unaffected. In a more complex realization the electronic contribution to heat transport could be used for fine-tuning the device. The effect is not only limited to Si, however. Any material exhibiting phonon mean free paths comparable to or longer than the dimensions of a hole array as described here and in which the heat transport is dominated by phonons should show rectification.

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Acknowledgments

Appendix

We use a standard microscopy setup in transmission geometry operating at a magnification of $10\times$. The Si membrane is clamped to the cold finger of a ^{4}He flow-cryostat, covering a temperature range between 6 and 350 K. As the light source, an ultra-bright white light-emitting diode (LED) is implemented. Light from a laser diode ($\lambda = 660$ nm, $P_{max} = 130$ mW) is confocally coupled into the detection beam by a polarizing beam splitter cube and is synchronized to the LED source. Both the LED and laser diode can be operated pulse-wise, allowing for time-resolved measurements as well. The transmitted intensity is then detected by a CCD camera with a resolution of 12 bit in depth. As the detection has to be done at a specific wavelength of the light, we use an optical filter ($\lambda_{center} = 480$ nm, FWHM = 10 nm) in front of the CCD in order to cut out only the most sensitive wavelength.

The Si membranes are fabricated from Si-on-insulator wafers by wet chemical etching techniques described elsewhere [3, 4].

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