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Performance evaluation and optimization of a high-efficient phonon rectifier

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Abstract. We report rectification enhancement of acoustic waves through a double array of periodic triangular holes embedded in an elastic medium of an acoustic phonon rectifier. We numerically investigate the transmission rates of waves and hence the efficiency of the rectifier using the Finite-Difference-Time-Domain (FDTD) method. We alter the position of the arrays and investigate the optimal position for high-efficient rectification to facilitate practical applications.

1. Introduction

Geometric effects on electron and phonon transport have attracted attention since asymmetric potential or scatterers can rectify electron and phonon transport[1-3]. In a previous work, the present authors investigated transverse acoustic(TA) wave transmission through an array of triangular holes periodically put in an elastically isotropic material. We numerically confirmed rectification effects of the asymmetric scatterers on the TA wave transmission. Very interestingly, the Bragg reflection owing to the periodic structure enhances the rectification. In spite of the finding, the efficiency of the rectification is 35% at most. In the present work, we propose a new system that shows large difference in energy transmission of acoustic waves and investigate the transmission properties in the system.

2. Model

Aiming for a perfect rectifier structure, we look for a periodic arrangement of scatterers that reflects perfectly all the waves impinging perpendicularly on the scatterers. We give a candidate for a perfect rectifier in Fig. 1(b). The system is composed of equilateral triangular holes of base length a drilled in an elastically isotropic and homogeneous material. The holes are periodically set in the y -direction with spacing equal to $2a$, and another array of aligned holes are put in the right of the first one. The second array is shifted by a in the y -direction and $b + \delta$ in the x -direction, where $b = \frac{\sqrt{3}}{2}a$ and δ is an adjustable structural parameter. Within the ray-acoustics, the transmission rate $T = 0$ for case (I) and $T = 0.5$ for case (II). We simulate the wave propagation across the scatterers, using a Finite-Difference-Time-Domain (FDTD) [5] method. We examine the transmission in the system by changing δ to find the optimized position of the arrays of scatterers for perfect rectification. When $\delta = -b$, the paths for the acoustic waves are pinched off, and then there is no transmission in both the directions.

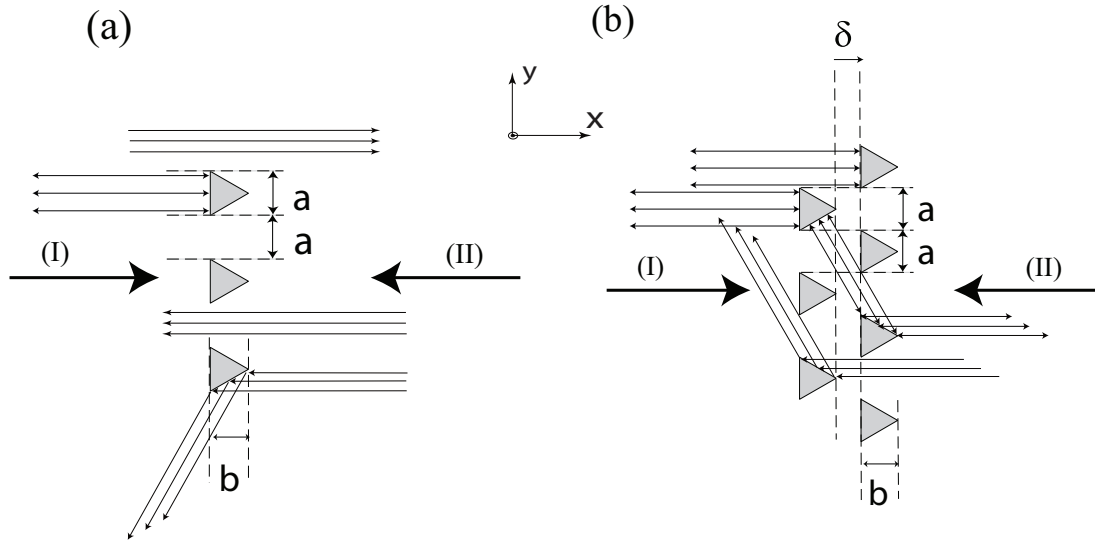


Figure 1. An acoustic wave rectifier with (a) single and (b) double array of triangular holes. Thick arrows (I) and (II) indicate the incident wave directions. The thin arrows illustrate reflection of waves based on the ray-acoustics. The parameters a and b are base length and median of the triangles respectively. δ is the length between the summits of the first array and the bottoms of the second one.

We investigate z -polarized transverse acoustic (TA) wave propagation in the $x-y$ plane. The wave equation of u_z is given by

$$\frac{\partial^2 u_z}{\partial t^2} = c^2 \nabla^2 u_z, \quad (1)$$

where c is the velocity of sound waves. Assuming vacuum in the holes, we employ stress free boundary condition on u_z , i.e. $\sigma_{z\alpha} n_\alpha = 0$. n_α is a component of the unit vector normal to the surface of a scatterer and $\sigma_{z\alpha}$ is the stress tensor defined by $\sigma_{z\alpha} = \mu \partial_\alpha u_z$, where μ is one of the Lamé constants. The acoustic Poynting vector $\mathbf{J}$ in the present system is defined from the continuity of energy flow as $\mathbf{J} = -\dot{u}_z(\sigma_{zx}, \sigma_{zy}, 0)$. The total energy flow is described in terms of the Fourier components of the displacement $\hat{u}_z(\omega)$ and the stress tensor $\hat{\sigma}_{z\alpha}(\omega)$ as $\int_{-\infty}^{\infty} \mathbf{J} dt = -4\pi \Im \left[\int_0^\infty \omega \hat{u}_z(\omega) (\hat{\sigma}_{zx}^*(\omega), \hat{\sigma}_{zy}^*(\omega), 0) d\omega \right]$. The total energy at ω is given by, $\hat{\mathbf{J}}(\omega) = -4\pi \Im \left[\omega \hat{u}_z(\omega) (\hat{\sigma}_{zx}^*(\omega), \hat{\sigma}_{zy}^*(\omega), 0) \right]$. Here $\Im[A]$ means the imaginary component of A . We define the transmission rate $T(\omega)$ as the ratio of the x -component of $\hat{\mathbf{J}}(\omega)$ integrated over the $y-z$ plane to that in the absence of scatterers.

$$T(\omega) = \frac{\int \hat{J}_x(\omega) dy dz}{\int \hat{J}_x^0(\omega) dy dz} \Big|_{x=x_D}, \quad (2)$$

where x_D is the detecting position which is in the right side of the scatterers for case (I) and in the left side of the scatterers for case (II).

We introduce the following rectifier efficiency to quantify rectification as

$$\eta(\omega) = \left| \frac{T_{(I)}(\omega) - T_{(II)}(\omega)}{T_{(I)}(\omega) + T_{(II)}(\omega)} \right|, \quad (3)$$

where $T_{(I)}$ and $T_{(II)}$ is the transmission rate for cases (I) and (II) respectively. The efficiency varies in the range $[0, 1]$, and $\eta = 0$ means no rectification and $\eta = 1$ the perfect rectification.

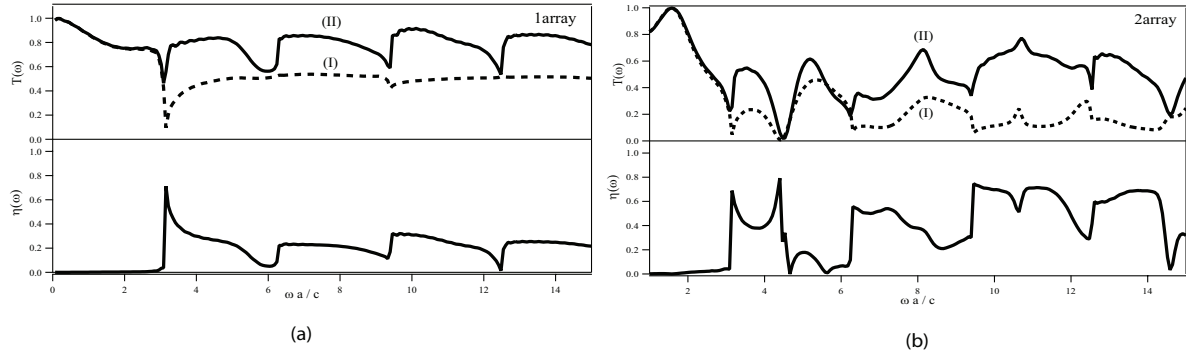


Figure 2. (a) and (b) Top: Transmission rate versus frequency for single-array and double array of triangular holes respectively. Case (I) and case (II) are indicated by dashed lines and solid lines respectively. Bottom: Efficiency versus frequency for the above model.

3. Transmission Rates and efficiency

Figure 2(a) and (b) shows the transmission rates and η versus frequency for the single and double arrays of scatterers with $\delta = 0$ respectively. There arises a threshold frequency $\omega_0 = \pi$, below which there is no difference in transmission rates for case (I) and (II). Above ω_0 , they show obvious difference in the energy transmission and there is periodic dips at multiples of π i.e) $\frac{\omega a}{c} = m\pi$ where m is an integer. The threshold frequency and the dips in the transmission rate arise from the Bragg diffraction due to the periodic arrangement of the scatterers in the y -direction. As a result of elastic scattering of the acoustic waves, $|\mathbf{k}'| = |\mathbf{k}|$, where $\mathbf{k}$ and $\mathbf{k}'$ are the wavevectors of incident and scattered waves, respectively. The wavevector of scattered wave is given by $\mathbf{k}' = \mathbf{k} + \mathbf{G}$, where $\mathbf{G}$ is the reciprocal lattice vector. The scattering takes place when the Ewald circle [6] and the lines in the reciprocal lattice space intersect and the wavevector of the incident wave satisfies $|\mathbf{k}| = |\mathbf{k} + \mathbf{G}|$. The double-array has another dip in the transmission rates at $\frac{\omega a}{c} = 4.5$, this is owing to multiple scattering peculiar to the double-array.

The bottom figures of 2(a) and (b) show the efficiency versus frequency. Below ω_0 , there is no rectification and hence $\eta = 0$. The double-array shows complicated frequency dependence and its magnitude fluctuates around 0.5. On the other hand, η of the single-array is at most 0.3 except for the abrupt increase at the threshold frequency. These differences evidence that the double-array works as a rectifier better than the single-array. Figure 3 shows the transmission and the efficiency η versus frequency for (a) $\delta = \frac{b}{4}$, (b) $\delta = \frac{b}{2}$, (c) $\delta = b$, (d) $\delta = -\frac{b}{3}$, (e) $\delta = -\frac{b}{2}$ and (f) $\delta = -\frac{3b}{4}$. In comparison with the case of $\delta = 0$ (Fig. 2(b)), the transmission rates are spiky and the corresponding η fluctuates quickly with increasing frequency for $\delta > 0$. The behavior is owing to the interference among multiply scattered waves. In contrast, for $\delta < 0$, the frequency dependences of the transmission rate and η are not as complicated as those for $\delta > 0$. The transmission rates and η vary smoothly and the magnitudes are almost constant i.e) $\eta \approx 0.6$, for $\delta = -\frac{b}{3}$. In addition, although the efficiency η changes drastically at $m\omega_0$, where m is an integer, η is almost constant between the frequencies and its magnitude is high, e.g $\eta = 0.8$ in the frequency region $2\pi < \frac{\omega a}{c} < 4\pi$ for $\delta = -\frac{3b}{4}$. Thus when the two arrays are moved close to each other, they show better rectification effects. From the above results, it is evident that the system with $-b < \delta < 0$ has large efficiency compared to all other possible positions.

4. Summary

We numerically investigated acoustic wave rectifiers composed of a single and double arrays of triangular holes which act as scatterers. We showed apparent differences in the transmission

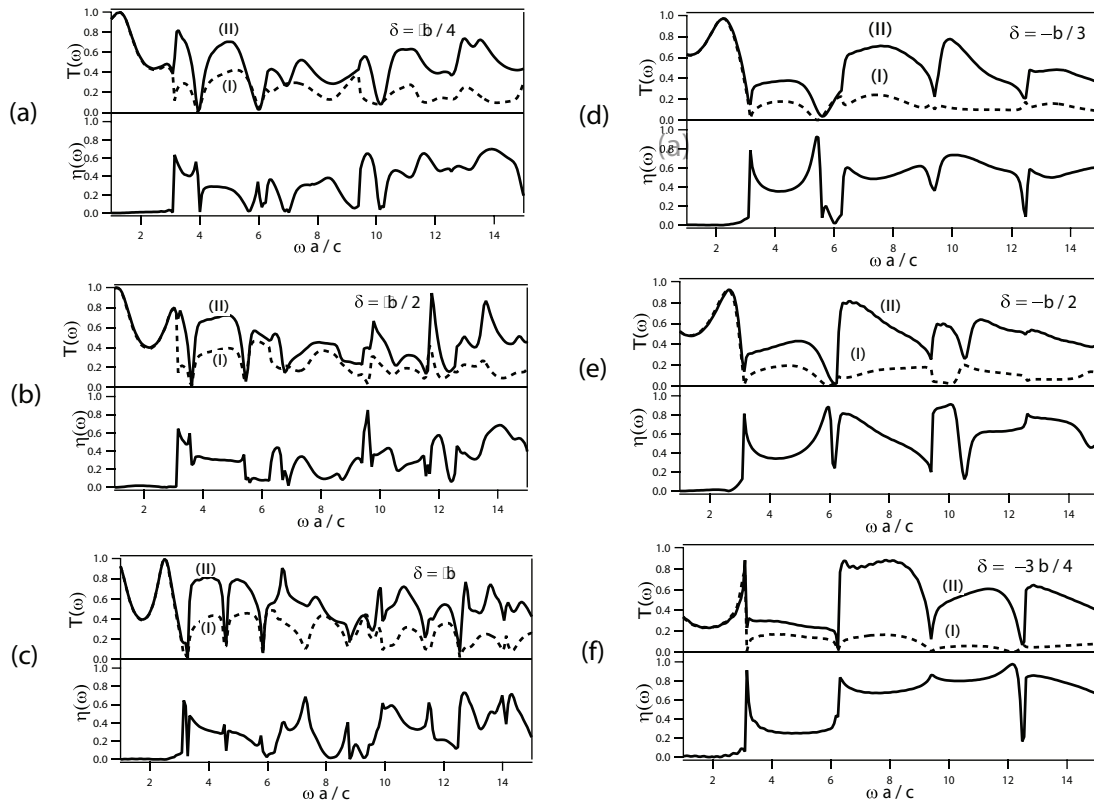


Figure 3. Efficiency versus frequency for different magnitudes of δ . (a) $\delta = \frac{b}{4}$, (b) $\delta = \frac{b}{2}$, (c) $\delta = b$, (d) $\delta = \frac{-b}{3}$, (e) $\delta = \frac{-b}{2}$, (f) $\delta = \frac{-3b}{4}$

rates, depending on the incident directions. The rectification is caused by directional scattering arising from the geometrically asymmetric scatterers. This kind of scattering is not realized by simple asymmetric structures such as a bilayer. In comparison with a single array rectifier, the double-array rectifier is found to have better rectification effects, judging from the efficiency of these two rectifiers. We optimized the position of the scatterers in the double array to improve the performance of the rectifier. The results show that the rectifier with $\delta = \frac{-3b}{4}$ is appropriate for a device application.

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