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Terahertz Acoustic Wave on Piezoelectric Semiconductor Film via Large-scale Molecular Dynamics Simulation

圧電性半導体薄膜における THz 弾性波伝搬の大規模分子動力学シミュレーション

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1. Introduction

Acoustic wave in bulk or in surface has been used as transmitting media in many technological applications. Particularly in communication equipment, it is applied to a frequency filter for noise reduction. Recently, the wireless communication in the terahertz (THz) region is attracting attention[1] as it has higher-speed and capacity than conventional technique. Practical application has been, however, hampered by noise. Development of an efficient and miniturized frequency filter in the THz rigion is thus desired. Since typical wavelength of acoustic waves in solid at THz is nanoscale, atomic-level modeling is inevitable for realistic design. We simulate acoustic wave propagation at THz in piezoeletric thin file using Molecular-Dynamics (MD) simulation. To control the acoustic wave at THz, we also introduce a phononic-crystal (PC) structure in the film. We examine the propagation property in the PC structure also via MD simulation.

2. Mode Analysis

To realized frequency filter for the THz rigion, we focus on the thickness longitudinal mode.

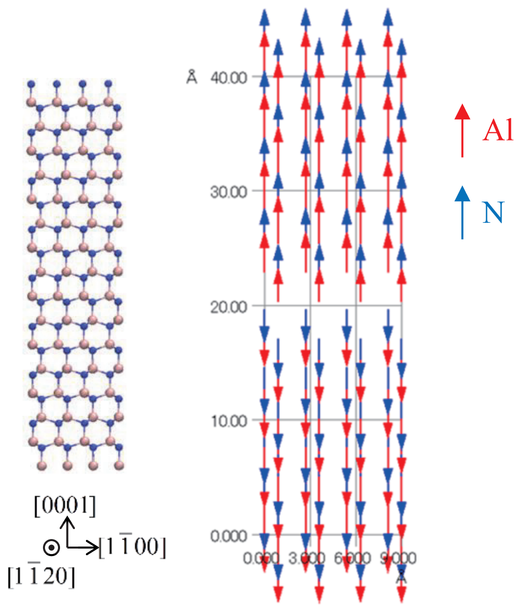


Fig. 1 THz thickness longitudinal vibration mode.

This mode has been used in the piezoelectric frequency filters at GHz regime and called Film Bulk Acoustic Resonator (FBAR). Since the present model is on the order of nanometer, we first examine if thickness longitudinal vibration mode at THz frequency in the thin film exists or not using mode analysis. The mode analysis in atomistic simulation is based on the following eigen value problem.

$$\mathbf{D}(\mathbf{k})\cdot\mathbf{u} = \omega\mathbf{u} \tag{1}$$

$$\mathbf{D}(\mathbf{k}) = \sum_n e^{-i\mathbf{k}\cdot\mathbf{R}_n} \frac{1}{\sqrt{M_i M_j}} \frac{\partial^2 V}{\partial\alpha_{ni}\partial\beta_{0j}}, \tag{2}$$

where $\mathbf{D}(\mathbf{k})$ is called dynamics matrix, $\mathbf{R}_n$ is lattice vector, M is mass of i, j th atom, α and β are direction component, and V represents interatomic potential. We adopt Aluminum Niteride (AlN) as the piezoelectric material, and its interatomic-potential model has bee taken from Ref. 2. The potential model is based on the two-body and three-body interaction. And it can reproduce the elastic constants, the cohisive energy, and other bulk properties of the material measured by experiments. Figure 1 shows displacement direction of each atom of a acoustic mode at 1.27THz. It clearly indicated that thickness longitudinal vibration exists in the nanoscale thin film of AlN. Also, the resonant frequency 1.27THz is close to a value (~1.3THz) obtained by a simple estimation of standing wave even in the nanoscale thin film.

3. MD simulation

We simulate acoustic wave propagation by the thickness longitudinal vibration of 1.27THz from induced area using MD tecnique as shown in Fig 2. Figure 2 shows snapshot of the propagation at the surface of AlN film and its cross-sectional view. The wavelength in this propagation mode is about 35Å. We thus confirm the plane wave of the thisckness longitudial mode at THz can propagate along the crystal direction.

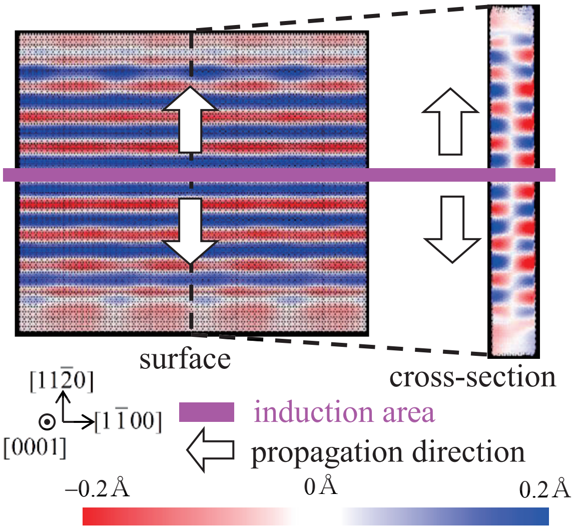
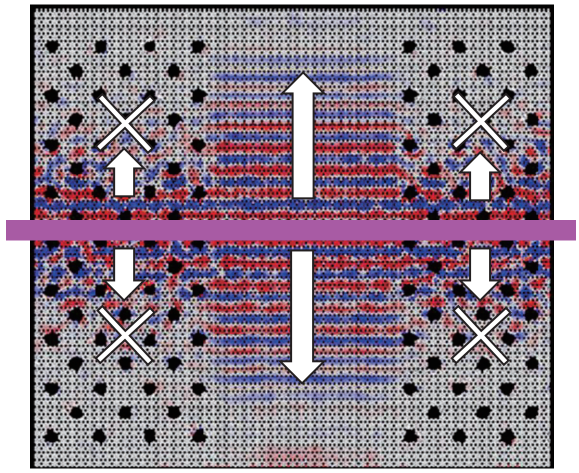


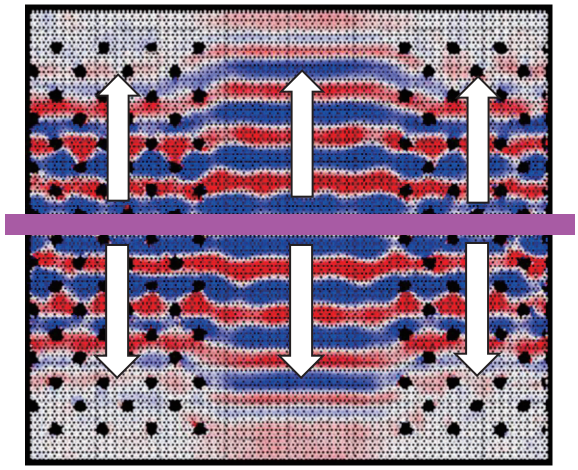
Fig. 2 Acoustic wave propagation at THz.

4. Phononic-Crystal Waveguide

To control acoustic wave, we focus on the Phononic Crystal (PC). Reallization of efficient filtering and waveguide of the surface acoustic wave at MHz frequency with a PC structure has been reported recently[3], We thus apply this structure to THz regime. The band-gap frequency in phonon dispersion with our PC structure is estimated to be near 2.54THz. We simulate acoustic wave propagation by MD method. Figure 3(a) shows acoustic wave propagation at the band-gap frequency. The propagation is localized in the waveguide region as shown in the figure. In contrast, at other frequencies, the waves propagate both in PC and waveguide regions, as shown in Fig. 3(b) for the frequency of 1.27THz. These results indicate designing and controlling THz thickness longitudinal vibration is possible with PC. Detailed analyses will be reported in the presentation.



(a) 2.54THz (band-gap frequency).



(b) 1.27THz.

Fig. 3 Acoustic wave propagation with PC

References

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