Epitaxial nanostructure design for control of phonon and electron transport

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Thermoelectric conversion efficiency is determined by a dimensionless figure of merit, $ZT=S^2\sigma T/\kappa$ in addition to the temperature difference, where S is Seebeck coefficient, σ is electrical conductivity, κ is thermal conductivity, and T is absolute temperature. For obtaining high ZT, high σ and low κ are required. However, this is difficult to achieve simultaneously because they are correlated. Therefore, the independent control of σ and κ has been a vital goal for long.

We proposed the two nanostructures composed of ultrasmall epitaxial nanodots (ND) as shown in Fig. 1. First one is the connected structure of epitaxial Si NDs. Carriers feel that connected NDs are single crystal because crystals of NDs are oriented, while phonon with long mean free path is scattered at the interfaces of NDs. The other is Si films containing epitaxial Ge NDs. In this structure, phonon is scattered effectively at the nanostructure interfaces while carriers go through them easily. Here, we fabricated the aforementioned structures using our original technique and measured electrical and thermal conductivity to show independent control of phonon and electron transports.

Ultrathin (~0.3 nm) SiO_2 films were formed by oxidizing clean Si surfaces at 500°C at the O_2 pressure of 2×10^{-4} Pa. Then Si or Ge atoms were deposited on the ultrathin SiO_2 films to form epitaxial Si or Ge NDs on Si substrates with ultrahigh density of ~10^{12} cm^{-2}. This detail is written everywhere [1-4]. In the Si ND case, Si NDs were oxidized again to form ultrathin SiO_2 cover film. These Si ND formation and oxidation processes were reported to form epitaxial connected Si ND structures. In the case of Si films containing Ge NDs, Si layers were epitaxially grown on Ge NDs. The aforementioned formation of Si layer/Ge NDs and the oxidization process were repeated to fabricate the ND stacked structures.

The thermal conductivity of these epitaxial nanostructures including NDs was measured by 2ω method. The κ value of the structure of connected Si NDs with 3 nm diameter was drastically reduced, which is close to the amorphous one In the case of Ge NDs, the κ value was also reduced compared with that of bulk Si. The Ge ND structures exhibited to similar σ to that of the bulk Si. This demonstrated the success in sustaining high σ and a reduction κ, indicating independent control of phonon and electron transports. This demonstrates the possibility of our nanostructure as a Si-based thermoelectric material.

This work was partially supported by JSPS KAKENHI Grant Number 16H02078 for Scientific Research (A) and 15K13276 for Challenging Exploratory Research. This work was also supported by CREST-JST.

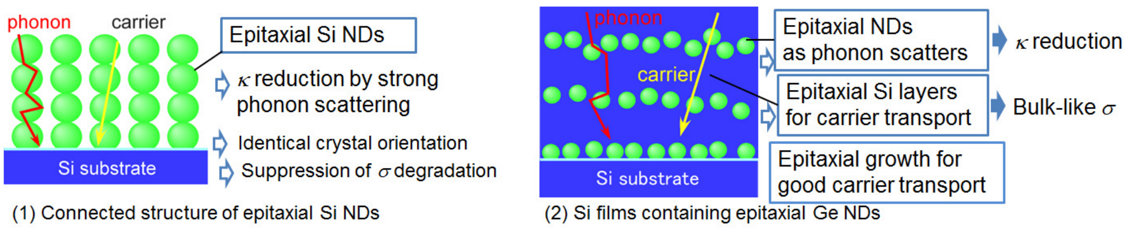

Fig. 1 Schematic of proposed nanostructures. (1) connected structure of epitaxial Si NDs and (2) Si films containing epitaxial Ge NDs.

References

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