Conference materials
UDC 536.2+537.32+539.21
DOI: https://doi.org/10.18721/JPM.173.220

Effect of diameter on lattice thermal conductivity of α-$FeSi_2$ and ε-FeSi nanowires

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Abstract. In this study the effect of α-$FeSi_2$ and ε-FeSi nanowires diameter on the lattice thermal conductivity was considered. *Ab initio* modeling was performed in the temperature range of 100–700 ˚K and nanowires diameter range of 6–48 nm. Results showed that at minimal considered diameter nanowires have 1.4–4.5 times lower lattice thermal conductivity than bulk material depending on temperature and nanowire elongate direction.

Keywords: silicon, Fe silicides, nanowires, *ab initio* calculation, thermal conductivity

Funding: This study was supported by the Russian Science Foundation, grant no. 22-12-00036.

Citation: Balagan S.A., Galkin N.G., Effect of diameter on lattice thermal conductivity of α-$FeSi_2$ and ε-FeSi nanowires, St. Petersburg State Polytechnical University Journal. Physics and Mathematics. 17 (3.2) (2024) 107–111. DOI: https://doi.org/10.18721/JPM.173.220

Материалы конференции
УДК 536.2+537.32+539.21
DOI: https://doi.org/10.18721/JPM.173.220

Влияние диаметра на решеточную теплопроводность нанопроволок α-$FeSi_2$ и ε-FeSi

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Аннотация. В данном исследовании рассмотрено влияние диаметра нанопроволок α-$FeSi_2$ и ε-FeSi на их решеточную теплопроводность. Моделирование из первых принципов производилось в диапазоне температур 100–700 ˚K и диапазоне диаметров нанопроволок 6–48 нм. Результаты показали, что у нанопроволок с минимальным из рассмотренных диаметров теплопроводность 1.4–4.5 раза ниже, чем у объемного материала в зависимости от температуры и направления, в котором вытянута нанопроволока.

Ключевые слова: кремний, силициды Fe, нанопроволоки, первопринципные расчеты, теплопроводность

Финансирование: Исследование поддержано Российским научным фондом, грант № 22-12-00036.

Ссылка при цитировании: Балаган С.А., Галкин Н.Г. Влияние диаметра на решеточную теплопроводность нанопроволок α-$FeSi_2$ и ε-FeSi // Научно-технические ведомости СПбГПУ. Физико-математические науки. 2024. Т. 3.2 № .17. С. 107–111. DOI: https://doi.org/10.18721/JPM.173.220

Introduction

The current technology evolution has resulted in high energy consumption. While it is necessary to increase energy efficiency, it is also important to look for new sources of energy [1]. Using heat released by burning fuel or electrical devices through the use of thermoelectric converters is one method of increasing energy efficiency. Another possible application of thermoelectrics is generating electricity for spacecraft [2]. The Seebeck coefficient, electrical conductivity, and thermal conductivity all affect a material's thermoelectric efficiency. In turn, thermal conductivity also encompasses phonon and electron thermal conductivity. The investigation of the lattice thermal conductivity of ε-FeSi and α-$FeSi_2$ is the main emphasis of this work.

Calculation details

The density-functional theory calculations were performed with the package VASP [3]. Generalized gradient approximation (GGA) to the exchange-correlation functional was used. Non-spherical contributions from the gradient corrections were included. The k-points and q-points grids were used with the center at the Γ-point and the cut-off energy was of 300 eV. Relaxation was performed with respect to the atoms' positions, volume, and the shape of the cell. For structure relaxation k-points grids were of 24×24×12 and 12×12×12 for α-$FeSi_2$ and ε-FeSi, respectively. The resulting lattice parameters was of $a = 2.704$ Å and $c = 5.138$ Å for α-$FeSi_2$ and $a = 4.448$ Å for ε-FeSi, which is in good agreement with the experimental data: $a = 2.684$ Å and $c = 5.128$ Å for α-$FeSi_2$ [4] and $a = 4.467$ Å for ε-FeSi [5]. Forces constants calculations were performed with the k-point grid of 3×3×3 for both materials and supercells were of 4×4×2 and 2×2×2 unit cells for α-$FeSi_2$ and ε-FeSi, respectively. The phonon properties were calculated within the harmonic approximation using Phonopy package [6]. The elements of dynamical matrix were determined by employing density-functional-perturbation theory. Lattice thermal conductivity was calculated by means of Boltzmann transport equation solving implemented in ShengBTE package [7]. Q-points grid was of 32×32×32 for both materials.

Results and Discussion

Phonon bands structures calculation results (Fig. 1) are in good agreement with that of in Refs. [8–9]. The results show that α-$FeSi_2$ has less acoustic phonon frequency value compared to ε-FeSi, which is one of the factors for lower lattice thermal conductivity, since usually the main contribution to lattice thermal conductivity comes from acoustic phonons.

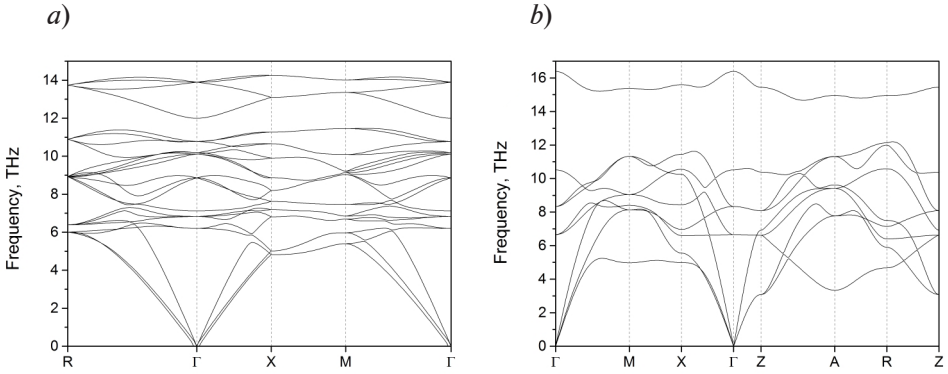

Fig. 1. Phonon band structure of bulk ε-FeSi (*a*) and bulk α-$FeSi_2$ (*b*) along high-symmetry *k*-points

Lattice thermal conductivity calculation show that approximately 80% of the contribution to lattice thermal conductivity comes from acoustic phonons in both materials, which as well means lower thermal conductivity value of α-$FeSi_2$ compared to ε-FeSi (Fig. 2, *a*). In the frequency range corresponding to the acoustic phonons on the one hand α-$FeSi_2$ and ε-FeSi have commensurable phonons group velocity (Fig 2, *b*) and on the other hand α-$FeSi_2$ has an order of magnitude higher scattering rate (Fig. 2, *c*), thereby one has an order of magnitude lower phonons mean free path (Fig. 2, *d*). This is the main reason why α-$FeSi_2$ has lower lattice thermal conductivity compared to ε-FeSi.

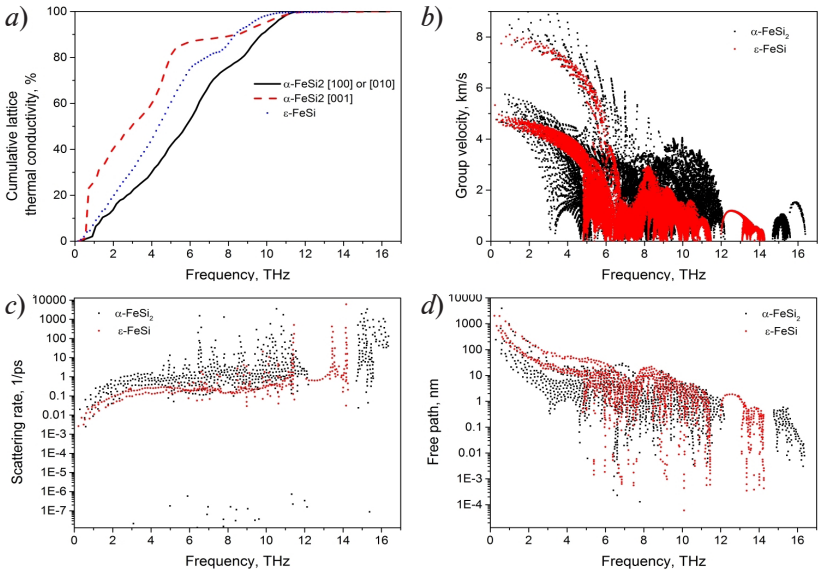

Fig. 2. Phonon transport properties of bulk α-$FeSi_2$ and bulk ε-FeSi: cumulative lattice thermal conductivity (*a*), group velocity (*b*), scattering rate (*c*) and free path (*d*)

Obtained lattice thermal conductivity values are shown in Fig. 3. The values of bulk materials are in agreement with results in Refs. [10–11]. Depending on temperature and heat spread direction bulk α-$FeSi_2$ has 2–4 times lower lattice thermal conductivity compared to that of ε-FeSi.

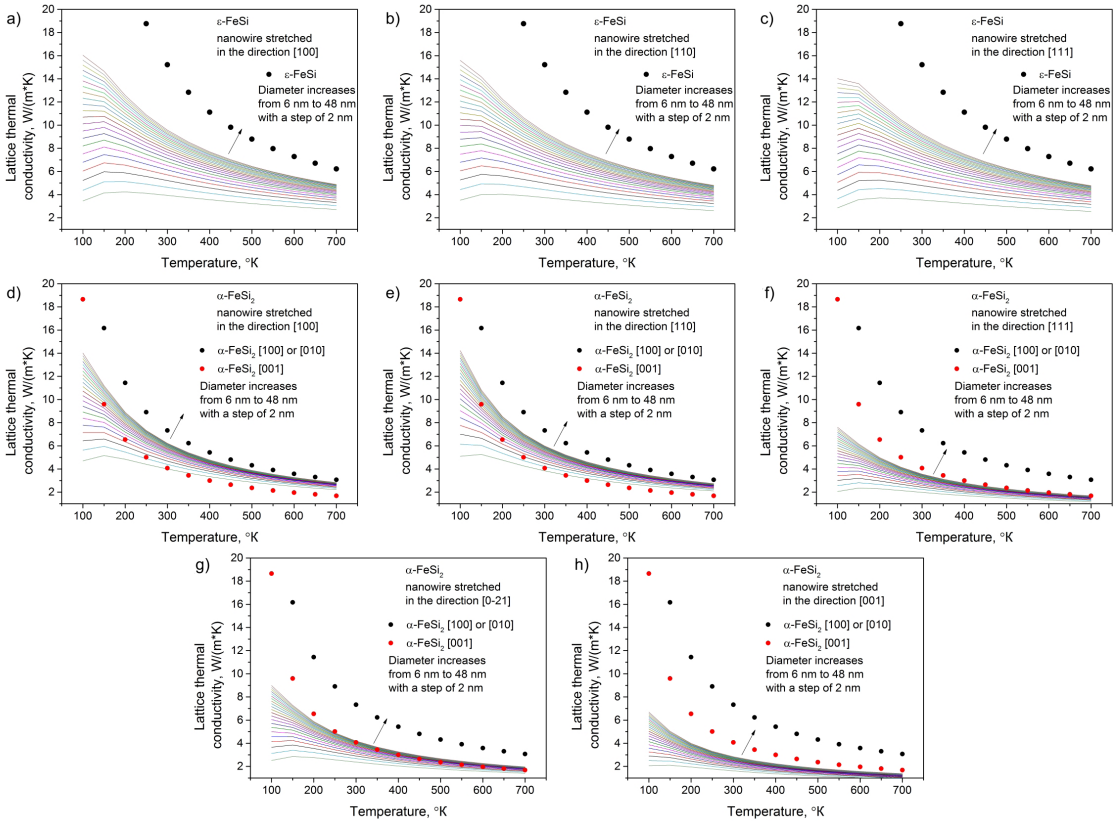

Fig. 3. Lattice thermal conductivity of ε-FeSi nanowires in directions: [100] (*a*), [110] (*b*), [111] (*c*) and that of α-$FeSi_2$: [100] (*d*), [110] (*e*), [111] (*f*), [$0\,\bar{2}\,1$] (*g*) and [001] (*h*). Black and red dots are bulk crystal data

Lattice thermal conductivity calculation of α-$FeSi_2$ nanowires showed significant dependence on the direction in which the nanowire is elongated: 2–2.5 times. The same calculations performed for ε-FeSi showed weak dependence of 1.02–1.20 times. On the other hand ε-FeSi lattice thermal conductivity shows stronger dependence on nanowire diameter compared to the α-$FeSi_2$ one. Depending on temperature ε-FeSi [100] nanowires show 95–56% lower lattice thermal conductivity at 6 nm diameter and 79–22% lower one at 48 nm diameter compared to bulk [100] value. Wherein α-$FeSi_2$ [100] nanowires show 84–28% lower lattice thermal conductivity at 6 nm diameter and 51–8% lower one at 48 nm diameter compared to bulk [100] value. α-$FeSi_2$ [001] nanowires show similar behavior: 89–45% lower lattice thermal conductivity at 6 nm diameter and 64–18% lower one at 48 nm diameter compared to bulk [001] value. It is associated with signification difference in phonons mean free path: α-$FeSi_2$ has lower value and therefore smaller phonons number reach nanowire surface and are scattered on it before scattering occurs inside the wire, similar to scattering in the bulk material. Results of the calculation were applied in Ref. [12].

Conclusion

The effect of α-$FeSi_2$ and ε-FeSi nanowires diameter on the lattice thermal conductivity was considered. Calculations showed strong dependence of α-$FeSi_2$ nanowires lattice thermal conductivity on the direction in which nanowire is elongated and weak one for ε-FeSi nanowires.

Acknowledgments

Boltzmann transport equation solving and quantum mechanics calculations were performed with the use of the computing facilities of IACP FEB RAS Shared Resource Center 'Far Easten Computing Resource' (https://cc.dvo.ru) and HPC cluster 'Academician V.M. Matrosov' (Irkutsk Supercomputer Center of SB RAS, https://hpc.icc.ru/), respectively.

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Received 26.07.2024. Approved after reviewing 06.08.2024. Accepted 08.08.2024.