

TSUBAME 共同利用 平成28年度 学術利用 成果報告書

利用課題名 ナノ構造界面における熱輸送特性の分子シミュレーション  
 英文: Thermal transport properties at nanostructured interfaces

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**邦文抄録** 近年, 材料科学に対する情報科学の応用 (マテリアルズ・インフォマティクス, MI) が試みられており, 材料の開発・設計の加速が期待されている. 本研究では MI を用いたナノ構造の設計を目的に, 原子グリーン関数とベイズ最適化を用いシリコン・ゲルマニウム界面の最適構造を探索した. その結果, 全候補構造数に対し数%の計算回数で最適構造を発見することに成功し, 非周期的な超格子構造により低熱伝導が実現できることを明らかにした. 本結果により, 材料の熱輸送特性制御を目的にしたナノ構造体設計に MI の技術が有効であることが示され, 今後のさらなる発展が期待される.

**英文抄録** Materials informatics (MI) is a new interdisciplinary research to provide efficient tools to accelerate the material discovery and design. In this work, we developed a new MI method combining atomistic Green's function approach and Bayesian optimization, which realizes highly efficient design of nanostructures with optimal thermal transport across Si-Si and Si-Ge interfaces. The optimal structures can be obtained with calculating only a few percent of the entire candidates. The obtained optimal aperiodic superlattice interfacial structures are non-intuitive and impacting. The present work shows the effectiveness and advantage of MI in designing nanostructures to control heat conduction, which can be extended to other structures.

**Keywords:** Boundary thermal transport, Atomic Green's function, Bayesian optimization, Machine learning

## 背景と目的 / Background

Designing nanostructures for phonon transport has been a challenging work due to the multi-freedom of choice (size, shape, material, etc.) as well as coupled effect such as constructive and destructive phonon interference. Informatics, the fourth paradigm of science in addition to theory, simulation, and experiment, is gaining a great attention in the general and interdisciplinary fields of physics as a powerful approach to search for optimal models, structures, and materials. In this research, we are trying to design nanostructures for phonon transport via materials informatics.

## 概要 / Overview

We have developed a new materials informatics

(MI) method combining atomistic Green's function approach and Bayesian optimization that realizes highly efficient design of nanostructures with optimal thermal transport, as shown in Fig. 1.

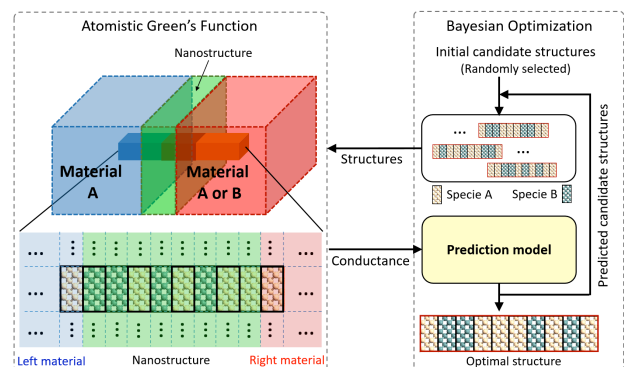


Figure 1: Schematics of the materials informatics method combining Atomistic Green's function (AGF) and Bayesian optimization.

As a case study, we have applied the developed method to design the Si/Ge-composite nanostructures that minimize or maximize interfacial thermal conductance (ITC) across Si-Si and Si-Ge interfaces which are important and realistic for instance in thermoelectrics. We formulate two optimization problems: the first part is optimization of relatively small interfacial region accounting for full degrees of freedom (as shown in Fig. 2) to demonstrate the validity and capability of the current method, and the second part move on to the optimization of larger interfacial region with layered superlattice structures, which is possible to do experiment measurement.

#### 結果および考察 / Results and Discussion

The optimal structures as shown in Fig. 2 (a)-(d) were obtained by calculating only a few percent of the total candidate structures, considerably saving the computational resources. In addition, the obtained structures are non-intuitive and impacting. The validity and capability of the method are demonstrated by identifying the thin interfacial structures with the optimal Si/Ge configurations among all the possible candidates. Based on the finding that the interfacial structures with minimum ITC take a form of aperiodic superlattice, we extended the search to thicker structures (up to 8.69 nm), and identified non-intuitive structures whose ITCs are significantly smaller than those of the optimal periodic superlattices.

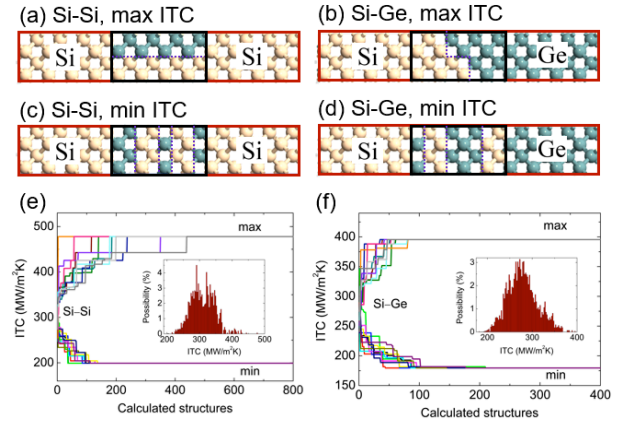


Figure 2: Interfacial Si/Ge alloy structure optimization. (a)-(d) Optimal structures with the maximum and minimum interfacial thermal conductance. (e), (f) The 10 optimization runs with different initial choices of candidates, where the insets show the probability distributions of ITC obtained from calculations of all the candidates.

Another merit of MI lies in possibility to explore new physics in the course of understanding its output. By performing further systematic analyses, we identified that the small thermal conductance in the aperiodic superlattices originates from their degrees of freedom to mutual-adoptively balance the two competing effects (as shown in Fig. 3): as the layer thickness in superlattice increases, the impact of Fabry-Pérot interference increases, and the rate of reflection at the layer-interfaces decreases. Aperiodic superlattice with spatial variation in the layer thickness has a degree of freedom to realize optimal balance between the above two competing mechanism. Furthermore, the spatial variation enables weakening the impact of constructive phonon interference in relative to that of destructive interference.

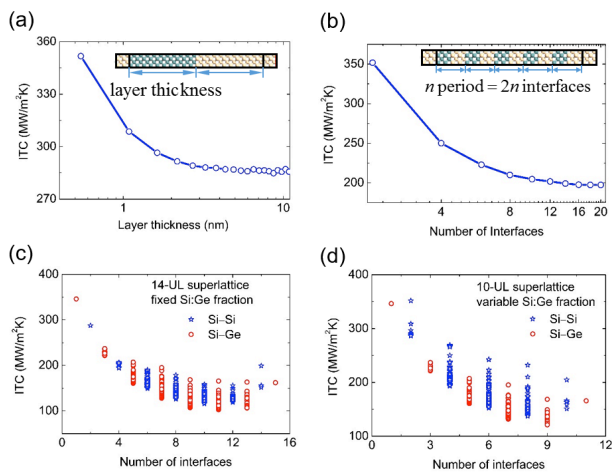


Figure 3: (a), (b) Interfacial thermal conductance versus the layer thickness and number of interfaces. (c), (d) Interfacial thermal conductance versus number of interfaces for cases of 14-unit layer (UL) superlattice with equal Si/Ge layer number and thickness and 10-UL superlattice with variable Si/Ge fraction.

#### まとめ、今後の課題 / Summary and Future Plans

In conclusion, we have developed a framework combining atomistic Green's function and Bayesian optimization to design the nanostructure for phonon transport with high efficiency. The present work shows the effectiveness and advantage of material informatics in designing nanostructures to control heat conduction. We believe that the developed novel method, which can be applied to nanostructure design of any materials in principle, would have a broad and impacting appeal to the general scientific and engineering communities, as well as to the general public. In the following work, we will try to apply informatics method to design more complicated structures in different fields such as thermoelectric, radiation, spintronic devices, etc.

#### References

S. Ju, T. Shiga, L. Feng, Z. Hou, K. Tsuda, J. Shiomi, *Physical Review X* **7**, 021024, 2017.