様　式　Ｃ－１９、Ｆ－１９－１、Ｚ－１９　（共通）

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研究課題名（和文）Thermal resonance induced by quasi-Casimir coupling for innovative nanoscale thermal management

研究課題名（英文）Thermal resonance induced by quasi-Casimir coupling for innovative nanoscale thermal management

研究代表者

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交付決定額（研究期間全体）：（直接経費）　　2,200,000円

研究成果の概要（和文）：真空中におけるナノギャップ間の熱輸送キャリアはフォノンである。界面層間の熱共振現象でナノギャップを介したフォノン輸送が促進されることを明らかになったが、吸着液体層や二原子分子層間における熱輸送のメカニズムは解明されていない。本研究では、非平衡分子動力学解析より、吸着液体層を有するナノギャップ、および異なる原子表面終端を持つSiC-SiCナノギャップを研究対象として、ナノギャップを横切るフォノン熱流束を調べました。その結果、固体表面に吸着した液体層間、または同一の原子終端を持つ界面層間に顕著な熱共振現象の発生によって、ナノギャップを介したフォノン熱輸送が促進されたことを明らかにした。

研究成果の学術的意義や社会的意義
This study provides a deeper understanding of phonon transmission across a nanogap in extreme near-field heat transfer, which is crucial for advancing thermal management systems. Enhanced thermal management strategies could realizing the energy-efficient devices with reduced energy consumption.

研究成果の概要（英文）：In vacuum, the gap distance is a key factor since phonon transmission dominates the heat exchange between two objects. Interfacial thermal resonance induced by quasi-Casimir coupling plays a critical role in facilitating extreme near-field heat transfer across a nanogap. However, the understanding of quasi-Casimir coupling between adsorbed liquid layers or diatomic molecular layers remains unclear. In this study, phonon heat transfer across a nanogap via adsorbed liquid layers and SiC-SiC nanogap with four kinds of atomic surface terminations were investigated. Our findings demonstrate that the thermal resonance exists between two adsorbed liquid layers or identical atomic terminated layers, resulting in the enhanced phonon transmission across the nanogap.

研究分野：熱工学

キーワード：準カシミヤカプリング　ナノギャップ　フォノン熱輸送　熱共振　分子動力学解析

１．研究開始当初の背景

In near-field heat transfer within a vacuum, the gap distance plays a critical role since phonon transmission dominates the heat exchange between two objects. The amount of heat transfer can be several orders of magnitude greater than Planck's blackbody limit when two objects are separated by a gap distance smaller than Wien's wavelength.[1] Experimentally, Casimir heat transfer between two Si_3N_4 membranes has been attributed to quantum fluctuations of electromagnetic fields.[2] Moreover, we proposed a new heat transfer mode to describe phonon transmission induced by quasi-Casimir coupling across a vacuum gap without electromagnetic fields.

２．研究の目的

(1) To investigate the effects of atomic surface terminations on phonon transmission across a nanogap between two SiC solid walls for achieving the enhanced extreme near-field heat transfer.

(2) To examine the phonon heat transfer across a nanogap via the liquid layers adsorbed on both the cooling and heating surfaces for verifying the possible quasi-Casimir coupling or thermal resonance.

３．研究の方法

Molecular dynamics simulations were performed to investigate thermal energy transport in various systems, utilizing a high-performance parallel computer on the supercomputing system of the Research Institute for Information Technology at Kyushu University and SQUID at the Cybermedia Center of Osaka University. The SiC–SiC system with nanogap (Fig. 1(a)) and the platinum–argon system with superhydrophilic surface (Fig. 1(b)) were simulated using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). Non-equilibrium molecular dynamics (NEMD) simulations were performed under various temperature difference between heating and cooling thermostats. The atomic vibrational displacements and vibrational density of states were analyzed to verify the existence of thermal resonance between interfacial layers. The spectral thermal conductance of interfacial layers was calculated to clarify the mechanism of enhanced phonon heat transfer across the nanogap.

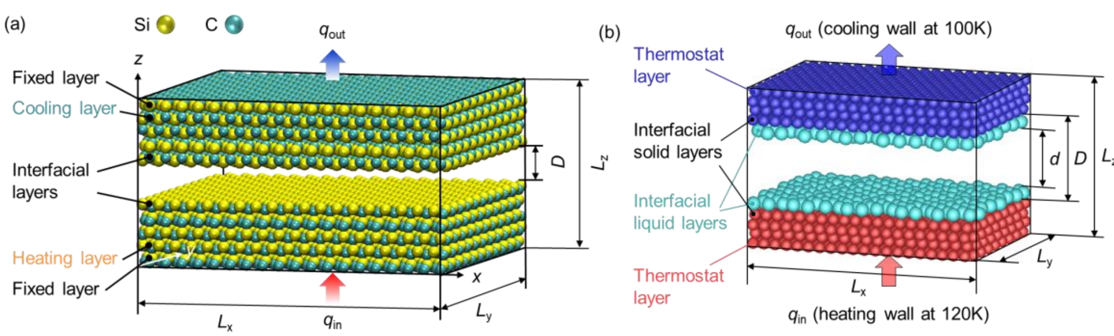

Fig. 1 NEMD simulation systems of (a) two separated SiC solid walls with a constant gap distance and (b) argon liquid layers adsorbed on platinum surface.

４．研究成果

(1) Interfacial thermal resonance in an SiC–SiC nanogap[4–9]

Phonon heat transfer across SiC–SiC nanogap with four kinds of atomic surface terminations was investigated by NEMD simulations, as shown in Fig. 1(a). The net heat flux across the nanogap in the cases of identical atomic surface terminations were remarkably larger than those in the nonidentical cases, as illustrated in Fig. 2. Thermal resonance occurs between identical atomic terminated layers, whereas it vanishes between nonidentical ones (Fig. 3). Moreover, Fig. 4 shows that the spectral thermal conductance of the nonidentical cases is

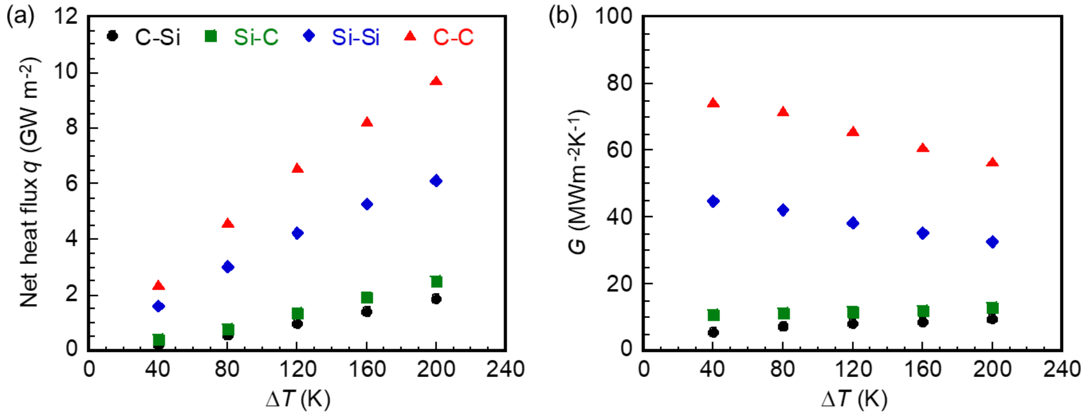

Fig. 2 Effects of temperature difference ΔT on net heat flux and thermal gap conductance.

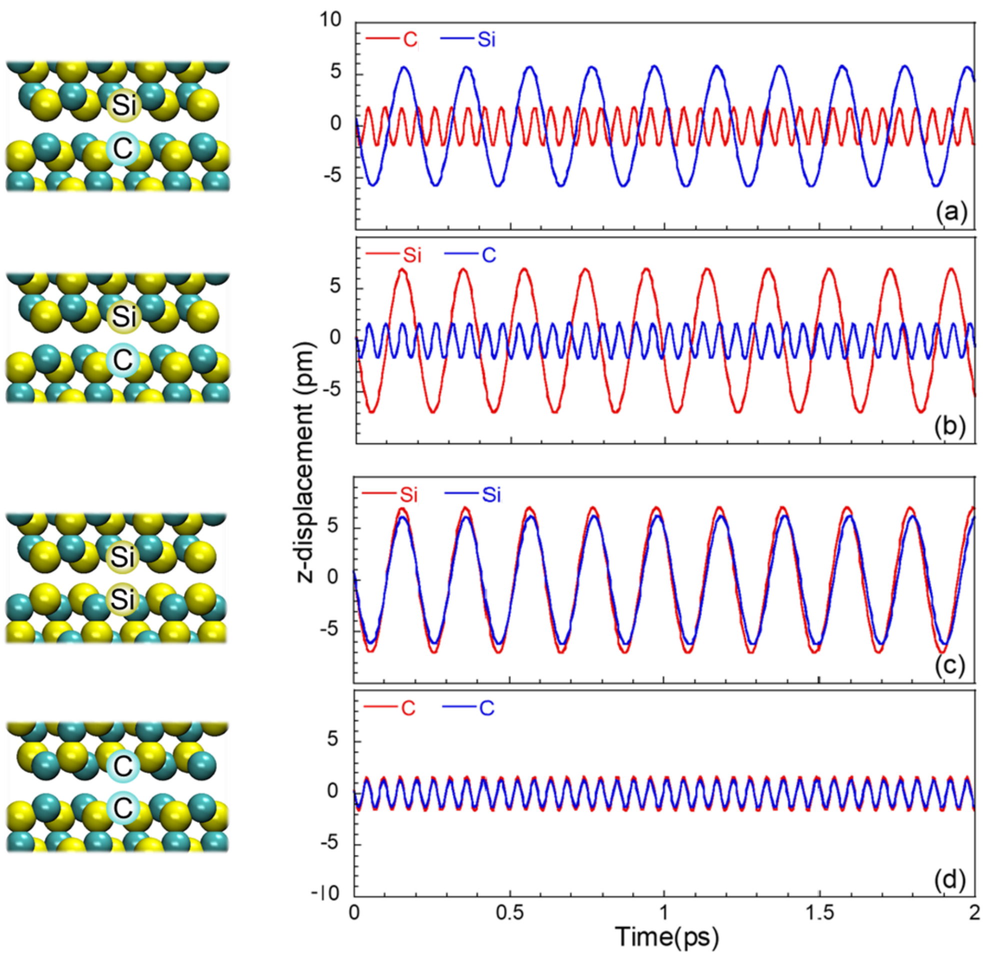

Fig. 3 Vibrational displacements of (a and b) nonidentical atomic surface terminations and (c and d) identical atomic surface terminations in the heating and cooling interfacial layers.

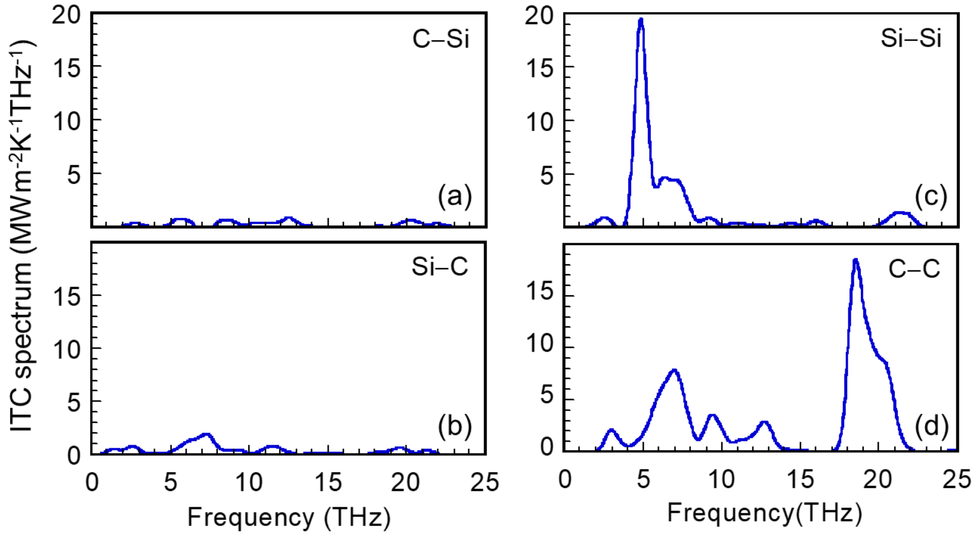

Fig. 4 Spectral thermal conductance in the cases with various atomic surface terminations of (a) C–Si, (b) Si–C, (c) Si–Si, and (d) C–C.

much lower than that of the identical cases, owing to the phonon mismatch between the heating and cooling interfacial layers in the nonidentical cases. A notable heat transfer enhancement in the identical case of C–C is due to optical phonon transmission, with interfacial thermal resonance between the C-terminated layers.

(2) Phonon heat transfer across a nanogap via adsorbed liquid layers[10–13]

NEMD simulations were carried out to verify the possible quasi-Casimir coupling or thermal resonance at solid–liquid interface in a nanogap, as shown in Fig. 1(b). The liquid monolayer adsorbed on the heating/cooling surface and two liquid layers adsorbed over both heating and cooling surfaces were focused on to clarify the effects of the liquid layers on phonon transmission across a nanogap. The existence of quasi-Casimir coupling at the solid–liquid

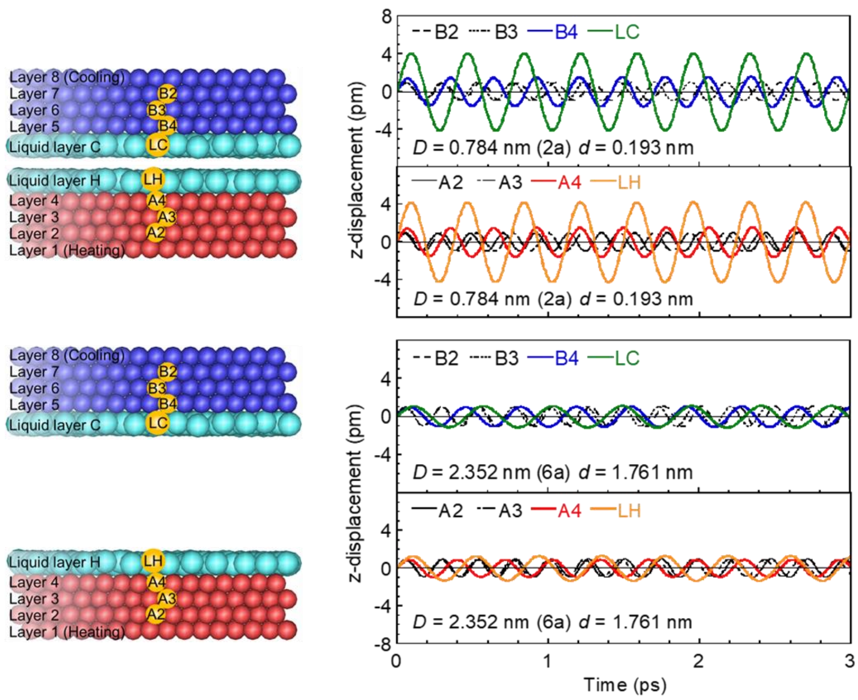

Fig. 5 Atomic vibrational displacements of specific atoms at interfacial solid layers and liquid layers adsorbed on the solid surfaces with various gap distance.

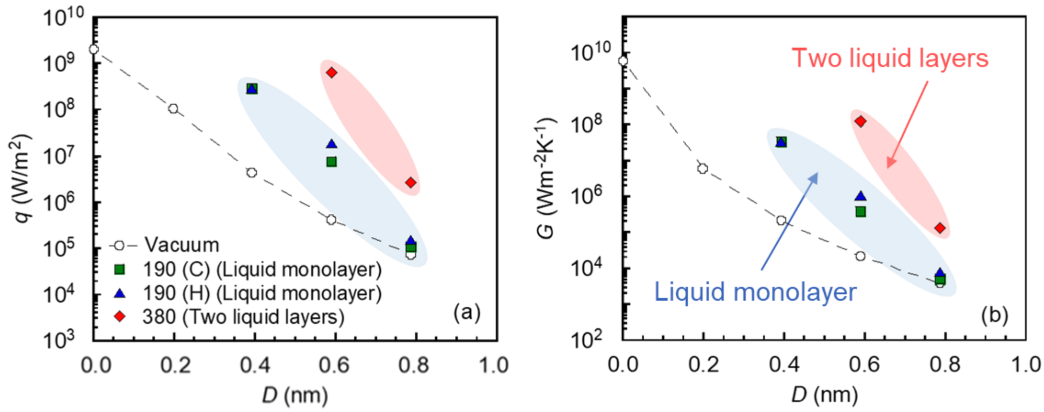

Fig. 6 (a) Heat flux and (b) thermal gap conductance versus gap distance *D* between the interfacial solid layers.

interface, between solid–liquid and liquid–liquid layers, was verified through modulating the gap distance to achieve the various molecular interactions (Fig. 5). The thermal resonance between two liquid layers can be induced by quasi-Casimir coupling, agitating the co-occurrence of thermal resonance between the interfacial solid layers. Figure 6 shows that the heat flux and thermal gap conductance are enhanced by thermal resonance between the two liquid layers compared with the case of vacuum gap and liquid monolayer.

＜引用文献＞

(1) A.I. Volokitin, *J. Phys. Condens. Matter*, 32, 215001, 2020.

(2) K.Y. Fong, H.-.K. Li, R. Zhao, S. Yang, Y. Wang, X. Zhang, *Nature*, 576, 243–247, 2019.

(3) W. Chen, G. Nagayama, *Proceedings of 14th International Conference on Computational Heat and Mass transfer*, No. 176, 2023.

(4) X. Li, W. Chen, G. Nagayama, *Proceedings of 14th International Conference on Computational Heat and Mass transfer*, No. 180, 2023.

(5) X. Li, W. Chen, G. Nagayama, *Proceedings of Thermal Engineering Conference 2023*, No. D114, 2023.

(6) X. Li, W. Chen, G. Nagayama, *Nanoscale*, 15, 8603–8610, 2023.

(7) X. Li, W. Chen, G. Nagayama, International Joint Seminar on Mechanical Engineering 2022, No. O323, 2022.

(8) X. Li, W. Chen, G. Nagayama, *Proceedings of Thermal Engineering Conference 2022*, No. A132, 1–5, 2022.

(9) X. Li, W. Chen, G. Nagayama, *Proceedings of 10th International Symposium on Applied Engineering and Sciences*, No. B21, 2022.

(10) W. Chen, G. Nagayama, *Proceedings of Thermal Engineering Conference 2022*, No. A131, 1–5, 2022.

(11) W. Chen, G. Nagayama, *Physical Chemistry Chemical Physics*, 24, 11758–11769, 2022.

(12) W. Chen, X. Li, G. Nagayama, International Joint Seminar on Mechanical Engineering 2022, No. I31, 2022.

(13) W. Chen, G. Nagayama, *Proceedings of 10th International Symposium on Applied Engineering and Sciences*, No. B20, 2022.

５．主な発表論文等

〔雑誌論文〕　計4件（うち査読付論文　2件／うち国際共著　0件／うちオープンアクセス　3件）

１．著者名 Chen Wentao、Nagayama Gyoko	４．巻 24
２．論文標題 Quasi-Casimir coupling can induce thermal resonance of adsorbed liquid layers in a nanogap	５．発行年 2022年
３．雑誌名 Physical Chemistry Chemical Physics	６．最初と最後の頁 11758～11769
掲載論文のDOI（デジタルオブジェクト識別子） 10.1039/D2CP01094A	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 －

１．著者名 Xiangrui Li, Wentao Chen, Gyoko Nagayama	４．巻 17
２．論文標題 Interfacial thermal resonance in an SiC－SiC nanogap with various atomic surface terminations	５．発行年 2023年
３．雑誌名 Nanoscale	６．最初と最後の頁 -
掲載論文のDOI（デジタルオブジェクト識別子） 10.1039/D3NR00533J	査読の有無 有
オープンアクセス オープンアクセスとしている（また、その予定である）	国際共著 －

１．著者名 Wentao Chen, Gyoko Nagayama	４．巻 1
２．論文標題 Interfacial thermal resonance between adsorbed liquid layers in a nanogap	５．発行年 2022年
３．雑誌名 Proceedings of Thermal Engineering Conference	６．最初と最後の頁 1-5
掲載論文のDOI（デジタルオブジェクト識別子） なし	査読の有無 無
オープンアクセス オープンアクセスとしている（また、その予定である）	国際共著 －

１．著者名 Xiangrui Li, Wentao Chen, Gyoko Nagayama	４．巻 1
２．論文標題 Effect of atomic surface termination on heat transfer across SiC－SiC nanogap	５．発行年 2022年
３．雑誌名 Proceedings of Thermal Engineering Conference	６．最初と最後の頁 1-5
掲載論文のDOI（デジタルオブジェクト識別子） なし	査読の有無 無
オープンアクセス オープンアクセスとしている（また、その予定である）	国際共著 －

〔学会発表〕　計9件（うち招待講演　1件／うち国際学会　4件）

1．発表者名 Wentao Chen
2．発表標題 Local Heat Flux of Resonant Layers at Solid-liquid Interface
3．学会等名 14th International Conference on Computational Heat and Mass transfer（国際学会）
4．発表年 2023年

1．発表者名 Xiangrui Li
2．発表標題 Spectral Analysis of Phonon Transport across an SiC-SiC Nanogap
3．学会等名 14th International Conference on Computational Heat and Mass transfer（国際学会）
4．発表年 2023年

1．発表者名 Xiangrui Li
2．発表標題 Effect of Electric Field on Phonon Heat Transfer Across an SiC-SiC Nanogap
3．学会等名 熱工学コンファレンス2023
4．発表年 2023年

1．発表者名 Xiangrui Li
2．発表標題 Effect of atomic surface termination on heat transfer across SiC－SiC nanogap
3．学会等名 熱工学コンファレンス 2022
4．発表年 2022年

１．発表者名 Wentao Chen
２．発表標題 Interfacial thermal resonance between adsorbed liquid layers in a nanogap
３．学会等名 熱工学コンファレンス 2022
４．発表年 2022年

１．発表者名 Wentao Chen
２．発表標題 Phonon Heat Transfer Induced by Quasi-Casimir Coupling in a Nanogap
３．学会等名 International Joint Seminar on Mechanical Engineering 2022（招待講演）
４．発表年 2022年

１．発表者名 Xiangrui Li
２．発表標題 Non-equilibrium Molecular Dynamics Simulation on Heat Transfer across SiC－SiC Nanogap
３．学会等名 International Joint Seminar on Mechanical Engineering 2022
４．発表年 2022年

１．発表者名 Xiangrui Li
２．発表標題 Dependence of Phonon Heat Transfer across a Vacuum Nanogap on Atomic Surface Terminations
３．学会等名 10th International Symposium on Applied Engineering and Sciences（国際学会）
４．発表年 2022年

１．発表者名 Wentao Chen
２．発表標題 Enhanced Heat Transfer across a Nanogap by Thermal Resonance between Adsorbed Liquid Layers
３．学会等名 10th International Symposium on Applied Engineering and Sciences（国際学会）
４．発表年 2022年

〔図書〕　計0件

〔産業財産権〕

〔その他〕

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６．研究組織

	氏名 （ローマ字氏名） （研究者番号）	所属研究機関・部局・職 （機関番号）	備考

７．科研費を使用して開催した国際研究集会

〔国際研究集会〕　計0件

８．本研究に関連して実施した国際共同研究の実施状況

共同研究相手国	相手方研究機関