

Large-scale Simulation for a Terahertz Resonance Superconductor Device

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This study is aiming at designing by large-scale simulations a new nano-scale devices of high temperature superconductor (HTC) that would emit the terahertz wave continuously, for the purpose of developing a new application fields of terahertz waves that have been abandoned so far as the untapped frequency range between photon and radio waves. As a new light source, the continuous and frequency tunable terahertz wave, especially in the range of 1-4 THz, would be applicable to the advanced research fields of material science, bioscience, medical and information technology. Our challenge is set to develop the device to generate the terahertz wave using high temperature superconductor. The mechanism of generating the continuous terahertz waves, its optimum conditions and the frequency control have been revealed so far through the large scale simulation that run on the Earth Simulator with vast computing power.

One of challenges we are tackling is to design a wave guide that lead the terahertz waves generated out of the device to the object for flexible irradiation. In the wave guide the terahertz wave propagates dynamically with varying wavelengths from nanometer to millimeters. Thus, for searching the optimum conditions of design, it is required to perform large and multi-scale simulation on the nonlinear dynamics of terahertz in the three dimensional space of the device and wave guide. In this term, we have developed a two dimensional simulation model for designing the way of emitting the terahertz waves as Josephson plasma out of the device to the outer-space.

Keywords: high-temperature-superconductor, device, generating terahertz waves, stable excitation, Josephson plasma, high performance computational resource, wave guide.

1. Introduction

Terahertz wave has been untapped as electromagnetic wave in the frequency range from 0.3 to 10THz. The range is overlapping the resonance frequencies of the molecules and the low-energy collective and elementary excitations such as carrier scattering, recombination, and transporting etc in substances. Thus, terahertz wave has some potential for being applied to the advanced research field of science and technology such as spectroscopic analyses on dense or soft materials and bio-molecules, medical diagnoses and information technology. Especially, the continuous, tunable and intense terahertz waves in the range of 1-4 THz are valuable for applications. But, it would be hard to generate the continuous, tunable and intense terahertz wave with 1-4THz, by conventional method such as quantum cascade laser and photo mixing.

It is therefore our challenge to develop a new device of generating the continuous and frequency-tunable terahertz waves in 1-4 THz for the realization of a new terahertz light source. Therefore, until last year, we have revealed the

mechanism and optimum condition of generating terahertz waves with new device of the high temperature superconductor, proposed in 1994 in Japan, by use of large-scale simulation with huge power of Earth Simulator.

The challenge for realization of the device generating terahertz waves of high temperature superconductor is the development of wave guide method that guides the terahertz waves from device inside to objects.

Themes are as follows as shown in Fig. 1;

- (a) Design of the connection from the inside of device to outer space: configuration, size and material of device, electrode, current source and wave guide for realizing the efficient emission of Josephson plasma without loss of power.
- (b) Design of the wave guide from the surface of device to targets: configuration, dimension and material of wave guide for realizing the efficient propagation of terahertz waves without reflection, decay of power.

It is indispensable to perform the optimum design of the

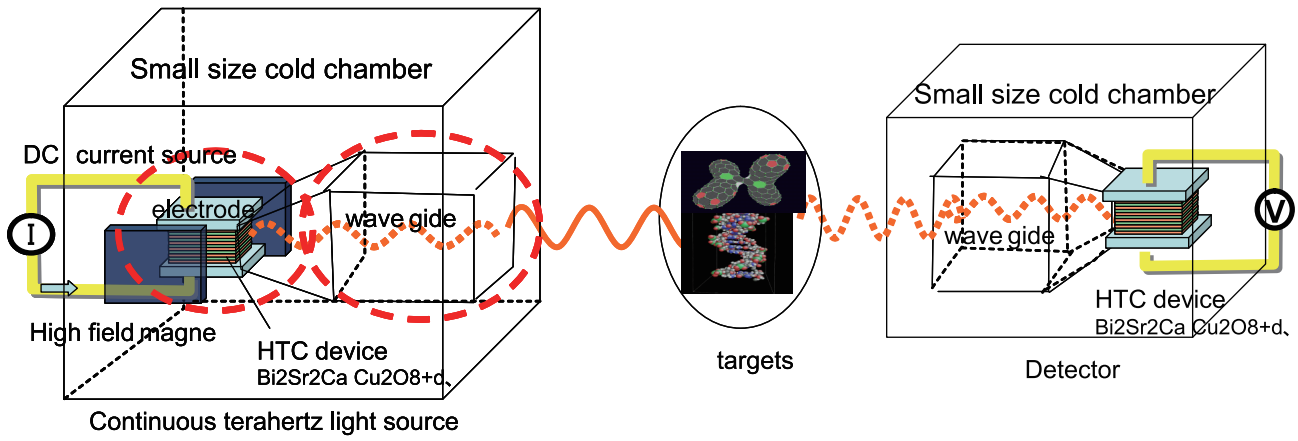


Fig. 1 Schematic diagram of measurement equipment using HTC device and the challenge of development of light source.

terahertz device by large-scale simulation of nonlinear dynamics of terahertz waves in the scale from nano-meter to milii-meter on the HTC device and wave guide system.

Until last year, we performed the basic study by focusing the Josephson plasma excitation inside the device and using quasi 2-dimensional mode of Josephson plasma dynamics for the development of new terahertz light source with HTC device. Hereafter, it is needed to perform the design of the optimum structure of connection between inside and outside of the HTC device and wave guide system from surface of device to targets in this study. Terahertz wave interact with 3-dimensional structure of hetero materials, emit and propagate the space. Therefore, (a) quasi 2-dimensional model must be extended to multi-dimensional model, (b) parallel model of coupling inside and outside of the HTC device must be developed to accurately and efficiently connect the inside and outside of the HTC device and (c) high performance tuning of that simulation code is needed to overcome the increase of calculation volume by multi-dimensional analysis.

In this year, we developed the large-scale 2D simulation model for deign of the method that enables the Josephson plasma to effectively emit as the terahertz waves from inside

of HTC device to outer-space for realization of continuous frequency tunable terahertz source using THC device. And we carried out a simulation of validation calculation.

2. Multi-dimensional model of generation of terahertz waves

2.1 Extension of quasi 2-dimensional model to multi-dimensional mode

Josphson plasma excites when it resonates with the array of fluxons and the most intense vibration of superconducting currents appears in parallel to layers (x-axis) and along layers (z-axis) near the surface of the device. These vibrating current fields on the surface of the device induce the terahertz wave in the outside of the device and then, the terahertz wave propagates to the space.

We have carried out so far the basic study on the HTC device by using a quasi 2-dimensional model neglecting the electric field parallel to the layers, because the electric field is induced by superconducting currents along to the layers (z-axis) generating intense terahertz waves. However, it is required that the vibration of superconducting currents is correctly analyzed on the layers (x-axis) and along layers (z-axis) for simulating the

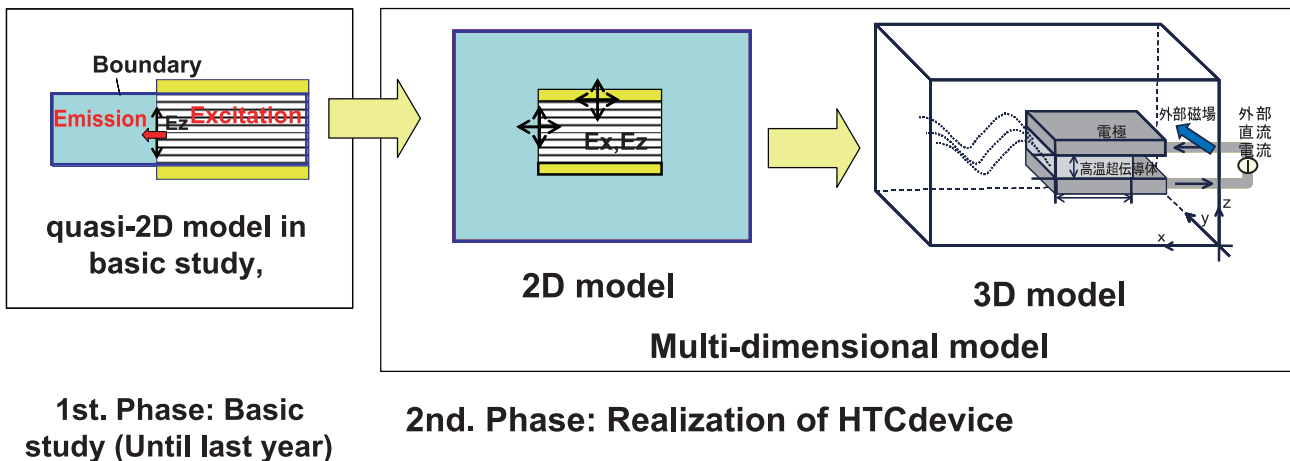


Fig. 2 Development of multi dimensional model

emission of the terahertz waves with a high degree of accuracy. Thus, in this term, the accurate 2-dimensional model of the generation of terahertz waves has been developed by taking the electric field parallel to the layers into consideration, as shown in Fig. 2.

2.2 Parallel model of coupling inside and outside of the HTC device

In this simulation, the equation of intrinsic Josephson plasma and Maxwell's equation of outer-space are solved inside and outside of the HTC device respectively, and the couple of equations are connected at the surface of the device for simulating the terahertz wave generation. The electromagnetic fields of inside /outside of the device are connected through solving the electric-field inside and the magnetic-field outside on the mesh shifted in half mesh as shown in Fig. 3.

Parallel coupling between inside and outside of the HTC device is carried out by partitioning two region each with good load-balance, and combining the electromagnetic field on the surface of the device by communicating between the inside of electric field and the outside of magnetic field. Communication table between IJJ and outer-space domain is automatically generated by the technique of DDM of unstructured grid as shown in Fig. 4.

3. Simulation

A simple simulation was carried out for validation of model as following; the simulation model is shown in Fig. 5.

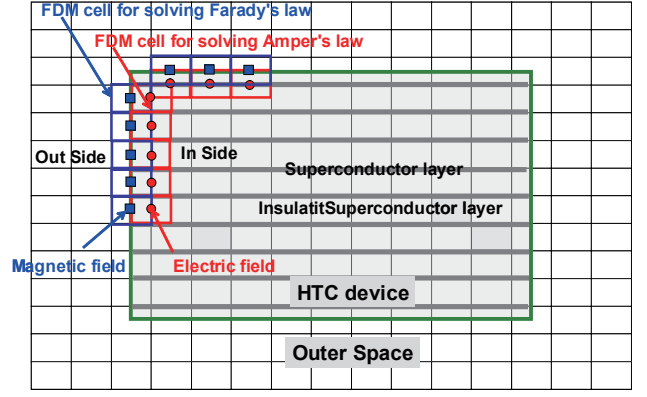


Fig. 3 Computational model of coupling the magnetic field with electric field on the surface of device on FDM cell.

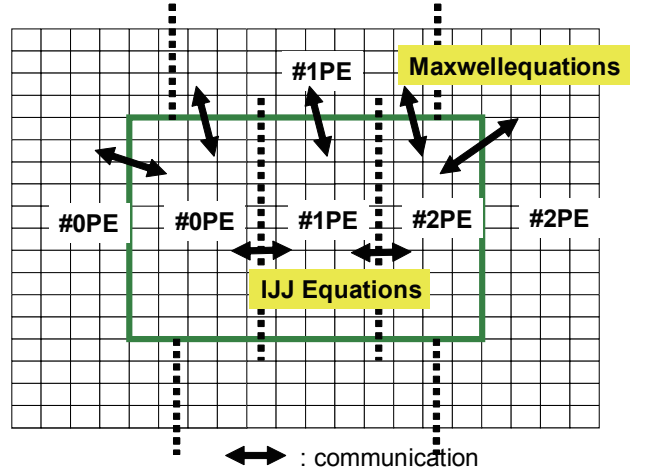


Fig. 4 Parallel model of coupling electromagnetic files inside and outside of the HTC device.

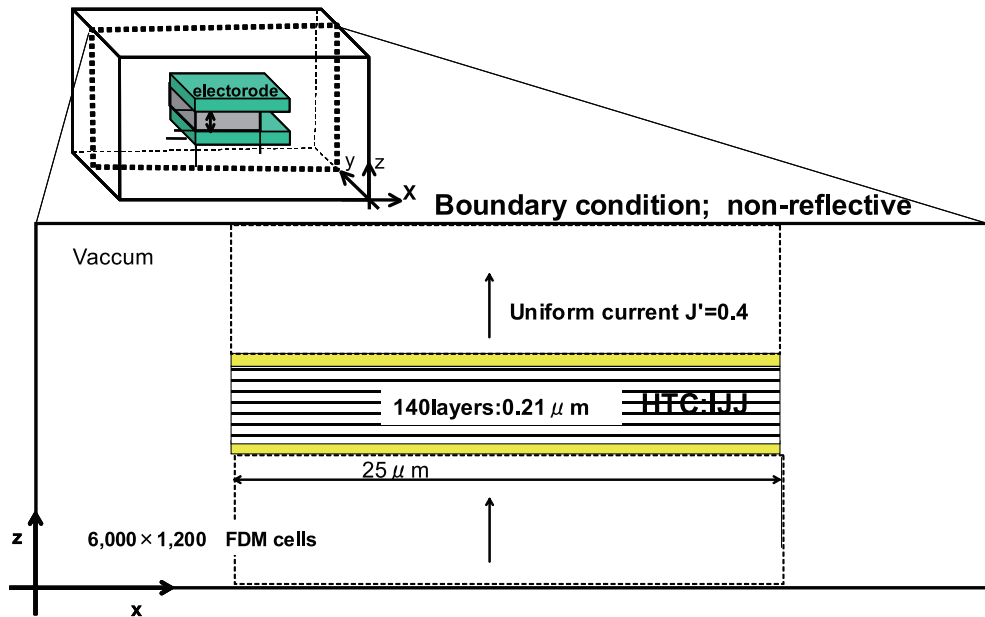


Fig. 5 Schematic diagram of the device generating terahertz waves. $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ forms IJJ. The device consists of HTC crystal and electrodes. The green part shows the IJJ sandwiched by electrodes. An external current flows uniformly in the junctions in the direction of the z axis. An external magnetic field is applied to y-direction.

We performed simulations with parameters: (a) Num. of layre:140, (b) Device length :25 μm , (c) Magnetic field penetration depth from the bc and ab surface plane: λ_c, λ_{ab} :150 μm , 0.212 μm , (d) Reduced quasi-particle conductivity along c-axis β : 0.02, (e) External magnetic field: B_y : 0.5T, External DC: $J=0.4$.

Simulation results are shown in Fig. 6 and Fig. 7. Emission of THz waves starts as Josephson plasma starts excitation and the intensity of emission increases as Josephson plasma increases excitation, as shown in Fig.6. Terahertz wave diffuses immediately after the emission from the edge of the device.

The simulation study with the two-dimensional model

has just started. It will be continued toward 3D simulation.

4. Conclusion and future work

In this term, the large-scale 2D simulation model has developed for deigning the effective emission of the Josephson plasma as the terahertz waves from the inside to the outside of HTC device. And validation has been carried out on the simulation models.

In the next phase, we will developed the large-scale 3D simulation model for deigning a terahertz light source that effectively guide the irradiation of terahertz waves from the inside of the HTC device to the object placed in the outer-

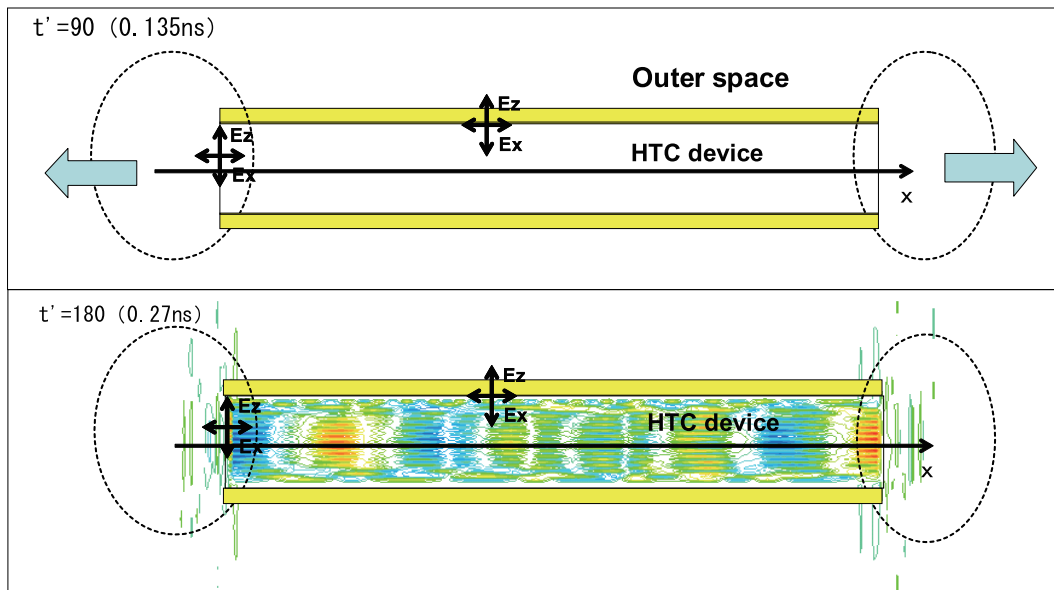


Fig. 6 Contour of Ez'/dt , that is oscillating part of Ez' . Ez' is electric field component propagating to x direction. Time is at 0.135ns and 0.2ns.

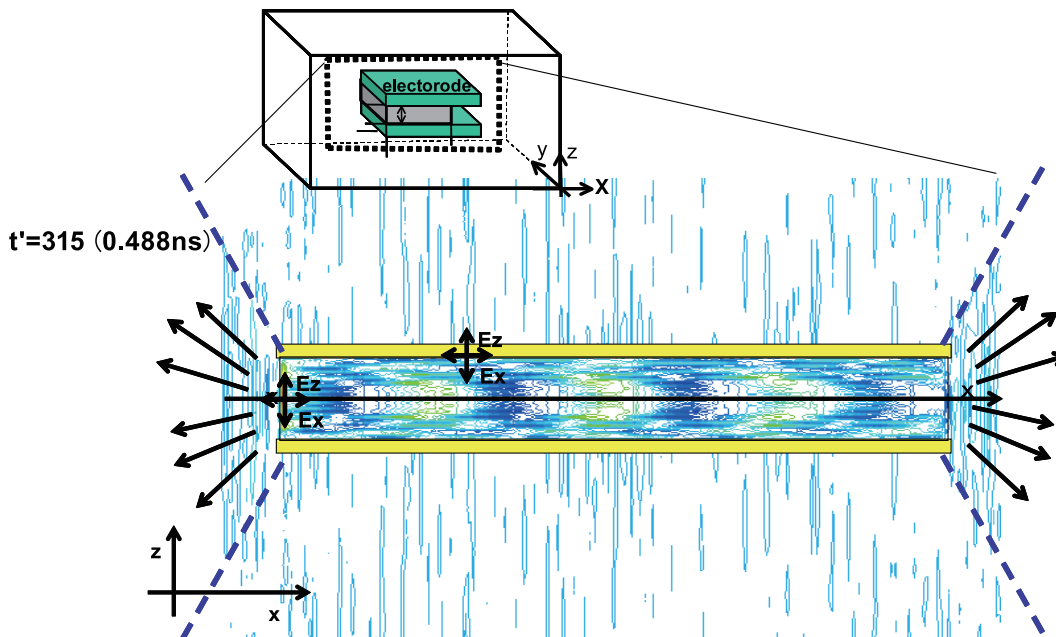


Fig. 7 Contour of Ez'/dt , that is oscillating part of Ez' . Time is at 0.488ns.

space and wave-guide.

The Earth Simulator shows clearly that the large-scale simulation with high performances is an effective methodology for developing new technologies.

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テラヘルツ発振超伝導素子に関する大規模シミュレーション

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本研究は、電波と光の間の未利用周波数帯域であるテラヘルツ波応用の開拓を目指し、連続波としてテラヘルツ波を発振する高温超伝導素子及びその利用システムを大規模シミュレーションにより設計するものである。

テラヘルツ波は光と電磁波の中間域（0.3 ～ 10THz）の未開拓領域にあり、物質、生体分子の励起振動数（～ 6THz）を含むことから、物性、癌細胞分子の分光分析、細菌・プラスチック爆発物の検出、X線よりも低エネルギーで透過性があるため安全な医療線源、また大容量通信等へ応用が期待される。特に、1 ～ 4THzでの周波数可変で高出力の連続波光源が無いことから、テラヘルツ波の実用化においては、この帯域の連続波の光源開発が課題となっている。そのため、昨年度まで、1994年に日本にて提案された高温超伝導体を使うテラヘルツ生成素子の開発を目的に、連続波テラヘルツ波を発振させる原理、その最適発振条件、さらに周波数制御法を地球シミュレータの計算力を生かした大規模シミュレーションから世界で始めて明らかにした。

さらに、実用化へ向けた克服すべき課題として、素子内で励起されたジョセフソンプラズマをテラヘルツ波として対象物に自在に照射するための導波技術がある。そこでは、素子及び導波システムにおけるナノからミリスケールまでのテラヘルツ波の非線形挙動を3次元空間で扱う大規模マルチスケールシミュレーションで明らかにし、最適設計条件を求めることが必須となる。そのため、今年度は、高温超伝導素子を使った周波数可変の高出力連続波のテラヘルツ光源の実用化へ向けて、素子内部発生ジョセフソンプラズマの外部への効率的放射法を設計するための2次元の大規模シミュレーションモデルを開発した。そしてその検証計算を実施した。これにより、素子端面からのテラヘルツ波放射の詳細な解析が可能となり、テラヘルツ波の反射、減衰を生じない素子と外部空間との接続法の設計が可能となった。また、3Dシミュレーションモデル（外部空間）の準備もできた。

今後は、3次元連続波テラヘルツ波の反射、減衰を考慮した素子・導波管系の大規模シミュレーションを行ない、連続波テラヘルツ波応用の基本となるシステム概要、その設計条件を定量的に明らかにする。また、これらの計算規模はペタスケールであり、そのためのモデル拡張、並列性能向上、演算性能向上へ向けた階層メモリ利用法向上、そのためのアルゴリズムの高度化等を含めた大規模モデルの研究開発も進めていく予定である。本研究は大容量情報伝送やエネルギー伝送の利用研究としての側面も持つことから米、独、中、韓等でも類する研究が盛んに行われており、厳しい競争状況にある。このため、本研究から得られる設計情報は、わが国の学界・産業界に優先的に提示し、日本独自の新しい産業技術の勃興に資する。

キーワード：テラヘルツ発振素子, 超伝導体, 大規模シミュレーション