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 teraherz waves that have been abandoned so far as the untapped frequency range between photon and radio waves. HTC naturally forms intrinsic Josephson junction (IJJ). So we call the device IJJ device. A new light source of the continuous and frequency 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 generating the terahertz wave using IJJ device. The mechanism of generating the continuous frequency tunable 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 method that flexibly leads the terahertz waves from inside of the device to the object being irradiated. In the wave guide the terahertz wave propagates dynamically with varying its wavelengths from nanometer to millimeters. Thus, for searching the optimum conditions of the design, it is required to perform large and multi-scale simulation on the nonlinear dynamics of terahertz wave in the three dimensional space of the device and wave guide.

Last year we made an assumption that the terahertz waves emit effectively if the ratio of the outside dielectric constant to the inside effective one of IJJ device increases. The effective dielectric constant of the inside of IJJ device can be controlled by the number of layers of IJJ. Therefore we have studied this year the effect of the ratio on the emission of terahertz waves by controlling the number of layers of IJJ.

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 electromagnetic wave, in the frequency range from 0.3 to 10 THz. The range is overlapping the resonance frequencies of molecules and the low-energy collective and elementary excitations such as carrier scatting, 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 tunable, continuous 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 1-4 THz, by conventional methods such as quantum cascade laser and photo mixing.

Our challenges are to develop a new device of generating the continuous and frequency-tunable terahertz waves in 1-4 THz as a first stage, and to realize a terahertz light source finally. Therefore, until 2009, we had revealed the mechanism and optimum conditions of generating terahertz wave with the new device of IJJ, by using large-scale simulation with huge power of the Earth Simulator [1, 2, 3, 4].

As a next step of our challenges, it was required to develop the wave guide that leads the terahertz waves to the objects being investigated. Thus, themes to be cleared are as follows as shown in Fig. 1: (a) Design of the optimum connection from the inside to outer space of device: configuration, size and material of device, electrode and current, etc. for realizing the efficient emission of Josephson plasma with less loss of power. (b) Design of the wave guide from space around the device to the targets: configuration, dimension and material of wave guide for realizing the efficient propagation of THz waves with less
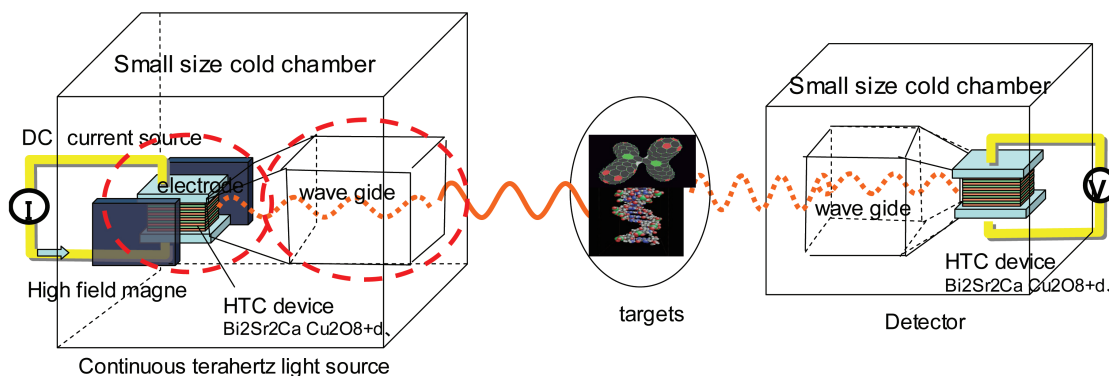
Fig. 1 Schematic diagram of measurement equipment using IJJ device.

reflection, less decay of power.

Until FY 2009, we had conducted the basic studies, focusing on the Josephson plasma excitation inside the device and using quasi two-dimensional model of Josephson plasma dynamics. Hereafter, it was made clear that it is required for us to design the optimum structure of connection or boundary among inside and outside of the IJJ device and wave guide system.

Terahertz wave emits and propagates through three-dimensional configuration of device and guide with hetero materials. Therefore, more accurate modeling efforts are requited as follows; (a) to develop accurate multi-dimensional one, (b) to develop a parallel model of coupling inside and outside of the IJJ device for connecting the inside and outside of the IJJ device accurately and (c) to tune those models to high performance computer for overcoming the vast increase of computational loads during multi-dimensional analysis.

Last year we studied the effect of arrangement of electrodes and dielectrics around IJJ device on emission of terahertz waves. And we made an assumption that the terahertz waves emit effectively if the ratio of the outside dielectric constant to the inside effective one of IJJ device increases. The effective dielectric constant of the inside of IJJ device can be controlled by the number of layers of IJJ. In this year, therefore we have studied the effect of the ratio on the emission of terahertz waves by control of the number of layers of IJJ.

2. Multi-dimensional simulation models of IJJ device for generation of terahertz waves

2.1 Multi-dimensional model of IJJ device

In this year, we use the advanced two dimensional model of IJJ device for generation of terahertz waves. Its model is more accurate than the model used to 2009 and has been developed until 2010 to study the optimum conditions of emission of terahertz wave from IJJ device. The reason why more accurate multi-dimensional models are required is as follows.

Josphson plasma excites when it resonates with the array of fluxons and the most intense vibration of electric field that is induced by vibrating superconducting currents appears in parallel to layers (x-axis) and along layers (z-axis) near the surface of the device. These vibrating electric 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. Until FY 2009, we had carried out the basic study on the IJJ device by using a quasi two-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 was required that the vibration of superconducting currents should be correctly analyzed on the layers (x-axis) and along layers (z-axis) for simulating the emission of the terahertz waves with a high degree of accuracy.
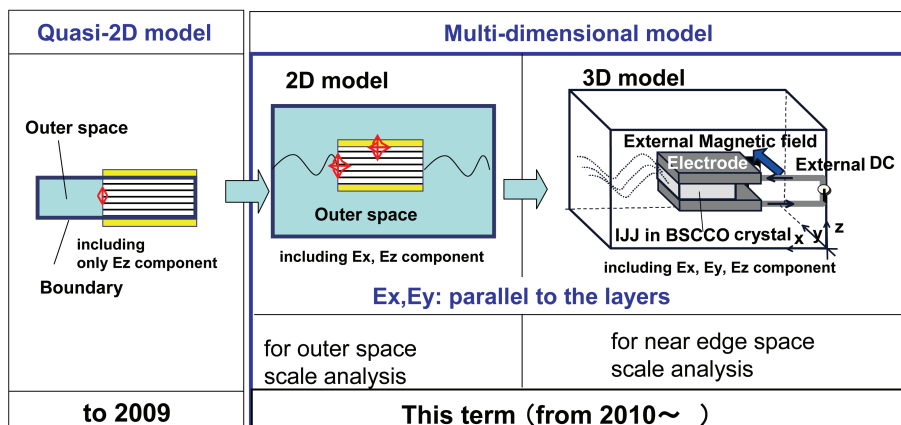

Fig. 2 Flow of development of multi dimensional models.

Thus the accurate two-dimensional model of the generation of terahertz waves was developed unitl 2010 by considering the electric fields that are parallel to the layers, as shown in Fig. 2.

2.2 Simulation model

Last year our simulation showed that IJJ device could emit effectively terahertz waves if it consists of the large number of layers, is enclosed by electrodes at up and down sides and the outside dielectric constant has high value. Considering the change of theoretical effective dielectrics in IJJ device, we assume that the number of IJJ layers has the most effect on the emission of terahertz waves by following mechanism. The effective dielectric constant ε^{eff} in IJJ device is expressed as follows:

$$\varepsilon^{eff} = \left(1 + 2\lambda_{ab}^2/(Ds)(1 - \cos(\pi q_c/(Nc + 1))) \right) \varepsilon_c \ ,$$
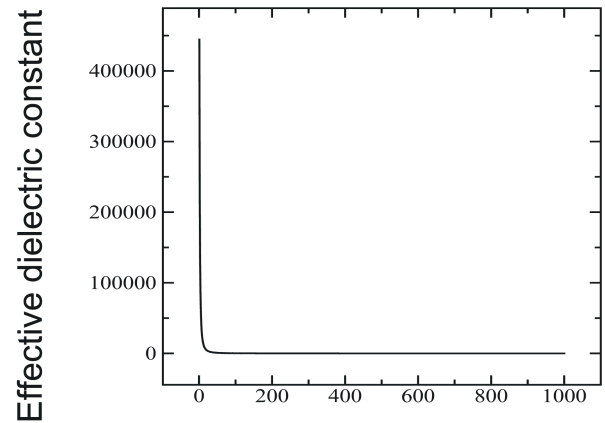
here, εc is dielectric constant along c-axis, q_c is wave number along c-axis of Josephson plasma and Nc is number of layers of IJJ device. The effective dielectric constant strongly depends on Nc as shown in Fig. 3.

The effective dielectric constant ε^{eff} of small number of layers is very large value in inside of IJJ device as shown in Fig. 3, and dielectric constant in air is value of one. Therefore the ratio of the outside dielectric constant to the inside effective one is very small. Increase of number of layers makes effective dielectric constant extremely decrease as shown in Fig. 3. Then

the reflectivity of Josephson plasma at the edge of the device decreases by increasing the ratio of outside dielectric constant to inside effective one. Therefore IJJ device of large number of layers is expected to cause intense emission of terahertz waves.

We change the ration of outside dielectric constant to inside effective one by the control of number of IJJ layers as follows. The ratio$\varepsilon/\varepsilon^{eff}$ is shown in table 1.

Based on these cases, we set the model of IJJ device and its simulation model as shown in Fig. 4.

Fig. 3 Dependence of effective dielectric constant on number of layers of IJJ device for the case of qc=1 that induces node-less coherent mode along c-axis.

Table 1 Simulation parameters.

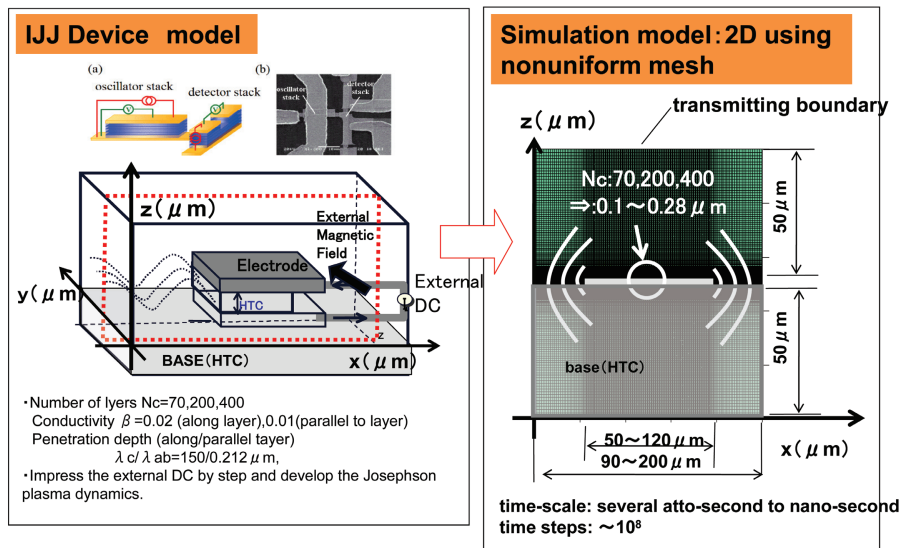| CASE No.	Dielectric Constant of outside	Nc	Effective dielectric constant ε^{eff} of inside	Ratio: $\varepsilon/\varepsilon^{eff}$
1	ε=1(air)	70	2379	1/2379
2		200	245	1/245
3		400	62	1/62
4	ε=10	70	2379	1/240
5		200	245	1/24.5
6		400	62	1/6.2

Fig. 4 IJJ device models and its simulation model.

Table 2 Summary of parameters for simulation.

Items	Value
Number of layers Nc	70, 200, 400
Device length	$50 \sim 120\mu m$
Space area of outside	$(90 \sim 200\mu m) \times 100\mu m$,
Magnetic field penetration depth from the bc (λc) and ab surface plane (λab)	λc=150μm, λab=0.212μm,
Reduced quasi-particle conductivity c-axis	along c-axis: $\beta = 0.02$ paralle to layers: βab= 0.01
External magnetic field	Byo= 0.5Testa
Reduced external DC	DC: J'=0.4. The reduced external DC is impressed as step wise at reduced time t'=0, and time development phenomena of Josphson plasma excitation was simulated up to t'=100 $\sim$ 200.

Simulations were performed with parameters shown in table 2.

3. Simulation results

Figure 5 shows terahertz waves in inside and outside of IJJ device for number of layers Nc and dielectric constant of outside of IJJ device based on simulation results.

Terahertz waves are stayed locally around the edge of IJJ device for case (1), (2), (3) and (4) . Ratios ε/ε^{eff} are 1/2379,

1/249, 1/240 and 1/62 for case(1), (2), (3) and (4). On the other, terahertz waves are traveling in the outside space of IJJ device for case (5) and (6). Ratios ε/ε^{eff} are 1/24.5, 1/6.2 for case (5) and (6). The results show that efficient emission of terahertz waves requires increasing ratioε/ε^{eff} to make its ratio close to value of one. The control of number of IJJ layers is effective for increasing ratioε/ε^{eff}.

Figure 6 shows that the power of terahertz waves were estimated from amplitude of traveling terahertz waves in the
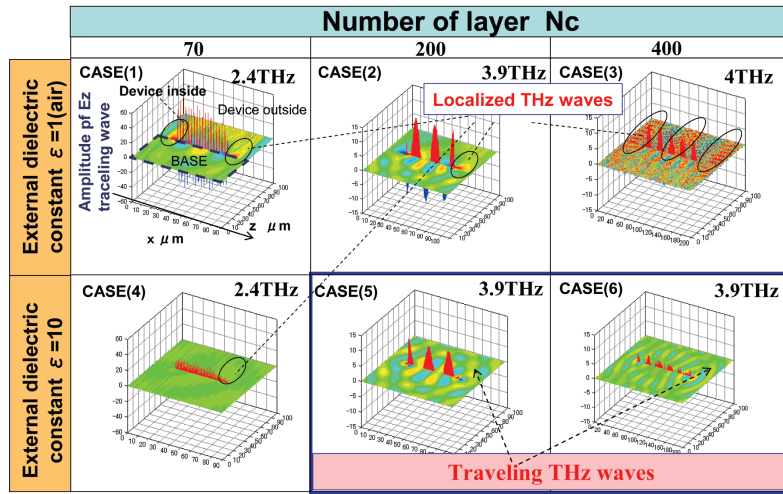

Fig. 5 Terahertz waves in inside and outside of IJJ device for number of layers Nc and dielectric constant of outside of IJJ device.
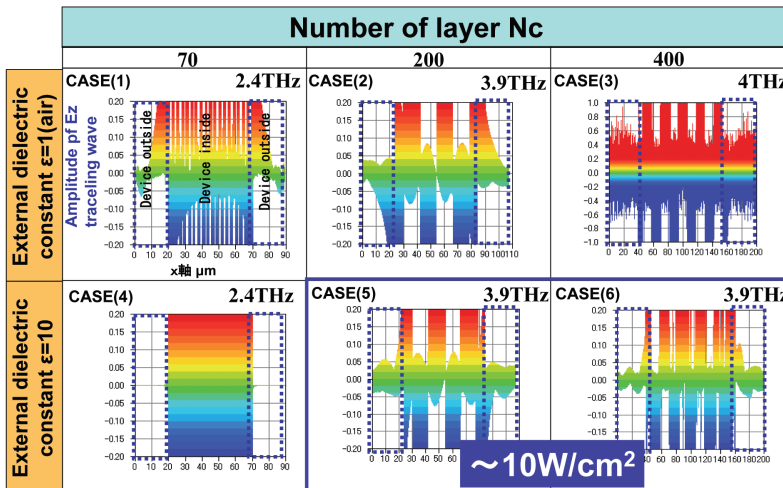

Fig. 6 Power of emitted terahertz waves.

outside space of IJJ device. The power of 10 W/cm^2 is double-digit lower than estimated power in previous study [3]. Next, therefore we would try to study the way that makes power of emission increase.

4. Conclusion and future work

This year, we have studied the effect of ratio $\varepsilon/\varepsilon^{eff}$ on emission of terahertz waves by controlling number of IJJ device layers. The results show that the traveling terahertz waves emit effectively from the edge of IJJ devifce when the value of the ratio$\varepsilon/\varepsilon^{eff}$ increases and is closing to one. The control of number of IJJ layers is mostly effective factor for increasing ratio$\varepsilon/\varepsilon^{eff}$.

Hereafter we would study how to increase the power of emission by using 2D, 3D simulation model, for investigating more design factors of a terahertz light source.

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体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。

　この課題を解決するため、平成 20 年度までに、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多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、昨年度までに、素子とその外部空間を含む 2 次元モデルにより、高温超伝導素子の電極配置や周りの誘電体配置のテラヘルツ波生成への影響を調べ、素子上下に電極を配置し、素子外部の誘電率と素子内部の有効誘電率の比を上げることによりテラヘルツ波を効率的に生成できるという仮説を得た。また、素子内部の有効誘電率は素子の層数により制御可能であることもつきとめた。

　そこで今年度は、素子の層数を制御し、素子外部の誘電率と素子内部の有効誘電率の比を上げて 1.0 に近づけることにより、この仮説を検証した。この成果は、素子端面からの効率的テラヘルツ波放射のための制御変数とその制御法を示し、実験側にとって有効な情報である。しかし、得られたテラヘルツ放射の強度は、$10\mu W/cm^2$ 程度で必要とされる強度に比べ 2 桁ほど低いため、今後、さらに放射強度を増す方法を地球シミュレータの大規模計算能力を利用し設計して行く。さらに、開発中の 3 次元コードを完成させ、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。この 3 次元の計算規模はより大規模な計算資源を必要とするため、現状ではモデルの規模が制限される。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。本研究は新しいセンサー技術やテラヘルツデバイス技術だけなく、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：高温超伝導体，デバイス，連続波テラヘルツ波発振，安定励起，ジョセフソンプラズマ，高性能計算資源，導波管