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. 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 efficiently 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.

In 2011 we developed an advanced two-dimensional parallel model that describes accurately the whole configuration of IJJ device with coupling the outside space of the device. And we reached to an assumption that the increment of the number of IJJ enhances the power of terahertz waves emitted from the IJJ device.

This year we have studied the emission of terahertz waves from the device edge with increasing the number of IJJ from 70 to 1000. As a result we have revealed a method for enhancing the emission power of terahertz waves and the device design for 1mW power of terahertz wave generation.

As shown here, we have attained to get the optimum conditions of the device design through large scale simulation by using Earth Simulator.

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 1-4THz, 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.

As a next step of our challenges, it was required to develop the wave guide that leads the terahertz waves to the objects

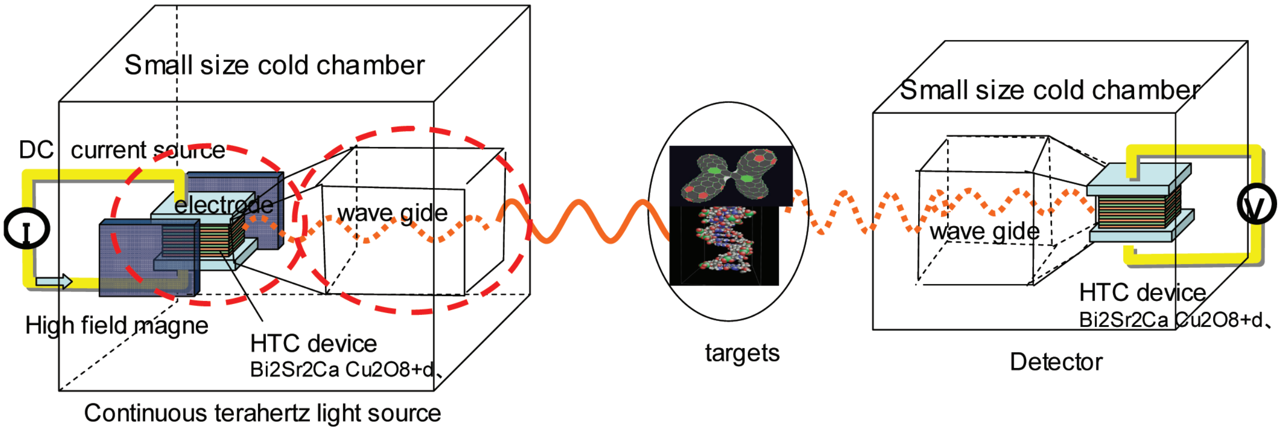


Fig. 1 Schematic diagram of measurement equipment using IJJ device.

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 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.

In 2011 we developed an advanced two-dimensional parallel model that describes accurately the whole configuration of IJJ device with coupling the outside space of the device. And we reached to an assumption that the increment of the number of IJJ enhances the power of terahertz waves emitted from the IJJ device.

It is expected that the increment of the number of IJJ reduces the dielectric constant of the inside of the device, increases the intensity of Josephson plasma excitation in the device and enhances the power of terahertz waves emitted from the edge of IJJ device

With increasing the number of IJJ of the device, the dielectric constant of the inside of the device approaches one of the outside of device. Therefore, the increment of the number of IJJ of the device is expected to make the ratio of dielectric constant of the inside and outside of the device approach to 1.0. This means that, reflections of the plasma wave at the edge of the device are reduced, Josephson plasma wave excited in the IJJ device is guided to the outside of the device and then the intense terahertz wave is generated. Increment of the number of IJJ is also expected to increase the amplitude of the excited Josephson plasma wave and lead to generate the intense terahertz waves.

This year we have studied the emission of terahertz waves from the device edge with increasing the number of IJJ from 70 to 1000. As a result we have revealed a method for enhancing the emission power of terahertz waves and the device design for 1mW power of terahertz wave generation.

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.

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

2.2 Condition of Simulation

The condition of simulation with increasing the number of IJJ is shown here. Table-1and 2 shows parameters and cases for simulation.

Based on these cases, we set the model of IJJ device and its simulation model of FDM as shown in Fig. 3.

3. Simulation results and discussion

Figure 4 shows snap shots of terahertz waves in the inside and outside of IJJ device, with regard to the number of layers Nc and the dielectric constant of the outside of IJJ device. Terahertz waves are locally characterized as *near-field light* staying around the edge of IJJ device, for cases (1), (2), (3) and (5) . On the other hand, terahertz waves are traveling to the outside space of IJJ device, for cases (4), (6), (7) and (8). In this way,

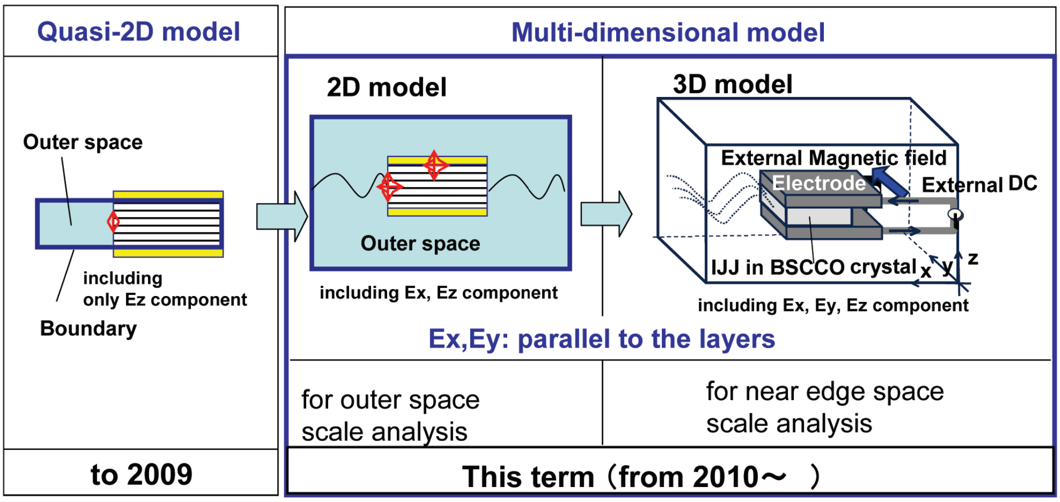


Fig. 2 Flow of development of multi dimensional models.

Table 1 Summary of parameters for simulation.

Items	Values of parameter
Number of layers Nc	70, 200, 400,1000
Device length	50,50,120,300μm
Space area of outside	(90,90,200,900μm)×100μm,
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: β= 0.02, 0.1 parallel to layers: βab= 0.001, 0.01, 0.1
External magnetic field	Byo= 0.5, 0.068, 0.0288Testa
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'=100~200.

Table 2 Cases of simulation.

CASE No.	Dielectric Constant of outside	Nc	Effective dielectric constantεeff 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		1000	11	1/11
5	ε=10	70	2379	1/240
6		200	245	1/24.5
7		400	62	1/6.2
8		1000	11	1/1.1

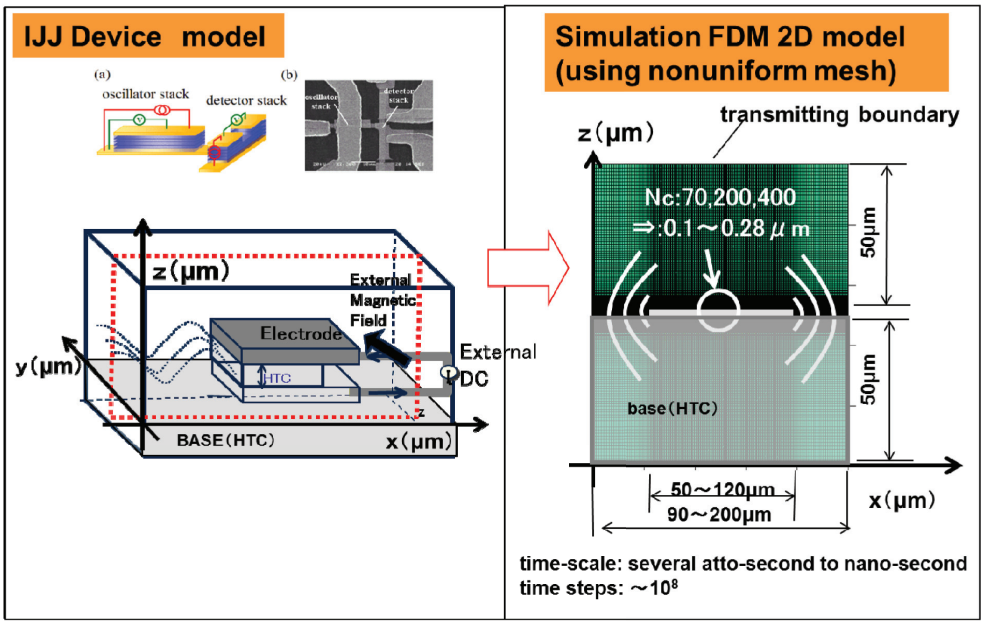


Fig. 3 IJJ device models and its simulation model.

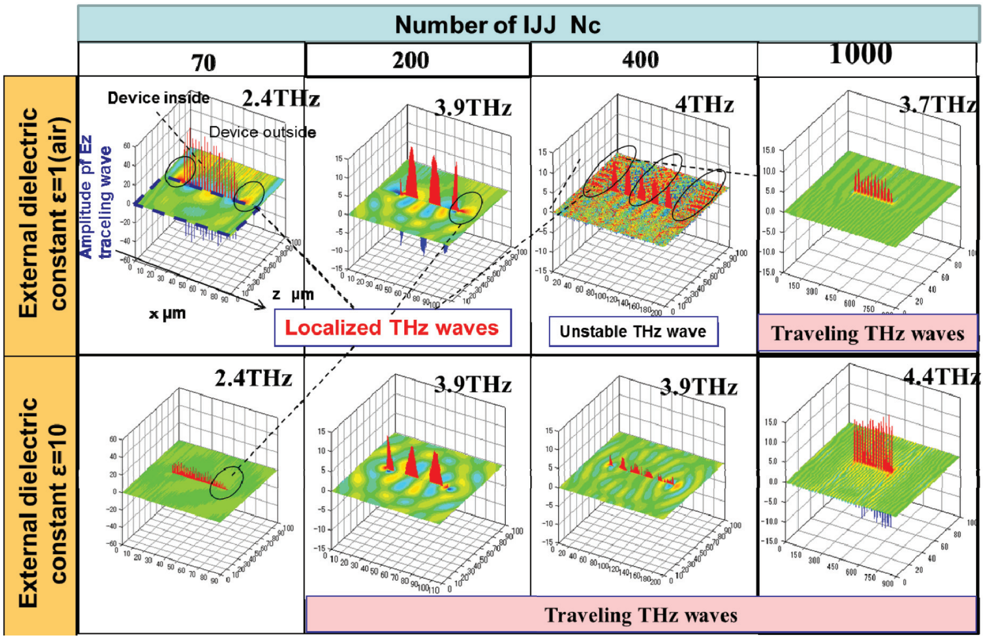
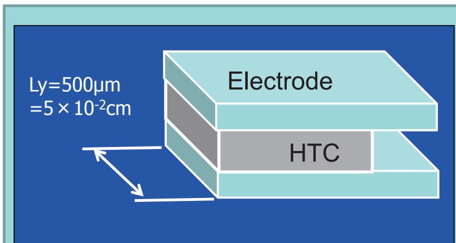


Fig. 4 Snap shots of terahertz waves in inside and outside of IJJ device for number of IJJ Nc and dielectric constant of outside of IJJ device.

Table 3 Effect of increasing number of IJJ.



Geometry Spec of IJJ device

Number of layers Nc	400	1000
Thickness	0.6 μm	1.5 μm
Edge area	3.0×10^{-6}cm^2	7.5×10^{-6}cm^2

Number of layers Nc	400	1000
Power/cm^2	8.4W/cm^2	135W/cm^2
Power /device	0.025mW/device (μW order)	1mW/device (mW order)

the .emission pattern of terahertz wave from IJJ device changes with increment of the number of IJJ.

Next we show in table-3 the effect of increasing number of IJJ on the emission power of terahertz wave. This result shows that increment of the number of IJJ from 400 to 1000 enhances the emission power by 16 times and the device with 1000 layers emits terahertz waves by 1mW/device.

From these results, it is evaluated that change of emission mode from near-field light to traveling light causes the increase of power of terahertz emission.

As shown above, this year we have studied the emission of terahertz waves from the device edge with increasing the number of IJJ from 70 to 1000. As a result we have revealed a method for enhancing the emission power of terahertz waves and the device design for 1mW power of terahertz wave generation.

4. Conclusion and future work

We have attained to get the optimum conditions of the device design through large scale simulation by using Earth Simulator. We will also support experiment works through supplying large-scale simulation with more real model of the device and the IJJ device design by using large-scale computers.

Along this study, Earth Simulator has shown 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、平成 22 年度昨年度までに、素子とその外部空間を含む正確な２次元の並列モデルを開発し、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、素子の層数により素子内部の有効誘電率を制御可能であることもつきとめた。

そこで昨年度と今年度、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高温超伝導体素子を使うテラヘルツ生成素子から放射されるテラヘルツ波の強度を急激に高めることが可能であることを示した。その結果、当初目的としていた、テラヘルツ波生成の制御法と 1mW/ 素子級の素子の最適な設計パラメータを明らかにすることができた。

今後も、スーパーコンピュータの大規模計算能力を利用した設計研究を続け、本素子の実用化を目指した実験的研究開発を支援して行きたい。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していく。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、ナノスケール通信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 : 連続波テラヘルツ波 , 高温超伝導体 , デバイス , ジョセフソンプラズマ , 導波法 , 大規模シミュレーション