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. 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.

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 using vast computing power of the Earth Simulator

One of challenges we are tackling is to design a wave guide that flexibly leads the terahertz waves 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 in the device and wave guide.

This year, we have studied the conditions of the Josephson plasma that emit effectively the terahertz waves from a device of BSCCO crystal to its outer-space, using 2 dimensional IJJ device model. Furthermore, we have developed 3 dimensional model of IJJ device.

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 10THz. 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 the high temperature superconductor, 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 being investigated. Thus, themes to be cleared are as follows as shown in Fig. 1:

(a) Design of the optimum connection from the device to the wave guide: 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 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 between inside and outside of the HTC device and wave guide system.

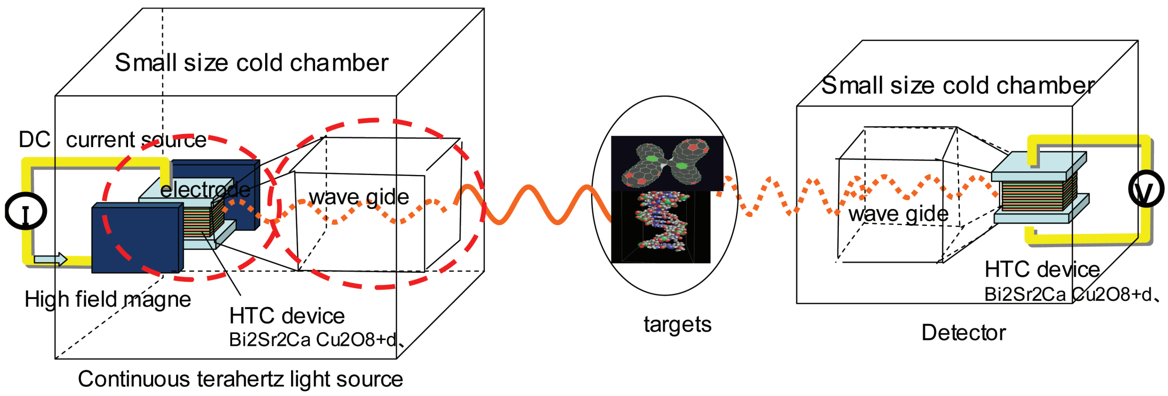

Fig. 1 Schematic diagram of measurement equipment using HTC device and the challenge of development of light source.

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 extend quasi 2 dimensional model to multi-dimensional one, (b) to develop a parallel model of coupling inside and outside of the HTC device for connecting the inside and outside of the HTC 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 this year, (a) we have studied more effective methods that emit the terahertz waves from inside of BSCCO crystal to the outer-space, using 2 dimensional model of IJJ device developed last year. As for (b), we have developed 3 dimensional model of IJJ device.

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

2.1 Extension of quasi 2 dimentional model to multi-dimensional IJJ device model

In this year, we applied the advanced two dimensional model of the generation of terahertz waves to study the optimum conditions of the Josephson plasma emission. The reason why the 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 outside 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 last year by considering that the electric fields are parallel to the layers, as shown in Fig. 2.

Base on the last year's activity, we have developed this year the accurate three-dimensional model of the generation of terahertz waves based on the accurate two-dimensional model.

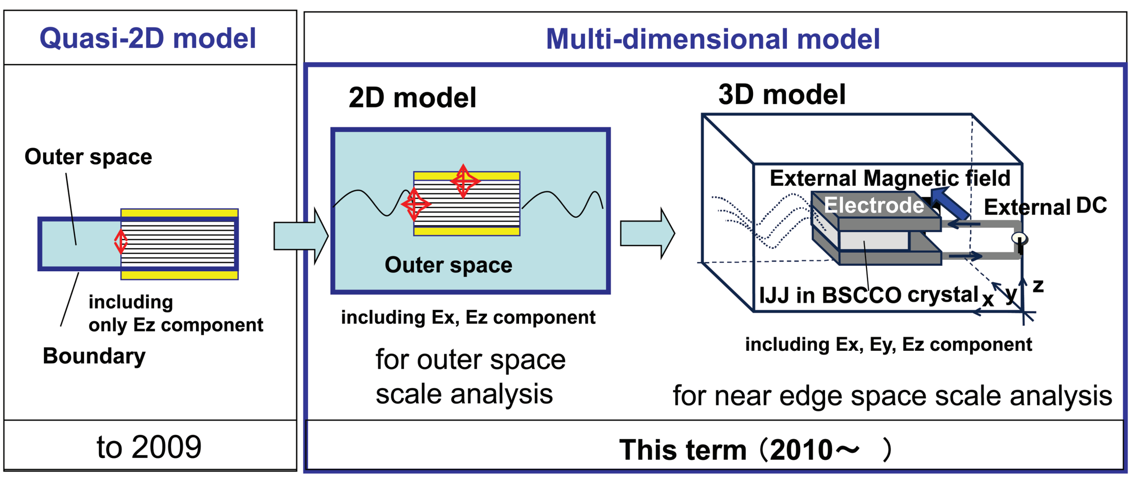

Fig. 2 Accurate multi dimensional models.

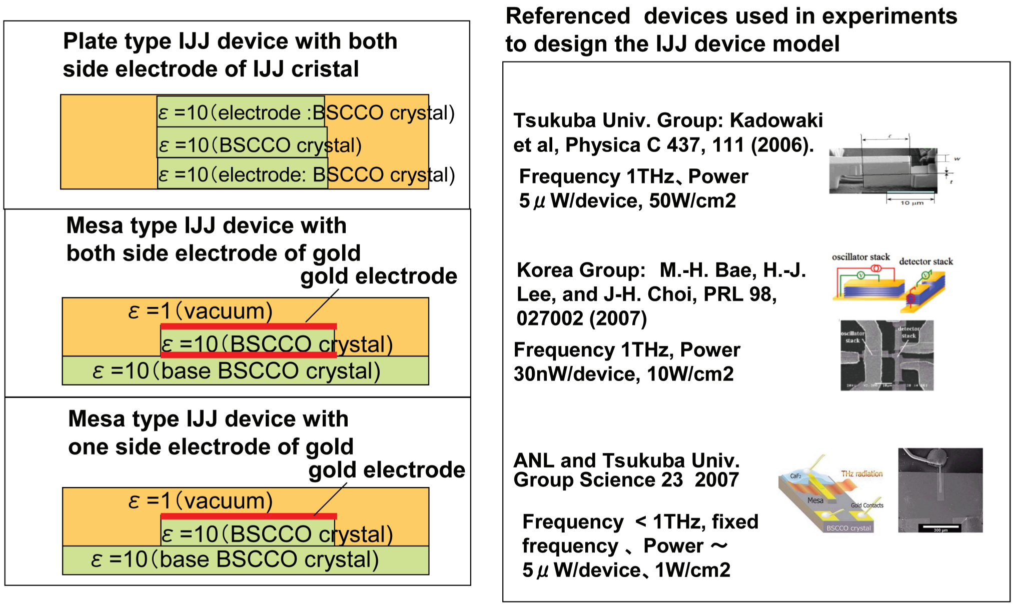

Fig. 3 IJJ device models for simulation.

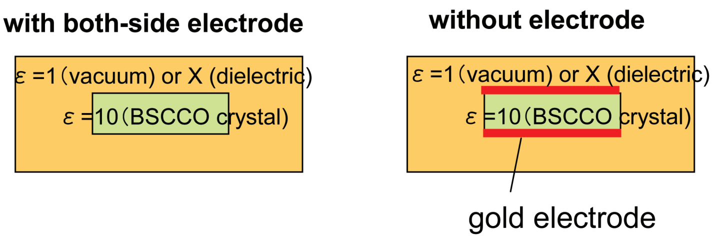

Fig. 4 Simple plate models of device.

2.2 IJJ device models for simulation

We set the IJJ device model for simulation, as shown in Fig. 3, referencing the examples of experiments of terahertz generation. In addition, we used simple plate models with both-side electrode and without electrode as shown in Fig. 4, for making clear the effects of configuration of electrode and dielectric on emission of terahertz waves.

We also set the 2 dimensional simulation model for analysis of terahertz emission from the surface of IJJ device as shown in Fig.5. Simulation was performed with the following parameters: (a) Number of layers: Nc=70, (b) Device length : L=50μm, (c) outer space area: about 100μm×100μm, (d) Magnetic field penetration depth from the bc and ab surface plane: λc, λab:150μm, 0.212μm, (e) Reduced quasi-particle conductivity along c-axis: β=0.02 and along layer: βab=0.01, (f) External magnetic field: By= 0.5Testa and reduced external DC: J'=0.4. The reduced external DC was impressed as step wise at reduced time t'=0, and time development phenomena of Josphson plasma

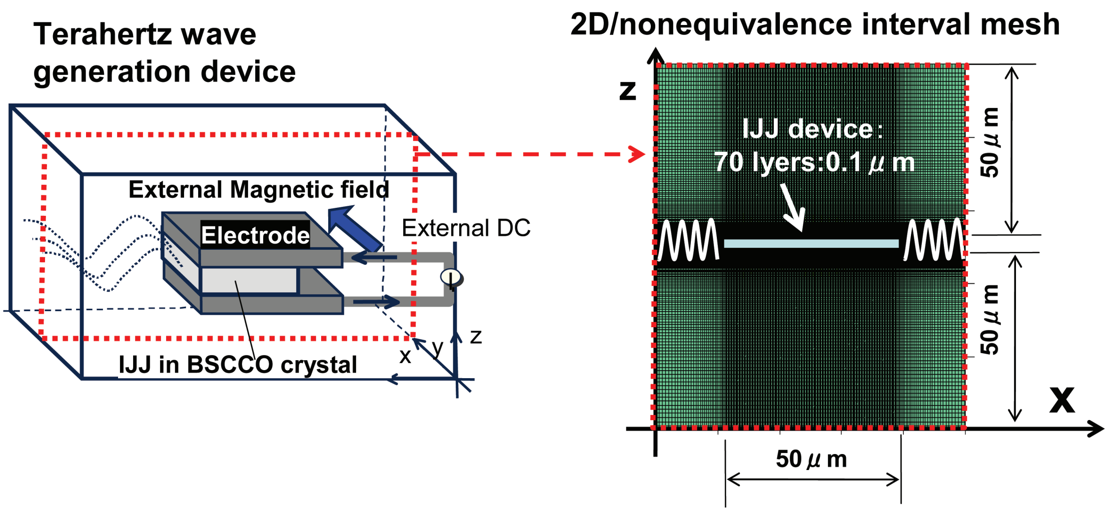

Fig. 5 Simulation model for analysis of terahertz emission from the surface of IJJ device.

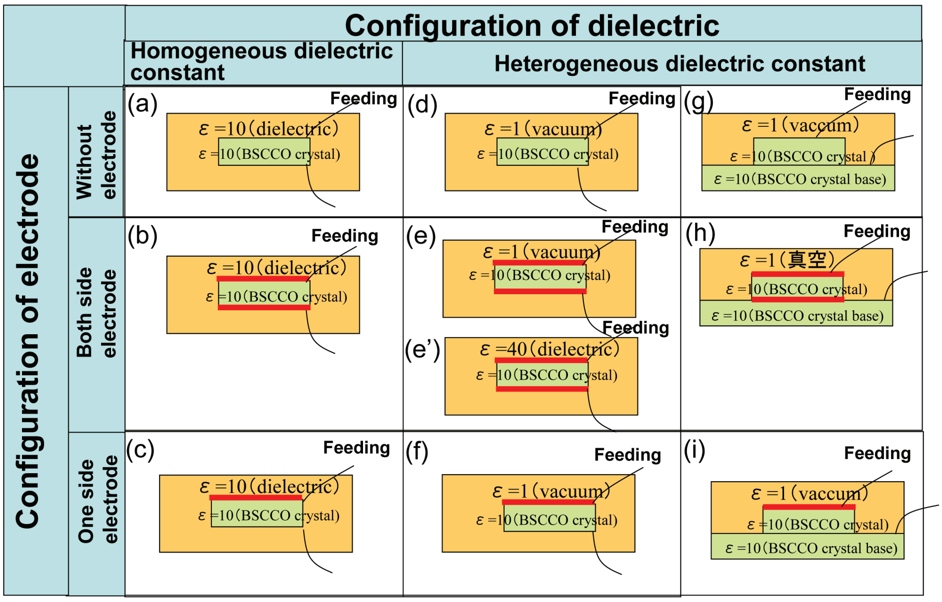

Fig. 6 Figure 6 Analysis cases for studying the affection of configuration of electrode and dielectric on emission of terahertz waves.

excitation was simulated up to t'=100~200.

2.3 Analysis cases for studying the affection of configuration of electrode and dielectric on emission of terahertz waves

In this year, we focused on studying the effects of configuration of electrode and dielectric on emission of terahertz waves. The analysis cases are shown in Fig. 6.

3. Simulation results and affection of configuration of electrode and dielectric on emission

We studied the effects of the configuration of electrode and dielectric on the emission as follows.

3.1 Affection of electrode configuration on the emission

We compared the case of IJJ device without electrode to the case of one with both-side electrode by checking the oscillation part of electric field of generated terahertz wave in outer-space as shown in Fig. 7.

As for the IJJ device without electrode, terahertz wave is out of phase between upper and lower of device. Then the intensity of terahertz wave in far field is canceled. On the one hand, in the case of IJJ device with both-side electrode, terahertz wave is in phase between upper and lower of device. And the intense terahertz wave propagates to far field.

Next, we simulated the Josephson plasma excitation by checking the oscillating part of electric field of Josephson plasma wave in the IJJ device. The simulation showed that, in the case of IJJ device without electrode, there is incidence of wave in an oblique direction from corner of IJJ device as shown in Fig. 8. This oblique direction wave disturbs the coherent Josephson plasma excitation. On the one hand, in the case of IJJ device with both-side electrode, there is no incidence of wave in

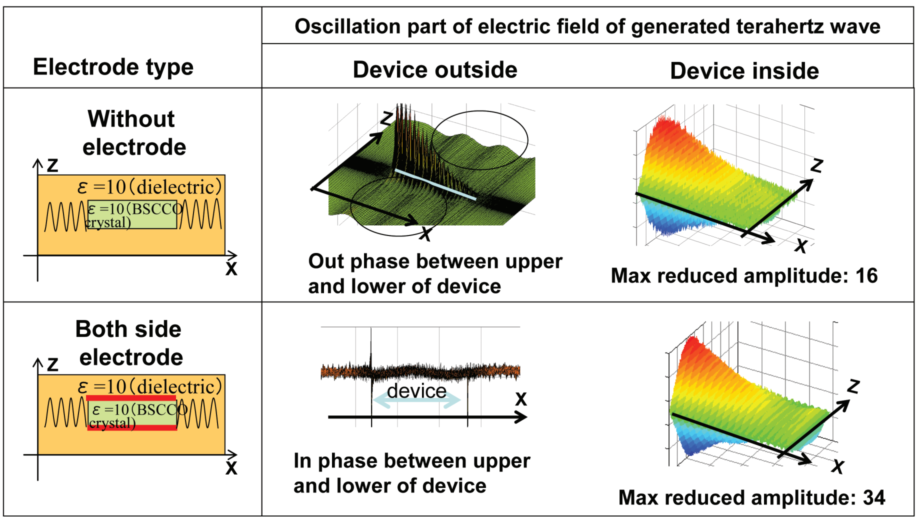

Fig. 7 Affection of electrode configuration on emission of terahertz waves.

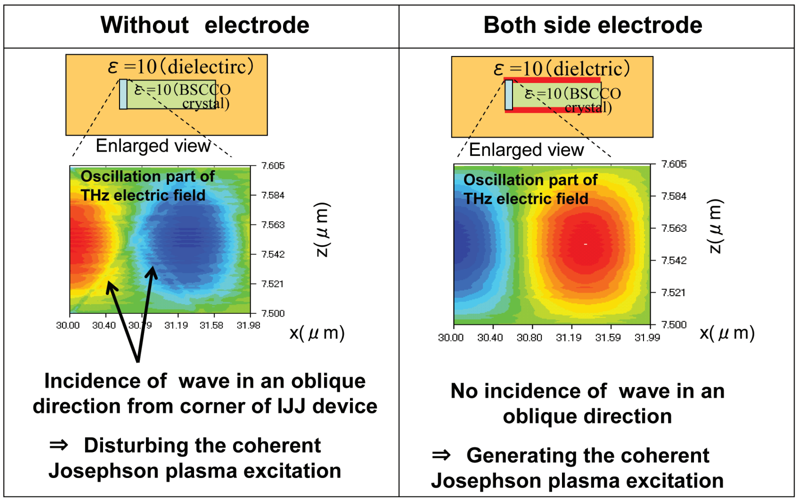

Fig. 8 Affection of electrode configuration on Josephson plasma excitation in the IJJ device.

Fig. 9 Affection of electrode configuration on Josephson plasma excitation.

an oblique direction from corner of IJJ device.

Furthermore, we also compared the case of IJJ device with one-side electrode to the case of one with both-side electrode as shown in Fig. 9.The simulation showed that, in the case of IJJ device with both-side electrode, the excitation of Josephson plasma excitation is stable. On the one hand, in the case of IJJ device with one-side electrode, the excitation is unstable.

From these studies, it is clear that, in electrode configuration, the type of both-side electrode IJJ device is favorable to emission of terahertz waves from the edge of IJJ device. Up to now, however, the IJJ device of one side electrode was used for the almost reported experiments because of easiness to fabricate the one side electrode device compared to both-side one. Therefore it is summarized that the both-side electrode IJJ device is suitable to generate the intense and coherent terahertz waves.

3.2 Effects of dielectric configuration on the emission

The case of homogeneous dielectric constant was compared to the case of heterogeneous dielectric constant, for studying the oscillation part of electric field as shown in Fig. 10. The simulation cleared that intensity of homogeneous dielectric constant is more than that of heterogeneous dielectric constant. It indicates that increase of dielectric constant of outer space strongly contributes to the emission of terahertz waves from edge of IJJ device.

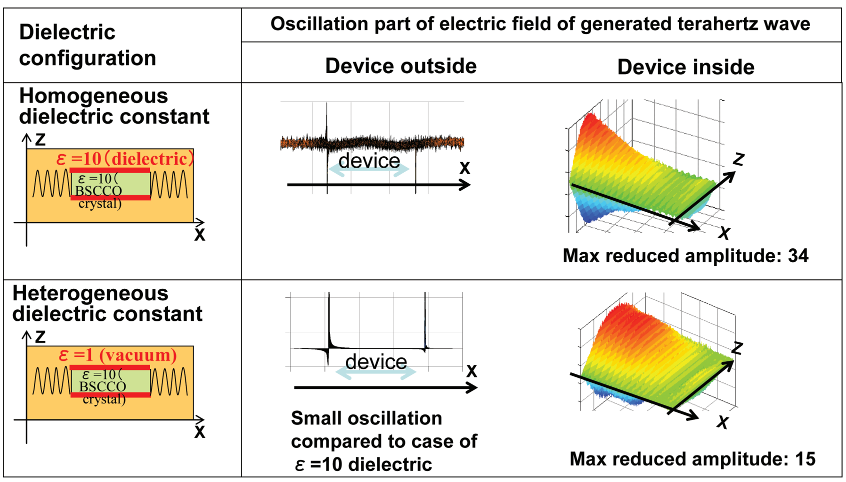

Fig. 10 Affection of dielectric configuration on emission of terahertz waves.

The ration of effective dielectric of IJJ in BSCCO crystal to dielectric in the outer-space is therefore very effective to the emission. Thus, the effect of dielectric of IJJ in BSCCO crystal was studied theoretically. The effective dielectric of IJJ is shown as follows:

$$\varepsilon^{eff} = \left(1 + 2\lambda_{ab}^2/(Ds)(1-\cos(\pi q_c/(Nc+1)))\right)\varepsilon_c$$

here, ε^{eff} is effective dielectric of IJJ, εc is dielectric of IJJ along c-axis, qc is wave number along c-axis of Josephson plasma. Dependence of effective dielectric on Nc: number of layers of BSCCO crystal strongly depend on number of layers as shown in Fig. 11. For example, 10layers: ε eff = 18,000, 23layers: ε eff = 3,810, 70layers: ε eff = 445,700~1000layers: ε eff = 14.5~12.2. This example shows that the difference of effective dielectric between inside and outside of the device decreases for large numbers of layers case.

The effective dielectric of IJJ in BSCCO crystal indicated to be sensitive to the numbers of layers of BSCCO crystal. It is therefore summarized that BSCCO crystal with large numbers of layers is favorable to emission of terahertz waves from edge of IJJ device.

3.3 Optimum design condition for intense coherent terahertz wave generation

From the results, it is concluded that the configuration of both-side electrode and large number of BSCCO crystal IJJ device are good conditions for realizing coherent and intense terahertz wave generation.

4. Conclusion and future work

In this term, the accurate two-dimensional simulation was performed, by large-scale simulation, for deigning the conditions of effective emission of the Josephson plasma as the terahertz waves from the inside to the outside of IJJ device. The results showed that the configuration of both-side electrode and large number of BSCCO crystal IJJ device is effective for coherent and intense terahertz wave generation.

In the next term, we run the large-scale 3D simulation model for deigning more details of a terahertz light source that could effectively guide the irradiation of terahertz waves from the inside of the HTC device to the object placed in the outer-space.

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

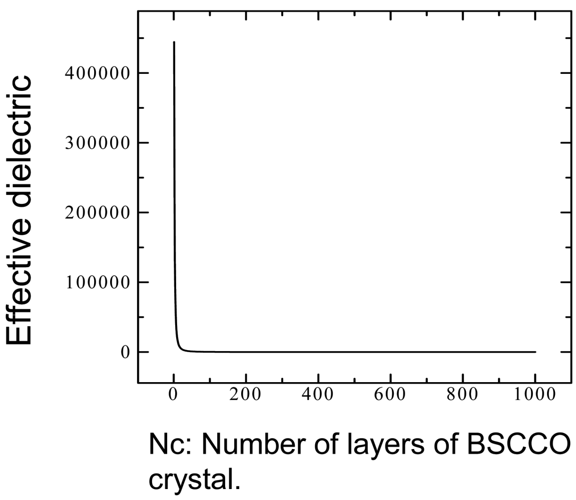

Fig. 11 Dependency of effective dielectric on number of layers of BSCCO crystal. The case of qc=1 is node-less coherent mode.

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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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本研究では、電波と光の間の未利用周波数帯域にあるテラヘルツ波の応用開拓を目指し、大規模シミュレーションを利用したテラヘルツ発振超伝導素子の利用システムの設計を行なっている。テラヘルツ波は、多くの物質に対し高い透過性を持ち、生命分子を含む多くの物質と強く相互作用するため、環境、医療、物質・生命科学などへの応用が期待されている。テラヘルツ波にはパルス波と連続波とがあり、連続波はパルス波より大出力で周波数が揃うことから利用価値はパルス波よりも遥かに大きい。このため、シリコン系半導体、非線形材料等を使う連続波発振が試みられたが、未だに性能が不十分であり、新原理による連続波発振が課題であった。そこで、本研究ではわが国の独自技術としてナノスケールの高温超電導体薄膜素子を使う連続波テラヘルツ発振を目指し、地球シミュレータの大規模シミュレーションにより、これまでにその発振原理、制御法を世界で初めて明らかにした。その後、本研究を参考にしつつ発振実験が行なわれ、発振原理が実証された。

これを計測システムとして実用化を目指すには、素子から発振される連続波テラヘルツ波を反射・損失・減衰を最小限にして計測対象物に照射するための導波管の構造、形状、媒質（誘電体）などに関するシステム的な最適設計が必要となる。そのため、昨年度までに、応用計測系の基本概念を固め、素子・導波管系の連続波テラヘルツ波の 3 次元空間放射の非線形挙動や大出力放射のための電極形状、配置などの最適条件等を明らかにした。そこで今年度は、実用化への開発実験等を加速するため、2 次元モデルで素子と誘電体配置条件や素子の元形状等とコヒーレントで強い放射との関係を明らかにした。

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。本研究内容は大容量情報伝送やエネルギ伝送の利用研究の側面も有し、米、独、中、韓等でも類する研究が盛んであり、国際的に厳しい競争状況にある。このため、本研究では防衛的に国内特許を確保した。本研究から得られる設計情報等は、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: 高温超電導体, 素子, テラヘルツ波生成, 安定励起, ジョセフソンプラズマ, HPC