Large-scale Simulation for a Terahertz Resonance Superconductors Device

Project Representative

Masashi Tachiki　Research Organization for Information Science and Technology

Authors

Mikio Iizuka [*1], Masashi Tachiki [*1], Kazuo Minami [*1], Syogo Tejima [*1] and Hisashi Nakamura [*1]

[*1] Research Organization for Information Science and Technology

We have carried out a large-scale simulation of the Josephson-coupled superconductor (intrinsic Josephson junctions: IJJ) device with a potential of terahertz resonance phenomena. This simulation needs high-performance computational resource, because this resonance phenomena is expected to be strong nonlinear and complex system behavior and the scale of space and time for simulation needs 1nm-several hundred μm and 10^8 step by 10as. It is estimated that the simulation takes two years to perform even a case of simulation through a personal computer. Thus, the Earth Simulator is needed for solving the simulation effectively. By the last year, we have studied new mechanism and condition of terahertz waves resonance and emission, and characteristic features of emitted terahertz waves. This year, we have investigated a mechanism and condition of terahertz waves resonance and emission, and found a new mechanism of frequency tunable, resonance dependence on parameters and new emission method.

Keywords: intrinsic Josephson junctions, terahertz resonance, high performance computational resource

1. Introduction

The unexpected plasma phenomenon with the low frequency in the crystal of the high temperature superconductors (HTC), was found by professor Uchida of The University of Tokyo in 1992. HTC is formed in a single high temperature superconductors crystals of CuO_2 and insulator layers which form a stack of many atomic-scale Josephson junctions called intrinsic Josephson junctions(IJJ). IJJ has two kinds of Josephson plasma, one is the longitudinal plasma vertical to layers(c axis direction), another is the transverse plasma along layers (ab plane).

Afterwards, professor Tachiki of Tohoku University developed the theory of new phenomenon, and showed that the plasma oscillation with terahertz order is theoretically possible. In addition, the electromagnetic wave absorption of the plasma oscillation of IJJ was observed by professor Matsuda of University of Tokyo. After that professor Tachiki predicted that the excited plasma wave is converted into a terahertz waves at an edge of IJJ [1], [2].

Terahertz wave has usefulness for important infrastructure technology in next generation; new spectroscopic analysis method for material and bio-science, medical diagnoses and treatment and information technology. Leading countries scurry to develop this technology now. Japan is now leading still on both sides of the experiment and the theory research.

If we practiced the use at first in the world, it brings a large advantage to Japan in the area of material and bio-science, medical diagnoses and treatment and information technology etc. and has the possibility to throw up the Japanese original new industry.

The development of the device for the terahertz waves emission is a very difficult only by the experiment, because IJJ have a very strong nonlinearity and the complex behavior. The development and research on the simulation base is indispensable. However, this simulation should deal with nonlinear and complex systems and requires high performance computational resource. This is because a scale of space and time for simulation is 1nm-several hundred μm and 10^8 steps by 10as. It takes two years to perform this simulation for only one case by a conventional computer. The Earth Simulator is therefore essentially needed for solving this problem through simulations.

By the last year, we have studied new mechanism and condition of terahertz waves resonance and emission, and characteristic features of emitted terahertz waves. At this year, we have investigated a mechanism and condition of terahertz waves resonance and emission, and found a new mechanism of frequency tunable, resonance dependence on parameters and new emission method. Let us to show our simulation results.

2. Model Equations

The physical system which should be solved consists of IJJ and the external medium. In IJJ, a coupling equation of the gauge-invariant phase difference φ_k, charge ρ and electric field E^z, which is derived from Josephson relation and Maxwell equation, is solved. The gauge-invariant phase difference is a phase difference between superconducting layer l + 1 and l layer. It is related to Josephson's superconducting current. Maxwell equation is solved at the outside of IJJ. Let us show a formulation for analysis model. The equations describing the dynamics of the phase difference, charge, electric field, magnetic field and super conducting current in ab plane are given by

$$\left(1-\frac{\lambda_{ab}^2}{sD}\Delta^{(2)}\right)\left[\frac{\partial^2\varphi_k}{\partial t'^2}+\beta\frac{\partial\varphi_k}{\partial t'}+\sin(\varphi_k)+\frac{\epsilon\mu^2}{sD}\left(\Delta^{(1)}\frac{\partial\rho'_k}{\partial t'}+\beta\Delta^{(1)}\rho'_k c\right)\right]=\frac{\partial^2\varphi_k}{\partial x'^2}+\frac{\partial^2\varphi_k}{\partial y'^2}, \quad (1)$$

$$\left(1-\frac{\epsilon\mu^2}{sD}\Delta^{(2)}\right)\rho'_{k+1/2}=\frac{\lambda_c}{s}\Delta^{(1)}\frac{\partial\varphi_{k+1/2}}{\partial t'}, \quad (2)$$

$$\left(1-\frac{\epsilon\mu^2}{sD}\Delta^{(2)}\right)E'^z_k=\frac{\partial\varphi_k}{\partial t'}, \quad (3)$$

$$\left(1-\frac{\lambda_{ab}^2}{sD}\Delta^{(2)}\right)B'^y_k=\frac{\partial\varphi_k}{\partial x'}, \quad (4)$$

$$\left(1-\frac{\lambda_{ab}^2}{sD}\Delta^{(2)}\right)B'^x_k=-\frac{\partial\varphi_k}{\partial x'}, \quad (5)$$

$$\left(1-\frac{\lambda_{ab}^2}{sD}\Delta^{(2)}\right)J'^x_{k+1/2}=\frac{1}{s'}\Delta^{(1)}\frac{\partial\varphi_{k+1/2}}{\partial x'}, \quad (6)$$

$$\left(1-\frac{\lambda_{ab}^2}{sD}\Delta^{(2)}\right)J'^y_{k+1/2}=\frac{1}{s'}\Delta^{(1)}\frac{\partial\varphi_{k+1/2}}{\partial x'}. \quad (7)$$

At outside of IJJ, Maxwell equation is as follows,

$$\frac{\partial E'}{\partial t'}=\nabla\times B'-J', \quad (8)$$

$$\frac{\partial B'}{\partial t'}=\nabla\times E', \quad (9)$$

where $\Delta^{(2)} A_k is A_{k+1} - 2A_k + A_{k-1}$, k: number of insulator layer between uperconducting layer l and l + 1, σ: conductivity of the quasiparticles, ε: dielectric constant of the insulating layers, μ: the Debye lenght, Φ_0: unit magnetic state, J_c: critical current density, s, D: superconducting and insulating layer thickness, φ_k: gauge-invariant phase difference in insulator layer k, $\rho_{k+1/2}$: charge density in superconducting layer in k + 1/2, E_k^z: electric field in z direction at insulator layer k, λ_{ab}:penetration depth in the ab-plane direction, $\lambda_c=\sqrt{\frac{c\Phi_0}{8\pi^2 DJ_c}}$: penetration depth in the c axis direction, $\beta=\frac{4\pi\sigma\lambda_c}{\sqrt{\varepsilon}c}$, $\omega_p=\frac{c}{\sqrt{\varepsilon}\lambda_c}$: Josephson plasma frequency, $t'=\omega_p t$: normalized time, $x'=x/\lambda_c$: normalized coordinate in x direction, $\rho'=\rho/(J_c/\lambda_c\omega_p)$: normalized charge density, $E'^z=E^z/(2\pi cD/\Phi_0\omega_p)$: normalized electric field, $E'=E/(2\pi cD/\Phi_0\omega_p)$: normalized electoric field, $B'=B/(2\Phi_0\omega_p/cD)$: normalized magnetic field.

These equations are solved by Finite Difference Method. Some research [3] has been done based on this model.

3. Computational Feature of IJJ Simulation

IJJ phenomenon is very strong nonlinear and complex. Many researchers try to understand IJJ phenomenon via experiments and analytical methods. But, it is very hard to understand IJJ phenomenon with only experiments and analytical method. IJJ simulation based on the model equation can show a detail of IJJ phenomenon mechanism and can allow researchers to easily change a conditions of numerical experiments to evaluate the effect of many conditions. Therefore, IIJ simulation opens up great possibilities for a development of IJJ technology.

A scale of space and time for simulation is 1nm-several hundred μm and 10^8 steps by 10as. It takes two years to perform this simulation for only one case by a conventional computer. In addition, many times IJJ simulation which are with combination of many different material properties, device shapes, current supply methods and current control etc is needed to design and optimize the Tera Hz resonance superconductors device. Therefore, IJJ simulation requires high performance computational resource.

We assume that the system is uniform along the y-axis and make two-dimensional calculation in the x-z plane for basic studies and use the 3 dimensional model for the design and development of device. We used the finite difference method to perform the numerical simulation. Figure 1 shows a performance of 2D simulation code, and figure 2

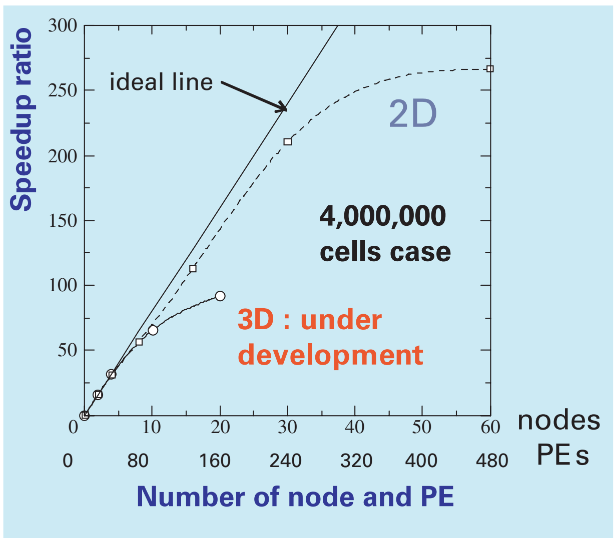

Fig. 1 Parallel performance of 23 code.

shows a performance of 3D code which is now under development. These figures show that ES drastically reduces the solution time.

4. Simulation Models and Results [4, 5]

Figure 2 shows a model of a terahertz emission device using, in this case, $Bi_2Sr_2CaCu_2O_{8-d}$.

We have simulated terahertz resonance with 2D in x-z plane of the model shown in Fig. 2. We impose the following boundary condition. To connect the Josephson plasma wave in the IJJ to the electromagnetic wave in the dielectric at the interface, We put the usual electromagnetic boundary condition; the electric and magnetic fields parallel to the interface are continuous at the interface. The electromagnetic wave in the dielectric is assumed to transmit freely to outer space at the end surface of the dielectric.

We chose $\frac{\lambda_{ab}}{sD}$ = 1 × 10^5, 2 × 10^5, 4 × 10^5, λ_c = 150 μm, s = 3$\AA$, d = 12$\AA$, μ = 0.6$\AA$, α = 0.1, β = 0.02, and the number of layers = 70 ~ 100, and take the dielectric constants along the z-axis in the IJJ and the dielectric constant of MgO to be ε = 10. We apply a magnetic field of 1, 2 Tesla along the y-axis. We change the normalized external current J/J_c from 0.0 to 1.5. The length of the IJJ is taken to be 50 ~ 100 μm along the x-axis and the length of the dielectric is taken to be 50 μm along the x-axis. For each external current, the time evolution is simulated until the system reaches a stationary state.

By the last year, we found the new mechanism of terahertz waves emission as follows. When an external current and a magnetic field are applied to the sample, fluxons flow induces voltage. At this time, Fluxons form as clusters with distorted fluxons. The voltage creates oscillating current through the Josephson effect and the current excites the Josephson plasma with terahertz frequency. The sample itself works as a cavity, and the input energy is stored in a form of standing wave of the Josephson plasma. A part of the energy is emitted as terahertz waves [4]. Figure 3 shows the relation between number of layers and fluxons distribution. When the number of layer increase, the fluxons have ordered distribution. The results show that the fluxons with disordered distribution can excite the coherent electromagnetic waves and the ordered fluxons didn't necessarily excite the coherent electromagnetic waves.

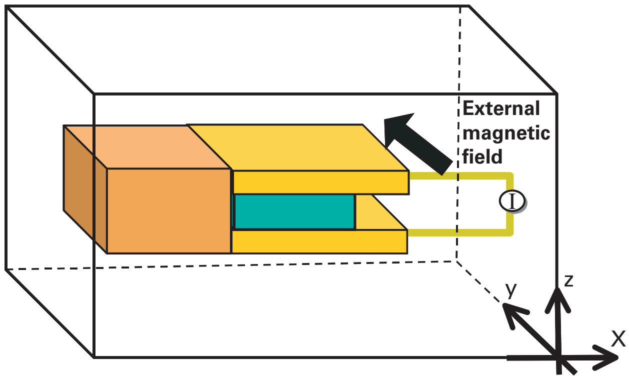

Fig. 2 Schematic diagram of prototype device for terahertz emission. $Bi_2Sr_2CaCu_2O_{8-d}$ forms an IJJ and electrodes. An external current flows uniformly in the junctions in the direction of the -z axis. An external magnetic field is applied to the direction of the y-axis. A dielectric wave guide elongates along the x axis from the left surface of the IJJ. The green part shows an IJJ sandwiched by electrodes made of the gold. The orange part shows the dielectric material, which guides terahertz electromagnetic waves from the device to the outer area.

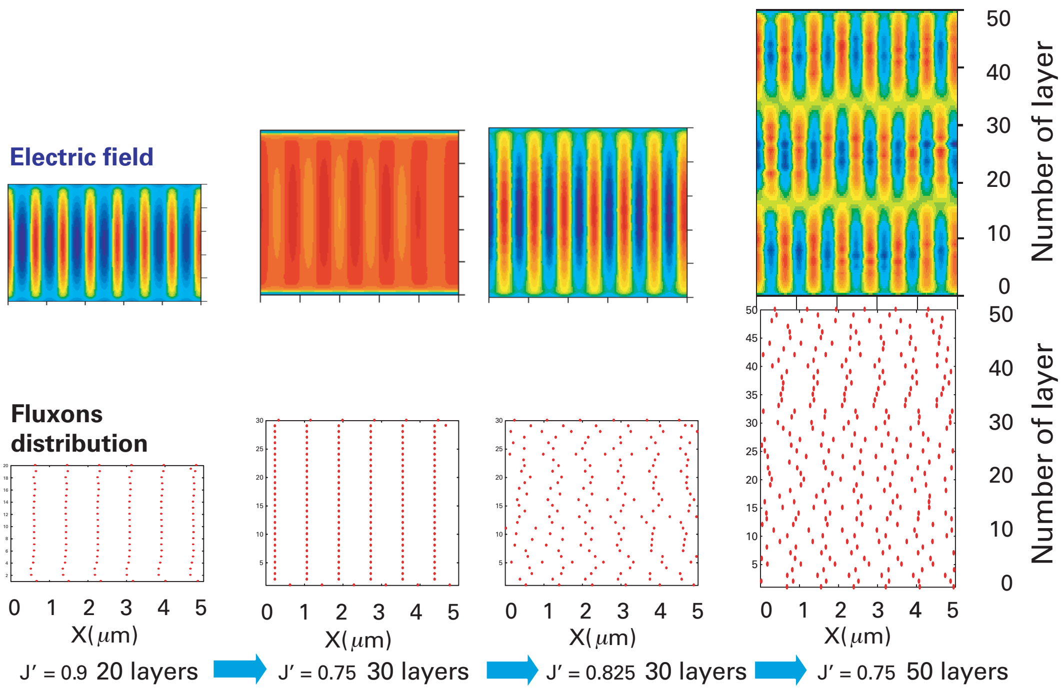

Fig. 3 Relation between number of layers and fluxons distribution.

At this year, we have investigated distributions of $sin\varphi_\kappa$ and $\frac{\partial\varphi_\kappa}{\partial x'}$. Figure 4 shows that the distributions of $sin\varphi_\kappa$ and $\frac{\partial\varphi_\kappa}{\partial x'}$ in 20, 35, 50 layers are disordered, on the one hand averaged distributions are ordered. This shows that the distributions in small scale (in layer or around fluxons) is disordered, in contrast the distributions in large scale (averaged along c-axis, whole device) is ordered. Therefore, we have suggested a hypothesis that the forces balance between small scale disordered force from fluxons interaction and large scale ordered force from electromagnetic waves, make the ordered electromagnetic waves from disordered distributions of fluxons.

Resonance of IJJ is cavity resonance. Cavity resonance makes discrete frequencies excitation. On the one hand, simulation results shows continuous frequencies excitation. We have investigated the details of oscillation of electric field $E^{x'}$. Figure 5 shows the average waves length along x-axis of $E^{x'}$ in 35th layer. The average waves length change in cycle. Figure 6 shows the amplitude and wave length of $E^{x'}$ along x-axis in 35th layer at $t' = 0.15$. Wave lengths at small amplitude of waves change. This result shows that average waves length could change via modification of waves length at small amplitude of waves and this mechanism makes frequency tunable of terahertz waves emitted from IJJ.

Figure 7 shows resonance dependence of IJJ on parameters that is important for experiments and design of IJJ device.

Large amplitude of superconducting current affects resonance in IJJ. We have investigated the oscillation of superconducting current. Oscillation of superconducting current makes the oscillation of $E^{x'}$. Figure 8 shows the $E^{x'}$ filed, in ac plane, that is oscillating in large amplitudes. We could expect the high power emission of terahertz waves from surface of ab plane because of wide area of ab plane surface. We will continue to investigate the emission from ab-surface.

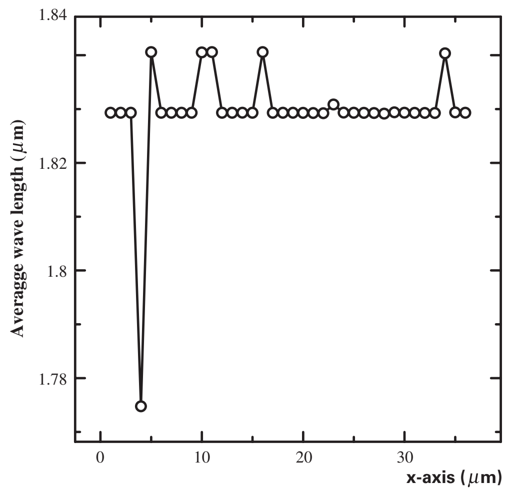

Fig. 5 Average wave length along x-axis in cycle.

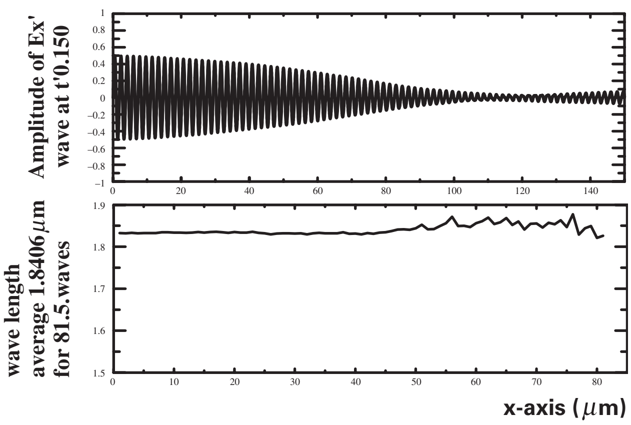

Fig. 6 Amplitude and wave length of $E^{x'}$ along x-axis in 35th layer at $t' = 0.15$

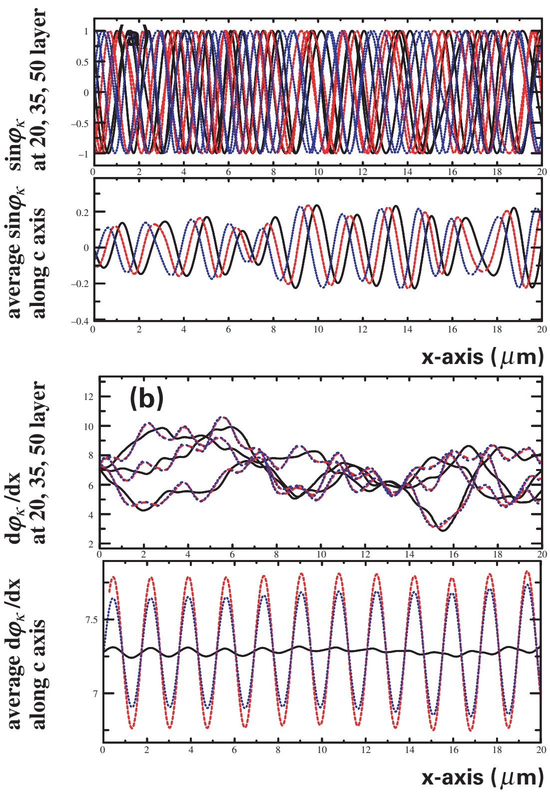

Fig. 4 Distributions of $sin\varphi_\kappa$ (a) and $\frac{\partial\varphi_\kappa}{\partial x'}$ (b) in 20, 35, 50 layers and average slong c-axis (b).

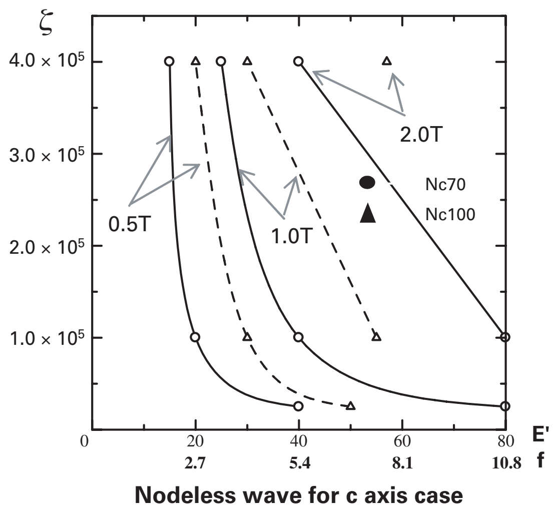

Fig. 7 Resonance dependence on parameters. $\zeta = \frac{\lambda_{ab}}{sD}$; 1×10^5, 2×10^5, external magnetic field; 1T and 2T, number of layers; 70, 100.

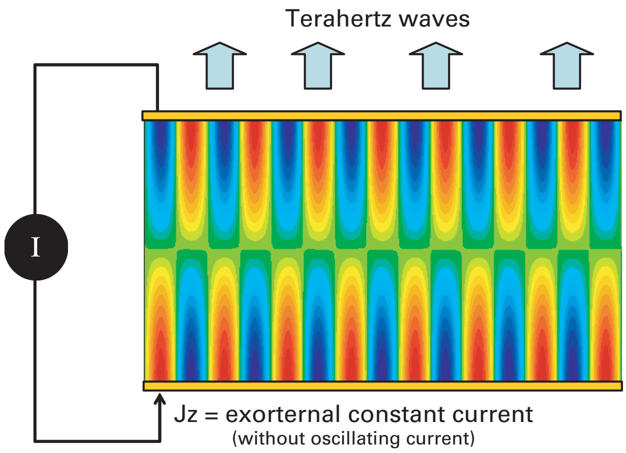

Fig. 8 emission from surface in ab-plene.

5. Future Work and conclusion

In this year, we have investigated a mechanism and condition of terahertz waves resonance and emission, and found a new mechanism of frequency tunable, resonance dependence on parameters and new emission method. Next stage, we will investigate the more details of mechanism and condition of terahertz waves resonance and emission, and ab-plane emission. We believe that Earth simulator class or over class high performance computational resource only enable us to research and design for terahertz resonance superconductors devices.

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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

プロジェクト責任者
立木　　昌　　財団法人高度情報科学技術研究機構

著者
飯塚　幹夫*1，立木　　昌*1，南　　一生*1，手島　正吾*1，中村　　寿*1
＊1　財団法人高度情報科学技術研究機構

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。しかし、分析、検出、解像、大容量通信に優れる連続波光源として、量子カスケードレーザ等があるが、1～4THzで低出力のため、実際の応用には、広帯域で単色、周波数可変、またmW級の高出力を得られる新光源が必要である。本研究では、磁場中のナノスケールの高温超伝導体に直流電流を印加するとジョセフソンプラズマが励起し連続波テラヘルツ波として発振するという理論に基づく大規模シミュレーションにより、テラヘルツ波広帯域でmW級の出力を可能とする連続波テラヘルツ波の発振条件を明らかにするとともに、デバイス開発のためのシミュレーションを行う。

平成16年度までに、新しい発振メカニズムと最適発振条件の発見、テラヘルツ発振メカニズムの詳細解明を行った。これら成果は国内外で認知され、本シミュレーション結果に基づき国内で実験が行われている。平成17年度は、不規則なフラクソンのクラスターが規則的な電磁場を励起する機構、周波数可変となる機構について解明し、実験に具体的指針を与えるデータの整備としてパラメータ(外部磁場、Inductive 係数、層数・・)が発振に寄与する因子の影響度把握、素子上面(<u>*ab*</u>面)より放射する新たな連続テラヘルツ波発生方法の考案を行った。

そこで、次年度以降は最適発振条件の解明を引き続き実施し、また昨年度発見した素子上面より放射する新発振方式の発振条件の解明を行う。これら成果を、論文、特許にまとめわが国の知的財産を確保すると共に、実験家に公開し我国の素子開発を先導する。

今後は、さらに、テラヘルツ波の応用にも着目し、テラヘルツ波と物質・生命分子との相互作用、大容量通信のための発振帯域拡大を目指す研究も行う。

キーワード：連続波テラヘルツ波，高温超伝導体，デバイス，大規模シミュレーション