Large-scale Simulation for a Terahertz Resonance Superconductor Device

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Terahertz wave (0.3-10THz) technology is unexplored and promising area for key infrastructure technology in the next generation. Bottleneck for the development of terahertz technology is a lack of light source for continuous terahertz waves. We have carried out a large-scale simulation of a high-temperature-superconductor device generating terahetz waves to develop a new light source for continuous terahertz waves. This simulation needs high-performance computational resource, because the phenomena, generating terahetz waves in high-temperature-superconductor is strong nonlinear and complex system in multi-scale of time and space. Thus, the Earth Simulator is needed for performing the simulation effectively.

By the last year, we found the new mechanism and the condition generating terahertz waves and revealed the characteristic of emitted terahertz waves. Japanese and Korean experimental scientists detected the terahertz waves using high-temperature-superconductor device, following our results of simulation. Next phase, the control and optimization of generating terahertz waves is needed to apply the high-temperature-superconductor device to industry. Therefore, in this year, we have studied the control parameters and optimum condition of generating terahertz waves.

Keywords: high-temperature-superconductor, device, generating terahertz waves, high performance computational resource

1. Introduction

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 researches. Terahertz wave technology brings a new science and technology 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 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. In addition, the electromagnetic wave absorption of the plasma oscillation of IJJ was observed by professor Matsuda of the University of Tokyo. HTC is formed in a single high temperature superconductor crystal 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, showed that the plasma oscillation with terahertz order is theoretically possible, and predicted that the excited plasma wave is converted into terahertz waves at an edge of IJJ [1, 2]. The development of the device for the terahertz waves emission is 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 require high performance computational resource. This is because s scale of space and time of 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 studied new mechanism, condition generating the terahertz waves, and characteristic of emitted terahertz waves[3]. Japanese and Korean experimental scientists have detected the terahertz waves using high-temperature-superconductor device, following our results of simulation. Next phase, the control and optimization of generating terahertz waves is needed to apply the high-temperature-superconductor device to industry. Therefore, in this year, we have studied the control parameters and optimum condition of generating terahertz waves. Here, we call the condition, in which terahertz waves of 1~4 THz are generated with high intensity and frequency tunable, the optimum condition of generating terahertz waves. The frequency band ranging from 1 to 4 THz is most profitable frequency band. Node-less Josephson waves along c-axis in the device could emit from the surface of the device with intense terahertz waves. Frequency tunable is needed from the view point of the usability of the device generating the terahertz waves.

2. Model Equation

The physical system 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 electric current. Maxwell equation is solved at the outside of IJJ.

The equations Eq.(1), Eq.(2) and Eq.(3) describing the dynamics of the phase difference, charge and electric field are given by,

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

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

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

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

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

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

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

At outside of IJJ, Maxwell equation is as follows,

$$\frac{\partial \boldsymbol{E}'}{\partial t'}=\nabla\times\boldsymbol{B}'-\boldsymbol{J}' \tag{8}$$

$$\frac{\partial \boldsymbol{B}'}{\partial t'}=-\nabla\times\boldsymbol{E}'. \tag{9}$$

where $\Delta^{(2)} A_k$ is $A_{k+1}-2A_k+A_{k-1}$, k: number of insulator layer between superconducting 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 thikness, φ_k: gauge-invariant phase difference in insulator layer k, $\rho_{k+1/2}$ charge density in superconducting layer in k+1/2, E^z_k: 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. These equations are solved by Finite Difference Method.

3. Computational feature of simulation for generating terahertz waves using superconductor device

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

A scale of space and time of simulation is 1nm ~several hundred m and 10^8 steps by 10as. We assume that the system is uniform along the y-axis and makes two-dimensional calculation in the x-z plan for basic studies of the device generating terahertz waves. We used the finite difference method to perform the numerical simulation. The simulation uses very large sized nonlinear equations heretofore difficult to compute; for a simulation using 10^6 spatial cells in the x-z two-dimensional model, it would take two years to simulate one case using a personal computer with a 2GHz processor. In addition, many times of simulation, which are with combination of many different material properties, device shapes, current supply methods and current control etc, are needed to design and optimize the superconductor device generating terahertz waves. Therefore, the simulation requires high performance computational resource.

4. Simulation

(1) Simulation model

Terahertz waves of Josephson plasma excite in the high-temperature-superconductor device and emit from the edge of the device. Therefore, study of Josephson plasma excitation in the device is a key to understand the optimum condition of generating the terahertz waves, and here we focus on the excitation of Josephson plasma in the device. We use the model of Josephson plasma waves perfectly reflecting at the device surface to focus on the studying the excitation of Josephson plasma in the device. This model simulates the device in the vacuum, in which Josephson plasma waves reflect at the surface almost perfectly. We can model the boundary condition of Josephson plasma reflecting perfectly at the device surface by setting the constant external magnetic field at the surface of the device. When Josephson plasma waves reflect perfectly at the device surface, the part of inputted energy converts to the energy of excited Josephson plasma waves and then to the heat energy. We assume that the device is well cooled and the temperature of the device is constant. Figure 1 shows a model of the device of $Bi_2Sr_2CaCu_2O_{8-d}$ generating the terahertz waves.

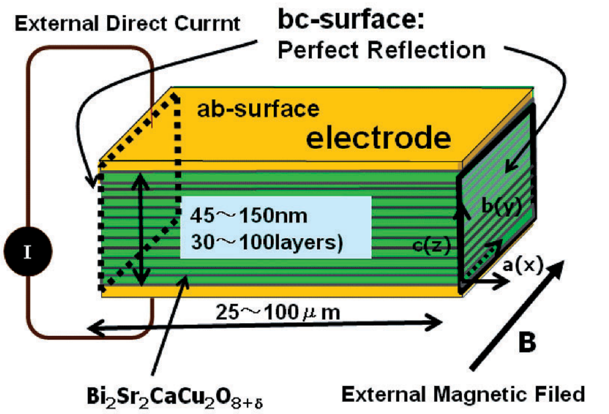

Fig. 1 Schematic diagram of the device generating terahertz waves. $Bi_2Sr_2CaCu_2O_{8-d}$ forms IJJ. The device is consists of the IJJ and electrodes of gold. The green part shows the IJJ sandwiched by electrodes. An external current flows uniformly in the junctions in the direction of the z axis. An external magnetic field is applied to the direction of the y-axis. Perfect reflection of Josephson plasma waves at device surface is imposed by setting the constant external magnetic field at the surface of the device.

(2) Setting the range of parameters

Fixed parameters

We set the parameters constant; $s = 3Å$, $D = 15Å$, $\mu = 0.6Å$, $\alpha = 0.1$, $\beta = 0.02$.

Variable parameters

Here, we set the range of variable parameters based on dispersion relation using perturbative method for Eq. (1). We apply perturbative method to Eq. (1) and get the dispersion relation;

$$\omega' = \sqrt{1 + \frac{B^{y'}}{1 + 2\frac{\lambda_{ab}^2}{sD}\left(1 - \cos\left(\frac{\pi q^z}{N+1}\right)\right)}} \quad (10)$$

Using this dispersion relation, we have the relation between frequency of Josephson plasma excitation and parameters as follows:

$$f \approx \sqrt{\left(\frac{\omega_p}{2\pi}\right)^2 + \left(1 - \cos\left(\frac{\pi q^z}{N+1}\right)\right)^{-1}\left(\frac{cD\sqrt{sD}}{\sqrt{2\varepsilon_c}\,\Phi_0}\frac{B^y}{\lambda_{ab}}\right)^2}, \quad (11)$$

where we used $\frac{\lambda_{ab}}{\lambda_c} \ll 1.0$, and N is a number of layers. We could estimate the range of parameters that cause the excitation of Josephson plasma over the range of 1~4 THz based on Eq.(11); $B^y = 0.25 \sim 2.0T$ for typical value of $\lambda_{ab} = 0.202\mu m$, $N = 30 \sim 100$. However Eq.(11) suggest that λ_c, the length of device along x-axis L_x do not have an influence on the frequency of Josephson plasma excitation, we assign the values to $L_x = 25, 50, 100\mu m$ to make sure that.

(3) Numerical simulation

We have performed the simulation using the equations (1)~(7) to simplify the numerical equations. We apply a magnetic field along the y-axis. We change the normalized external current J/J_c from 0.0 to the excess current that passed the value causing the node-less Josephson plasma wave.

5. Results

(1) Relation between Josephson plasma excitation and static part of electric field $\bar{E}^{z'}$ averaged in ac-plane

Figure 2 shows an example of the relation between static and oscillation part of reduced electric field $E^{z'}$ averaged in ac-plane in device. The static part of reduced electric field $\bar{E}^{z'}$ means the external voltage impressed on the device and causes AC Josephson effects. The oscillation part of $\Delta E^{z'}$ reduced electric field $E^{z'}$ averaged in ac-plane of the device represents the intensity of Josephson plasma excitation in the device. We are interested in the excitation of node-less plasma waves that emit from the surface of the device to space as terahertz waves with high intensity. Static parts of $\bar{E}^{z'}$ for node-less waves of Josephson plasma excitation state are bandwise as shown in Fig. 2 in most cases. Therefore, we have measured the range of static part of $\bar{E}^{z'}$ corresponding to Josephson plasma excitation state of node-less waves, in which oscillation part $\Delta E^{z'}$ has significant value, by changing each parameters; $\frac{\lambda_{ab}}{B^{y'}}$, λ_c, N, $L_{x'}$.

(2) Relation between the frequency range of Josephson plasma excitation and $\frac{B^y}{\lambda_{ab}}$.

The range of static part of $\bar{E}^{z'}$ is corresponding to Josephson frequency. Then, using the relation between static and oscillation part of reduced electric field $E^{z'}$, we show the relation between the frequency range for Josephson plasma excitation of node-less waves and $\frac{B^y}{\lambda_{ab}}$ in Fig. 3. Figure 3

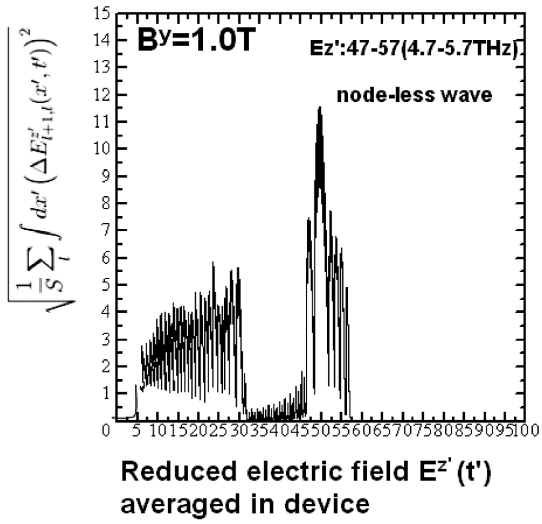

Fig. 2 Relation between static part of reduced electric field $\bar{E}^{z'}$ and $\sqrt{\frac{1}{s'}\sum_l \int D'dx'(\Delta E^{z'}_{l+1,l}(x',t'))^2}$ root mean square of amplitude of oscillation part $\Delta E^{z'}$ for reduced electric field $E^{z'}$ averaged in ac-plane in device, by changing the external current $J' = J/J_c$ = 0 ~ 1.2 with λ_c = 150μm, λ_{ab} = 0.202μm, $L_{x'}$ = 50μm.

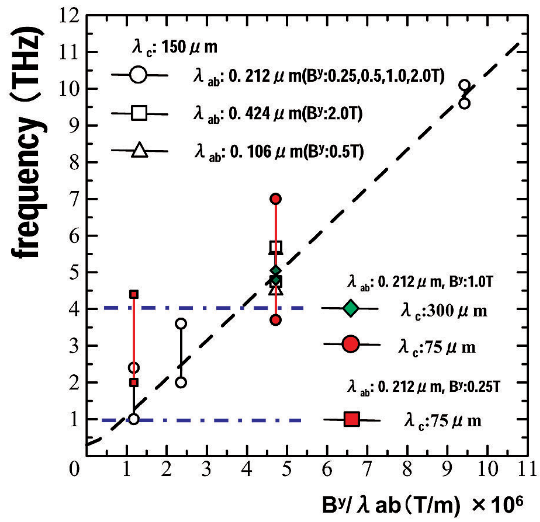

Fig. 3 Relation between the frequency range of Josephson plasma excitation and $\frac{B^y}{\lambda_{ab}}$. Dashed line shows the curve from Eq. (11).

show that we could qualitatively control the excitation frequency of node-less Josephson plasma waves by the parameter $\frac{B^y}{\lambda_{ab}}$. Therefore, using Fig. 3, we could control the parameter $\frac{B^y}{\lambda_{ab}}$ to generate the terahertz waves of 1~4THz. When $\frac{B^y}{\lambda_{ab}}$ or λ_c is large, the excitation frequency from simulation is well corresponding to that of Eq.(11). On the other hand when $\frac{B^y}{\lambda_{ab}}$ or λ_c is small, the excitaiton frequency from simulation deviates from that of Eq.(11), and the range of excitaiton frequency expand. Therefore, we could control the range of frequency tunable by λ_c with fixed frequency.

6. Conclusion and future work

In this year, we have performed many simulations and shown the control parameters and optimum condition of generating terahertz waves. This result will accelerate putting the high-temperature-superconductor device generating terahertz waves to practical use in industry. Next stage, we will focus on the applications of terahertz waves such as development of practical device generating terahertz waves, the use of interaction between terahertz waves and matter that is base for research of the new spectroscopic analysis method for material and bio-science. A large-scale and high-performance simulation using the Earth Simulator as high-end computers is an effective methodology for finding novel phenomena and developing new technologies in the forefront of emerging science and technology.

References

[1] M. Tachiki, T. Koyama, and S.Takahashi, Electromagnetic phenomena related to a low frequancy plasma in cuprate superconductors, Phys. Rev. B 10, 7065 (1994).

[2] M. Tachiki, T. Koyama, and S. Takahashi, in: G. Deutcher, A. Revcolevshi (Eds.), Coherent I High Temperature Superconductors, World Scientific, Singapore, 371 (1996).

[3] M. Tachiki, M. Iizuka, K. Minami, S. Tejima, and H. Nakamura, Emission of continuus choherent terahertz waves with tubnable frequency by intrinsic Josephosn junctions, Phys. Rev. B 71, 134515 (2005).

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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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発振条件の発見を行った。平成17年度においては、本シミュレーション結果に基づく国内、韓国での実験により発振が確認され、発振理論とデバイス設計概念が検証された。

平成17年度は、実用的素子開発に具体的指針を与えるためのシミュレーションを実施し、発振制御パラメータ(外部磁場、Inductive 係数、層数‥)の影響把握、最適発振条件の解明を実施した。

次年度以降は、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。さらに、今後は、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