Large-scale Simulation for a Terahertz Resonance Superconductor Device

Project Representative
Masashi Tachiki Research Organization for Information Science and Technology

Authors
Mikio Iizuka *1, Masashi Tachiki *1 and Hisashi Nakamura *1
*1 Research Organization for Information Science and Technology

The terahertz wave, especially in the range of 0.3-10THz, is one of key technology seed for the next generation of industries. It is well known that the wave has a high potential to be applied to the novel detectors by which one could find some kind of material such as explosives indirectly or easily in various packages at security scenes. However nobody has developed yet that wave generator, then there is still lack of the fundamental knowledge on the interaction between terahertz wave and material for identification of spectral line with the detectors.

We have carried out so far the simulation researches on the generation of the continuous terahertz waves in high-temperature superconductor, in order to develop a new generator. Theoretical analysis has shown that the terahertz wave has strong nonlinearity and complex behavior over multi-scale of time and space as generating wave in the high-temperature superconductor. For dealing with those phenomena our simulation researches need the high-performance supercomputer such as the Earth Simulator for large scale simulations. With the help of this computing power, we have revealed so far the new mechanism and the conditions on generating terahertz wave as well as characteristics of the emitted terahertz wave from the device. As result, we have succeeded in making clear the control parameters and the optimum condition for generating the continuous waves in the range of 1-3 terahertz.

Based on these progresses, our next theme is to develop a practical device. Before that, we need to make clear the condition of generating the terahertz wave stably. The stable generation can be due to the stable Josephson plasma excitation. Thus, in this term, we focused on studing the condition for the stable excitation of Josephson plasma wave in a wide range of frequency.

Keywords: high-temperature-superconductor, device, generating terahertz waves, stable excitation, Josephson plasma, high performance computational resource

1. Introduction

The electromagnetic wave in the terahertz region has been recognized as a new light-source of spectroscopic analyses for dense or soft materials and bio-polymers, medical diagnoses and information technology. Most of leading countries in the world have already pushed to develop terahertz technology as the next-generation infrastructure for sciences and industries. It is however pointed out that there is still lack of generator of the continuous terahertz wave in the world. In our research on the new light-source by the continuous terahertz waves, we have proposed to use high-temperature superconductor, HTC, as a device for generating the terahertz wave. In HTC, CuO_2 layers as superconductor and insulating layers are alternately stacked up and form layers of Josephson junction, so called intrinsic Josephson junctions (IJJ).

The theory [1, 2] has already predicted a possibility that there exists the plasma oscillation in the frequency range of terahertz and that the plasma wave could excite and emit as terahertz wave out of the edge of the device. The theory also indicated that Josephson plasma behaves in strong nonlinearity as complex system. Thus it had been very hard way for experimentalist to verify the theory through developing the IJJ device for generating the terahertz wave.

Simulation appears to be a reasonable approach for the complex phenomena such as the IJJ device and emission of Terahertz wave. This is because it is able to make clear numerically system dynamics in detail through parametric survey. Complexity requires simulation with high capability and large capacity of computer. For example, simulation in this case has to cover the broad space from 1nm to several hundred μm and huge time steps of 10^8 steps by 10as step width. This means that it takes a couple of year to make the simulation only for a case if one uses a personal computer. The Earth Simulator is therefore expected to be a reasonable computer for solving this problem.

Our simulation approach has been revealed out so far some mechanisms on excitation of Josephson plasma and continuous emission of terahertz waves out of the IJJ device under external magnetic field [3, 4]. Along our simulation research Japanese or Korean experimentalists [5] had announced in 2006 that they succeed to detect the terahertz wave emitted from the IJJ device.

Thus, in this term, we focused on stable excitation of terahertz wave, in order for experimentalists to develop their IJJ device.

2. Model equations

A device of the intrinsic Josephson junction of the high temperature superconductors and its surrounding external space was modeled for our simulation.

As for the IJJ device, some coupling equations of the gauge-invariant phase difference φ_k, charge, electric field and magnetic field were derived from Josephson relations and Maxwell's equations.

The gauge-invariant-phase difference is a phase-difference of wave function in insulating layer k between superconducting layer l + 1 and l layer. It is related to Josephson's superconducting electric current. For the external space, Maxwell's equations were used for describing the emission of electromagnetic wave. Let us show our model equations for simulation.

Eqs.(1), (2), (3) and (4) describing the dynamics of the phase difference, charge, electric field and magnetic field are given by

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

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

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

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

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 quasi-particles, ε dielectric constant of the insulating layers, μ the Debye length, Φo flux unit, Jc critical current density, s, D conducting and insulating layer thickness, $\rho_{k+1/2}$ 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, $\lambda_c = (c\Phi o/8\pi^2 D\, Jc)^{1/2}$ penetration depth in the c axis direction, $\beta = 4\pi\sigma\,\lambda_c/(\varepsilon^{0.5} c)$, $\omega_p = c/(\lambda_c\,\varepsilon^{0.5})$ Josephson plasma frequency, $t' = \omega_p\, t$ normalized time, $x' = x/\lambda_c$ normalized coordinate in x direction, $\rho' = \rho(Jc/\lambda_c\omega_p)$ normalized charge density and $E'^z = E^z(2\pi cD/\Phi o\ \omega_p)$ normalized electric field.

3. Computational feature of simulation

Based on the model equations, we carried out simulation in order to make it clear various effects on stable excitation of Josephson plasma by varying conditions of numerical experiments. In this simulation, the space is scaled from 1nm to several hundred μm and time from atta to nano second. Thus it is assumed that the system is uniform along the y-axis, and two-dimensional simulation in the x-z plane appears to be reasonable for studies of the device exciting Josephson plasma. The time dependent finite difference method was adopted for solving its numerical processes.

Our simulation needs to treat nonlinear equations with large space and time steps; approximately 10^6 spatial meshcells for the x-z two-dimensional model and by 10^8 time steps of 10as. Many parametric simulations are also required to study the effects of various conditions on the excitation of Josephson plasma, with combination of different material properties, device shapes, current supply methods and current control etc.

Hence it becomes large- scale simulation.

4. Simulation

We studied the conditions for the stable excitation of Josephson plasma in the wide range of frequency, using simulation model as shown in Fig. 1.

The excitation of Josephson plasma in the IJJ device was studied by simulating various interactions between fluxons

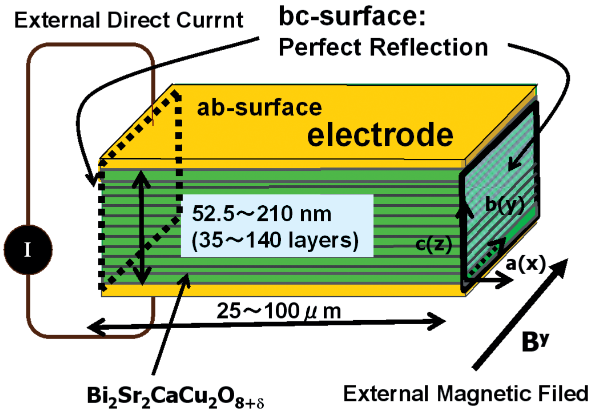

Fig. 1 Schematic diagram of the device generating terahertz waves. $Bi_2\,Sr_2\,CaCu_2\,O_{8+\delta}$ forms IJJ. The device is consists of HTC crystal and electrodes. The green part shows the IJJ sandwiched by electrodes. An external current flows uniformly in the junctions in the direction of the z axis. An external magnetic field is applied to y-direction.

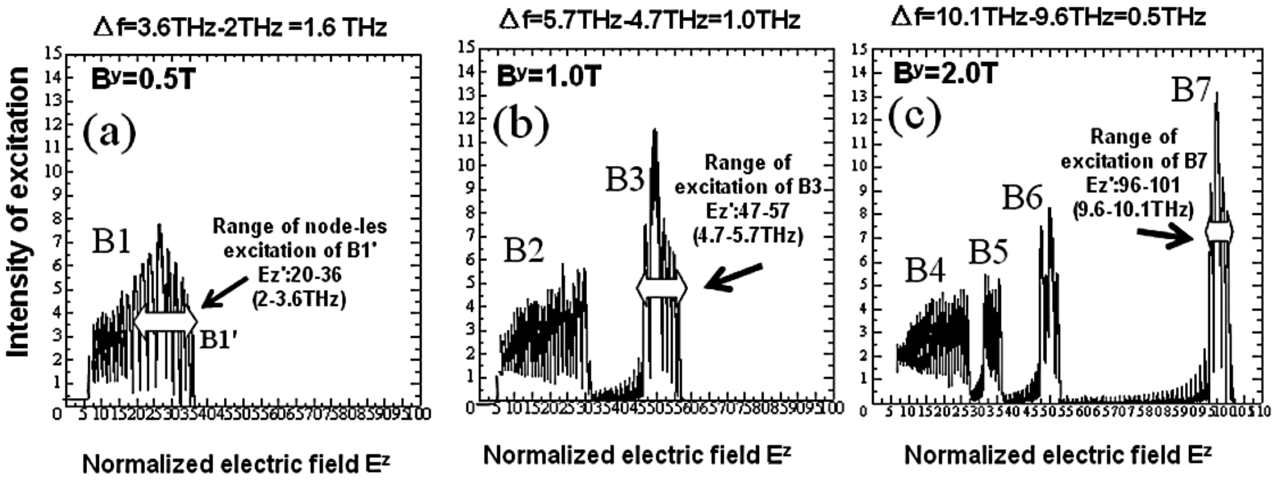

Fig. 2 Relations between the intensity of Josephson plasma excitation and the normalized constant part of electric field $E^{z'}$ averaged in device. External magnetic field B^y: 0.5, 1.0, 2.0T. λc = 150μm, λab = 0.2μm, Lx = 50μm, N = 70.

and Josephson plasma reflected at the inner wall of the device.

We performed simulation with many combinations of parameter: different material properties, device length, current supply methods and current control etc. Parameters are as follows: (a) constant parameters s = 3Å, D = 15Å, β = 0.02, μ = 0.6μm and α = 0.1, (b) variable parameters λc = 75 ~ 300μm, λab = 0.1 ~ 0.4μm, Lx = 25 ~ 100μm, N = 35, 70, 140 layers. The normalized external current J/Jc was varied from 0.0 to Jc and Jc to 0 to study the effect of increasing and decreasing path of external current.

5. Result

Figure 2 shows the relations between the intensity of Josephson plasma excitation and the normalized constant part of electric field $E^{z'}$ under the external magnetic fields; B^y: 0.5, 1.0, 2.0T. The intensity of excitation is defined as amplitude of oscillating part of normalized electric field of Josephson plasma. The frequency of Josephson plasma is described as $f = 2e/h(s+D)E^z$ in relation to the constant part of electric field E^z. It is found that there are some 'peaks' of the excitation of Josephson plasma. Thus we tagged those peaks as B1 in (a), B2 and B3 in (b), and B4, B5, B6 and B7 in (c).

In the device, Josephson plasma are oscillating with forms of node-less to (N/2–1)-nodes wave as shown in Fig. 3. Number of nodes along c-axis depends on value of $E^{z'}$.

The Josephson plasma wave is emitted out of the device and transformed into terahertz wave. If Josephson plasma wave shows oscillation with one-node to (N/2-1)-nodes, terahertz wave decreases its intensity due to interfering between the oscillation phases of different sign at the edge of the device. On the other hand, the oscillation phase of Josephson plasma wave with node-less wave indicates the same sign at the edge of the device. Thus, Josephson plasma wave with node-less wave is transformed into intense terahertz wave more than that those of one-node to (N/2-1)-nodes wave.

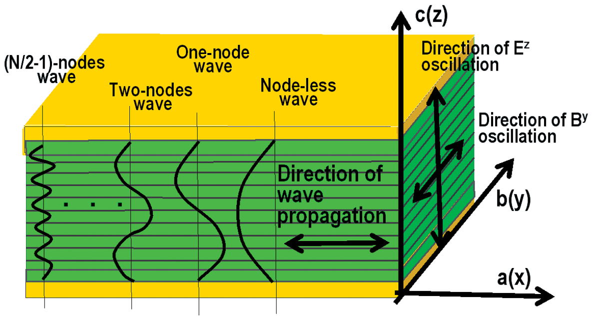

Fig. 3 Schematic diagram of waves along c-axis. Each Josephson plasma wave has no-node to (N/2-1)-nodes along c-axis in ab-plane of IJJ device.

In Fig. 2, Josephson plasma wave shows node-less wave in B1', B3 and B7, one-node wave in B6 and two-node wave in B5. In addition, large amplitude of oscillation is also observed on these points of 'peaks.' Therefore the peaks in B1', B3 and B7 are regarded as stable excitation.

In Fig. 2 we defined a frequency band for the stable excitation of Josephson plasma wave as Δf on B1', B3 and B7. Comparing with these frequency bands as shown in Fig. 4, it is clear that Δf is in inversely proportion to intensity of the external magnetic field B^y. This means that a control parameter for the stability of Josephson plasma excitation is determined with regard to external magnetic field B^y. As example shown in Fig. 2(a) for B^y = 0.5T, Δf extends its band up to 1.6THz , corresponding to the stable excitation with 2 ~ 3.6THz that might be in applicable range of terahertz wave for real usage.

6. Conclusion and future work

In this year, we studied the conditions for the stable exci-

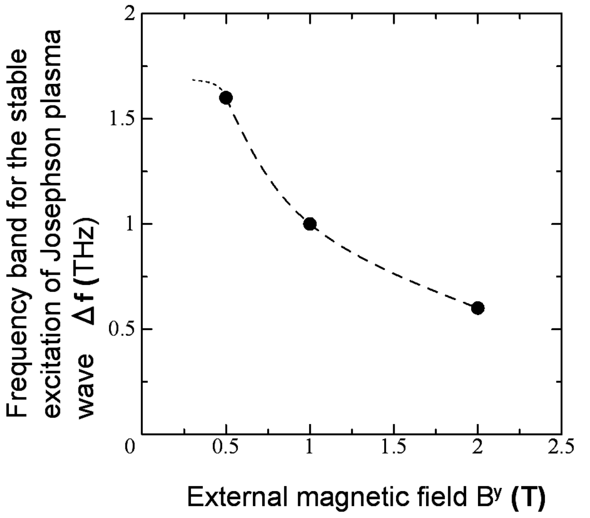

Fig. 4 The external magnetic field B^y dependency of the frequency band width of stable Josephson plasma excitation. λc = 150μm, λab = 0.2μm, Lx = 50μm, N = 70.

tation of Josephson plasma wave over the wide range of frequency. The result would be useful for scientists and industries to design or develop IJJ device generating the continuous terahertz wave for real applications.

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

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) Masashi Tachiki, Mikio Iizuka, Kazuro Minami, Syogo Tejima, and Hisashi Nakamura, Emission of continuus choherent terahertz waves with tubnable frequency by intrinsic Josephosn junctions, Phys. Rev. B 71, 134515 (2005).

(4) M. Iizuka, K. Minami, S. Tejima, M. Tachiki and H. Nakamura: Large-scale simulation on a high-temperature-superconductor device generating the continuous terahertz wave continuously, Journal of the Earth Simulator, Vol.8, Nov. (2007).

(5) M.-H. Bae, H.-J. Lee, and J-H. Choi, PRL 98, 027002 (2007).

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　高度情報科学技術研究機構

著者
飯塚　幹夫[*1]，立木　昌[*1]，中村　寿[*1]
＊1　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、テラヘルツ波技術の発展の課題として(a)良い連続波テラヘルツ光源の開発と(b)物質とテラヘルツ波相互作用の詳細の理解がある。本研究ではこの課題解決に向け地球シミュレータを用いた大規模シミュレーションを用いて取り組む。具体的には、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き、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デバイス開発のための大規模シミュレーションを行う。また、物質とテラヘルツ波相互作用解析のために量子効果を取り込みつつ大規模な分子動力学計算が可能な強結合モデルをベースとした解析モデルを開発し大規模シミュレーションを行なう。

平成17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ない、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18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。平成19年度には実用的素子開発のための安定発振条件を研究した。

次年度は、昨年度より開始した産業応用に向けた研究をさらに進め、多様な発振方式、導波管、テラヘルツ波と物質の相互作用など光源及び応用システム開発へ向けた大規模シミュレーションにより基礎的設計知識を得ることを目指し、3次元解析でのペタスケール大規模シミュレーションの要件をモデル、計算規模、計算機資源等の観点からまとめ、次ステップの準備とする。この成果を学界、産業界へ提示する。

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