Large-scale Simulation for a Terahertz Resonance Superconductors Device

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We have carried out a large-scale simulation of the Josephson-coupled superconductor device with a potential of teraherz resonance phenomena. This simulation needs high-performance computational resource, because 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 μ m and 10^8 steps 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. Last year, we succeed to find that there is a new mechanism of terahertz waves emission, the emission power is high with milli watt (mW) order and the frequency is easily tuned by varying the applied current, via simulation. This year, we have studied further the details of emitting mechanism and developed a three-dimensional code for designing the device system of terahertz wave emission.

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 (HTSC) that have connected multi layered structure, was found by professor Uchida of The University of Tokyo in 1992. HTSC 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 (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 systematized the new phenomenon in the theory, and showed that the plasma oscillation wtih terahertz order is theoretically possible [1],[2]. 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 coverted into a terahertz electromagnetic wave at an edge of IJJ.

IJJ has a potential for an important industrial infrastructure technology in next generation; the super-high-speed computer, the storage elements, and high-capacity and high-speed optical communication conversion devices in the highly-networked information society. 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 could put this technology to practical use in the world, it brings a large advantage to Japan in the area of a high-speed computer and the information on telecommunications equipment, etc. and has the possibility to throw up the Japanese original new industry as a strategic technology in Japan.

The development of the device for the terahertz electromagnetic wave generation is a very difficult only by the experiment, because IJJ have a very strong nonlinearity and the complex behavior. The development 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 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. So to speak, it can be said that only the earth simulator will enable the next generation super-high-speed computer to develop. At this year, we have studied detail of the new mechanism of terahertz waves emission and have developed 3 dimentioanl code for a design and develpment of terahertz waves emisson device. Let us to show our simulation results.

2. Model Equation

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 electric 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, and electric field, magnetic field and superconducting current are given by

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

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

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

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

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

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

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

At outside of IJJ, Maxwell equation is as fallws,

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

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

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_k^z : electric field in z direction at insulator layer k, λ_{ab} : a parameter related to the current in the CuO$_2$ superconducting layer, $\lambda_c=\sqrt{\frac{c\Phi_0}{8\pi^2DJ_c}}$: penetration depth from the bc

surface plane, $\beta=\frac{4\pi\sigma\lambda_c}{\sqrt{\varepsilon}c}$, $\omega_p=\frac{c}{\sqrt{\varepsilon}\lambda_c}$: 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 electoric field, $\boldsymbol{E}'=\boldsymbol{E}/(2\pi cD/\Phi_0\omega_p)$: normalized electoric field, $\boldsymbol{B}'=\boldsymbol{B}/(2\Phi_0\omega_p/cD)$: 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, 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 IJJ simulations 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 terahertz 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 plan for basic studies and use the 3 dimentional model for the design and development of device. We use the finite difference method to perform the numerical simulation. The simulation uses very large sized nonlinear equations heretofore difficult
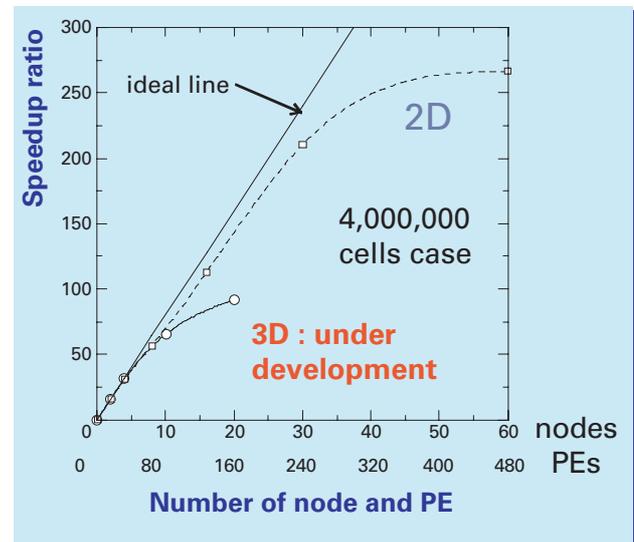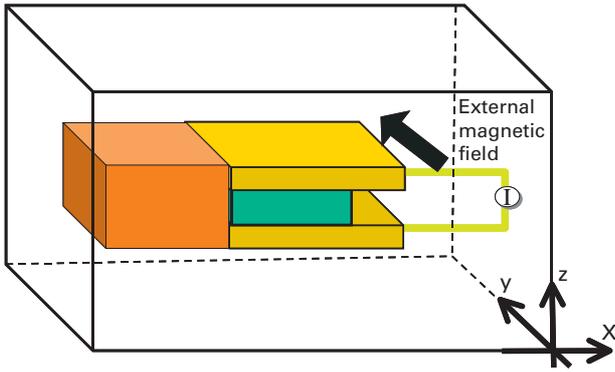

Fig. 1 Parallel performance of 2D, 3D code.

Fig. 2 Schematic diagram of prototype device for terahertz emission. $Bi_2Sr_2CaCu_2O_{8-d}$ forms an IJJ. 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.

to compute. Figure 1 show a performance of 2D simulation code, and figure 2 shows a performance of 3D code which is now under develpment. These figures show that ES drastically reduces the solution time.

4. Simulation Models and Results

At this year, we have studied detail the new mechanism of terahertz waves emission using 2D model as follows. Figure 2 shows a prototype unit of a terahertz emission device using, in this case, $Bi_2Sr_2CaCu_2O_{8-d}$.

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 λ_{ab} = 0.4 μm, λ_c = 200 μm, s = 3Å, d = 12Å, μ = 0.6Å, α = 0.1, β = 0.01 ~ 0.05, and the number of layers = 20 ~ 1000, 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 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 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.

Let us consider a case of the node-less Josephson plasma wave along the z-axis (the transverse plasma) that can be converted into the electromagnetic wave with the same frequency. In this case the emitted electromagnetic wave propagates approximately in the negative direction of the x-axis.
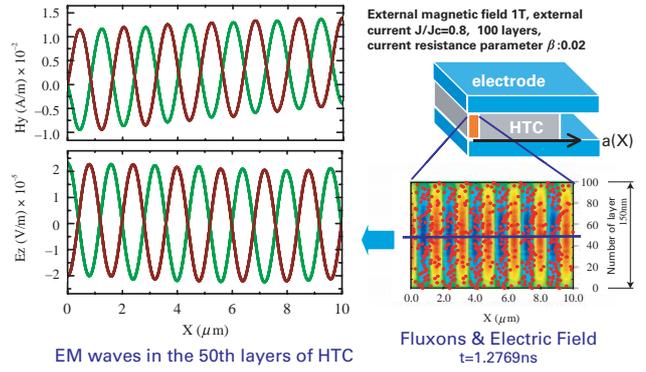

Fig. 3 Excited electromagnetic field and cluster of distorted fluxons.

We found that the stacking number that fulfill the condition is 100 layers under the magnetic field of 1 Tesla. From that results, we found the new mechanism of terahertz waves emission as fllows. 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 as shown in Fig. 3. 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 is small, the fluxons have ordered distribution. When the number of layer is large, the fluxons form clusters with disordered fluxons. Many researcher of this area predict and belive that the ordered fluxons only excit the coherent electromagnetic waves. Figure 3 shows that the fluxons with disordered distribution can excit the coherent electromagnetic waves and the ordered fluxons didn't necessarily excit the coherent electromagnetic waves.

5. Future Work and conclusion

In this year, we have studied detail of the mechanism of terahertz waves emission and have found the new mechnism. We have developed 3 dimentioanl code for a design and develpment of terahertz waves emisson devices.

Next stage, 3 dimentonal code for design and develoment of devices will be optimized for ES. 3 dimantional fluxons dynamics in IJJ of 3D model will be studied. A more wide and general condition for generation of continuous coherent terahertz waves will be studied.

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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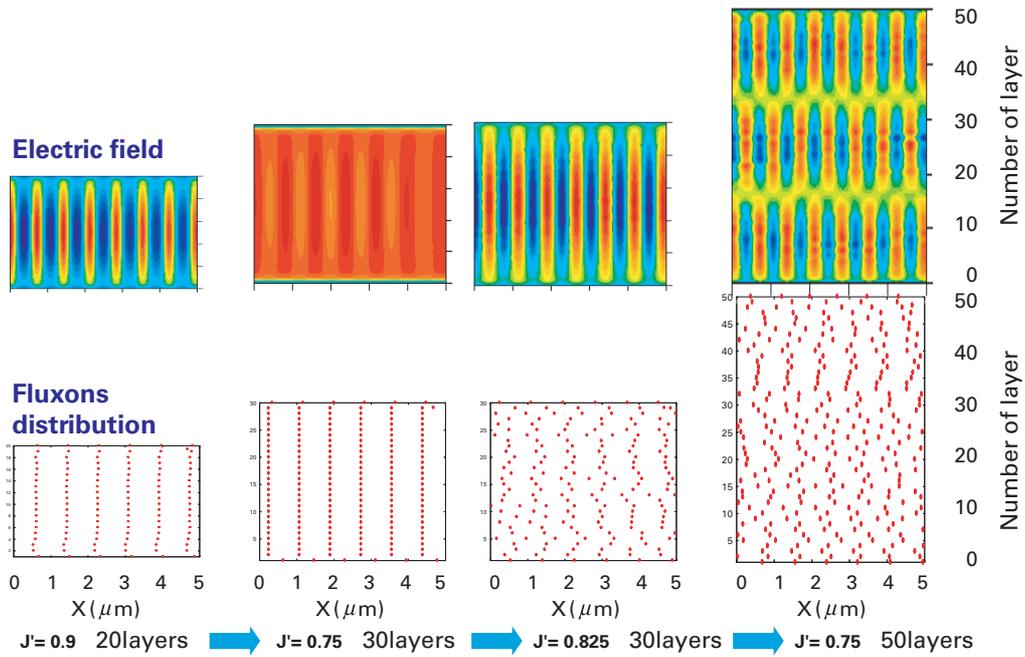[1] M.Tachiki, T.Koyama, and S.Takahashi, Electromagnetic phenomena related to a low frequency plasma in cuprate

Fig. 4 Relation between number of layers and fluxons distribution.

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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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　テラヘルツ波は光と電磁波の中間域($0.3\sim10$THz)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、$1\sim4$THz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14/15年度で新しい発振メカニズムと最適発振条件を発見し、平成16年度では、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、米国物理学会誌(PRB)に掲載された。さらに、本シミュレーション結果に基づき国内で行われた実験により、本発振原理の基本的部分実験的に確認された。また、平成16年度では、設計・開発用3Dコードの開発を実施した。

　平成17年度は、平成16年度の成果に基づき、さらに広範囲なパラメータでの発振条件の解明、設計・開発用3Dコードを用いて実デバイス開発のためのシミュレーション技術開発を行う予定である。

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