Large-scale Simulation for a Terahertz Resonance Superconductor Device

Project Representative
Masashi Tachiki University of Tokyo

Authors
Mikio Iizuka [*1], Satoshi Nakamura [*1], Masashi Tachiki [*2] and Hisashi Nakamura [*1]
*1 Research Organization for Information Science and Technology
*2 University of Tokyo

The terahertz wave, especially in the range of 0.3-10 THz, is one of key technology seed for the next generation of industries. It is well known that the wave has 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 an enough light source of the wave, then there is still lack of the fundamental knowledge on the interaction between terahertz waves and materials 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 the high-temperature superconductor, in order to develop a new light source. Theoretical analysis has shown that the phenomena of generating terahertz wave have strong nonlinearity and complex behavior over multi-scale of time and space in the high-temperature superconductor. For dealing with those phenomena our simulation researches need the high-performance supercomputer as the Earth Simulator and large scale simulations. With the help of this computing power, we have revealed so far the new mechanism and the conditions on generating terahertz waves as well as the characteristic of the emitted terahertz waves from the device. And we have succeeded in making clear the control parameters and the optimum condition for generating the continuous waves in the range of 1-4 terahertz.

Following the progress of study of IJJ device for generating the terahertz wave, we have studied terahertz applications. An understanding of interaction between terahertz waves and material is base of developing the terahertz applications such as terahertz sensing and terahertz high-tech devices. The interaction is also under strong nonlinearity and complex behavior over multi-scale of time and space. Therefore, we have studied the large-scale simulation model for the interaction between terahertz waves and nano-carbon material as first step of this research.

Based on these progresses, we have summarized the results of large-scale simulation for generating terahertz wave with IJJ device as design information of practical terahertz light source. And we have developed the large-scale simulation model of interaction between terahertz waves and nano-carbon material. As mentioned, we made preparations for next step of R & D for terahertz technology applications.

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

1. Introduction

The electromagnetic wave in the terahertz region has been recognized as the potential light for spectroscopic analyses on 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 technologies as the next generation infrastructure for sciences and industries. It is however pointed out that there is still a lack of light source of the continuous terahertz wave and less understandings of the interaction behavior between material and wave toward the advancement of terahertz technology.

In our research on a new light source of the continuous terahertz waves, we utilize the high-temperature superconductor, HTC, as a device for generating the terahertz wave. In HTC, the strongly superconducting CuO_2 layers and insulating layers are alternately stacked along the *c* axis of the crystals in this system. Those layers form a stack of many atomic-scale Josephson junctions, so called intrinsic Josephson junctions (IJJ).

A theory proposed in 1994 [1] has shown a possibility that there exists the plasma oscillation in the terahertz band and that the excited plasma wave could emit as terahertz wave from the edge of IJJ device.

It had been very hard way for experimentalist to design and develop the IJJ device for generating the terahertz wave under the strong nonlinearity and the complex behavior. Thus the simulation becomes indispensable approach for developing and designing the IJJ device. However it required high capability and large capacity in these computing for simulations because the simulation has to cover the broad space from 1nm to several hundred μm and huge time steps of 10^8 steps by 10as step width. For example, by roughly estimated it would take two years to make the simulation only for a case by using a personal computer. The Earth Simulator is therefore essentially utilized for solving this problem.

Our simulation research has been revealed out the mechanism, some conditions of generating the continuous terahertz-wave, and characteristics of the emitted terahertz waves out of the IJJ device under the external magnetic field [3, 4].

In the last year some Japanese or Korean experimentalists [5] had announced that they succeed to detect the terahertz waves emitted from the IJJ device by following our simulation research.

And besides, following the progress of study of IJJ device for generating the terahertz wave, we have studied terahertz applications. An understanding of interaction between terahertz waves and material is base of developing the terahertz applications such as terahertz sensing and terahertz high-tech devices. The interaction is also under strong nonlinearity and complex behavior over multi-scale of time and space. Therefore, we have developed the large-scale simulation model for the interaction between terahertz waves and nano-carbon material as first step.

Based on these progresses, we summarize the results of large-scale simulation for generating terahertz wave with IJJ device as design information of practical terahertz light source. And we summarize the large-scale simulation model of interaction between terahertz waves and nano-carbon material. As mentioned above we made preparations for next step of R & D for terahertz technology applications.

2. Model equations

2.1 Equations of IJJ device [1, 2]

We consider the IJJ device of HTC crystal in the external medium. In the IJJ device, we solve the coupling equations of the gauge-invariant phase difference, charge, electric field and magnetic field. Those equations are derived from Josephson relations and Maxwell's equations. The gauge-invariant phase difference φ_k 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. In the external medium, we solve Maxwell's equations. Let us show model equations for simulation of IJJ device.

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

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

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

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

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

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 unit magnetic state, 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' = ωp t normalized time, x' = x/λ_c normalized coordinate in x direction, ρ' = ρ(J_c/$\lambda_c\omega_p$) normalized charge density and $E'^z = E^z(2\pi cD/\Phi o\omega_p)$ normalized electric field.

2.2 Equations of interaction between terahertz waves and nano-carbon material

First, we focus on the nano-carbon material which is most hopeful nano-block. We consider the nano-carbon material in the external medium. The utilization of simulation of interaction between terahertz waves and material in quantum phenomena is fruitful for advanced science and technology. However, first principle quantum calculation requires huge computational volume. Thus, we use the DFTB (density-functional tight-binding) model which requires less computational volume than that of first principle quantum calculation. We combine the DFTB model and Maxwell's equations to solve the quantum state of electrons in atomics system under external electro-magnetic field. We use the Green's function with recursion method for DFTB Hamiltonian to reduce the computational volume as O(N). The DFTB Hamiltonian under electro-magnetic field is as follows,

$$
\begin{aligned}
&H_{\mathrm{DFTB}} = \sum_{j\zeta}\sum_{j'\zeta'}\sum_{\sigma} \exp\{(-\mathrm{i}e/\hbar c)\,\theta_{jj'}(t)\} \\
&\Big[\delta_{jj'}\,\delta_{\zeta\zeta'} + t^{LDA}_{j\zeta j\zeta'\sigma} \\
&+ \delta_{jj'}\left\{\delta U^{H}_{j\zeta\zeta'}(\{\boldsymbol{R}(\boldsymbol{t})\}) + \delta V^{ex}_{j\zeta\zeta}(\{\boldsymbol{R}(\boldsymbol{t})\})\right\} \\
&+ \left\{\delta_{\zeta\zeta'}\{-e\delta\phi_o(\boldsymbol{R}_j(t),t)\} - e\boldsymbol{P}_{\zeta\zeta'}\cdot \boldsymbol{E}_{\boldsymbol{r}=\boldsymbol{R}_{j(t)}}\right\}\Big] \\
&a_{j\zeta\sigma}(t)^{\dagger}\, a_{j'\zeta'\sigma}(t) \qquad (5)
\end{aligned}
$$

where $\theta_{jj'}(t)$ is phase difference between j and j' atom by magnetic field, $t^{LDA}_{j\zeta j'\zeta'\sigma}$ tight binding parameter, $\delta U^{H}_{j\zeta\zeta'}$ Hartree term, $\delta V^{ex}_{j\zeta\zeta'}$ exchange and correlation term, $\delta\phi_o$ electric field, $\boldsymbol{P}_{\zeta\zeta'}$ polarization and ζ atomic orbital S, Px, Py, Pz.

3. Computational feature of simulation

Based on the model equations, we perform the simulation which makes clear the effects of various conditions on the stable excitation of Josephson plasma by using equations of IJJ device and develop the large-scale simulation model of interaction between terahertz wave and material for terahertz applications. In the simulation, the scale of space is 1 nm ~ several hundred μm and the scale of time nano second.

For simulation of IJJ device, we use the time dependent finite difference method to perform the numerical simulation. The simulation treats very large sized nonlinear equations heretofore difficult to compute with using order 10^6 spatial cells in the x-z two-dimensional model and 10^8 time steps by 10as step width. In addition, many cases of simulation are needed 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 became large-scale simulation.

For simulation of the interaction between terahertz wave and material, we use the O(N) method for DFTB model to reduce the computational volume for solving the quantum state of electrons in atomics system under external electromagnetic field. However, the simulation treats very large sized nonlinear equations and large-scale time & space as same as the simulation of IJJ device. Then, this also becomes the large-scale simulation.

4. IJJ simulation and information for design of IJJ device

We studied the excitation of Josephson plasma and emission of terahertz waves from IJJ device. Typical simulation model is shown in Fig. 1.

Results of many simulations gave us the information for design of IJJ device generating terahertz waves. Here we show the typical results. Figure 2 shows the relation between frequency of excited Josephson plasma and parameter $B^y/\lambda ab$ with changing λc. Symbols connected by line shows the range of frequency of excited Jpsephson plasma. The frequencies are almost proportional to parameter $B^y/\lambda ab$. The width of frequency range of excited Jpsephson plasma changes for value of λc. This results show that we can control the frequency of terahertz wave generated by IJJ device with parameter $B^y/\lambda ab$ and λc. Dash line shows an analytical solution of linearized gauge-invariant phase difference equa-

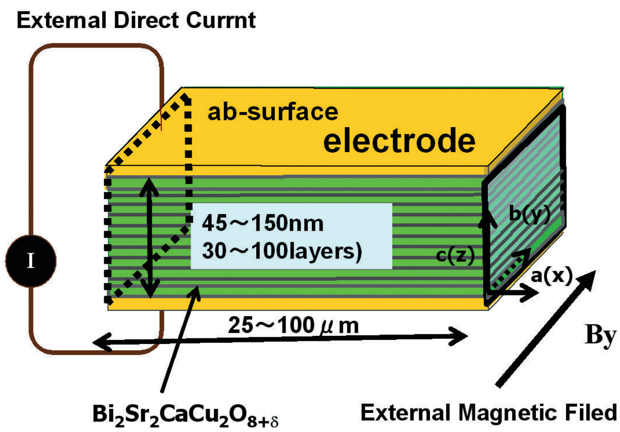

Fig. 1 Schematic diagram of the device generating terahertz waves. $Bi_2Sr_2CaCu_2O_{8+\delta}$ forms IJJ. The device is consists of HTC crystal and electrodes. The green part shows the IJJ sandwiched by electrodes. An external current flows uniformly in the junctions in the direction of the z axis. An external magnetic field is applied to y-direction.

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.

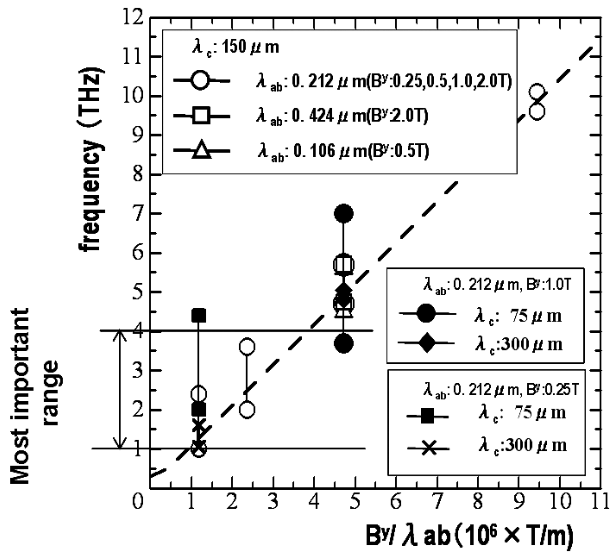

Fig. 2 Relation between frequency of excited Josephson plasma and parameter $B^y/\lambda ab$ with changing λc. Symbols connected by line shows the range of frequency of excited Jpsephson plasma. Dash line shows an analytical solution of linearized gauge-invariant phase difference equation.

tion. When $B^y/\lambda ab$ and λc are large value, results of simulation are correspond with the analytical solution. However, when $B^y/\lambda ab$ and λc are small value, results of simulation are not correspond with the analytical solution. $B^y/\lambda ab$ and λc are small value in the frequency range of 1 ~ 4 THz that is important frequency range for terahertz applications. Then, we can not use the analytical solution and must use the results of large-scale simulations for design of IJJ device.

5. Performance of large-scale simulation model of interaction between terahertz waves and nano-carbon material

We have developed the large-scale simulation model of interaction between terahertz waves and nano-carbon material. For the simulation of large-scale atomics system, O(N) attribute of analysis method is needed to achieve the reasonable time to solution. Figure 3. shows the relation between number of atoms and volume of calculation (Gflop/SCF) for DFTB model under external electro-magnetic field. This result shows that the developed large-scale simulation model is O(N) method.

6. Conclusion and future work

In this year, we have made preparations for next step of R & D for terahertz technology applications. Based on these progresses, we will develop the peta-scale large-scale simulation model with study of new algorithm for parallel and memory usage control etc. Those results would be useful for scientists and industries to design or develop their device of the continuous terahertz wave and real applications.

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

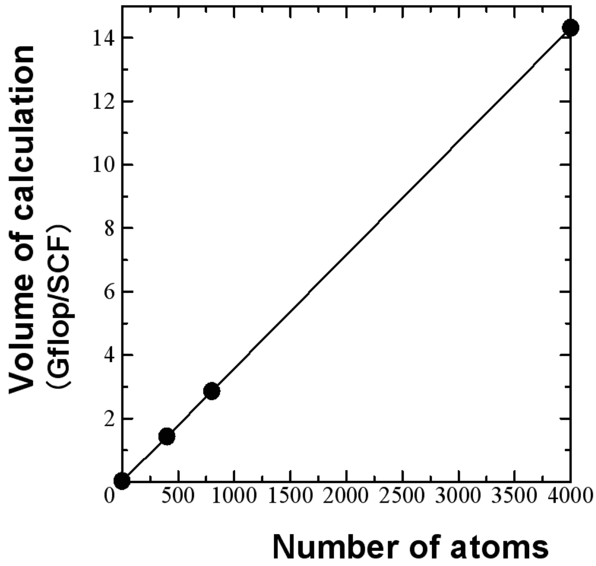

Fig. 3 Relation between number of atoms and volume of calculation for DFTB model.

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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　　東京大学

著者
飯塚　幹夫*1，中村　　賢*1，立木　　昌*2，中村　　寿*1
＊1　高度情報科学技術研究機構
＊2　東京大学

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)テラヘルツ波の応用へ向けた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とDFT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。

今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るともに次のステップへの準備を進めた。その結果、連続波テラヘルツ波光源として有望な高温超電導体を使った素子の設計要件が分かった。また、テラヘルツ応用のための、テラヘルツ波中に置かれた物質の応答計算の展望が開けた。また3次元解析でのペタスケール大規模シミュレーション要件が分かった。

今後は、実用化のための応用計算へ向かう。そのために実用的光源開発においては、高温超伝導体素子とそれに接続する給電ワイヤーや導波管等の3次元光源全システムの大規模シミュレーションモデルの開発を行なっていく。また物質・テラヘルツ波の相互作用理解では、多種原子系のテラヘルツ波と物質・生命分子相互作用(外場、内場応答)の大規模シミュレーションモデルの開発をおこなっていく。これらの計算規模はペタスケールであり、そのため、モデル拡張、並列性能向上、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を進めていく予定である。

キーワード：高温超伝導体素子，テラヘルツ波生成，大規模計算資源