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Large-scale Simulation on a High-Temperature-Superconductor Device Generating the Terahertz Wave Continuously

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Abstract Large-scale simulation has been carried out on a high-temperature-superconductor device generating terahertz waves, based on a theoretical prediction presented by Tachiki, et al. Since the resonance phenomena of Josephson plasma in the device are expected to show strong complexity by nonlinearity, we needed to trace it through large-scale simulation, dealing with the dynamic behavior of Josephson plasma in the device by solving a coupled model of Josephson plasma and Maxwell's equations under the time-dependent finite-difference method (TDFDM). The simulation treated multi-scale space ranging from nanometer to several hundred micron meter, and multi-scale time from 10 atto-second to nano-second with 10^8 steps respectively. As the simulation required large volume of memory and fast speed processing such as high-performance computing, we used the Earth Simulator to perform the simulation effectively. Until now, we have investigated the mechanism emitting terahertz waves and its controllability through parametric simulation. In this report, the recent results are summarized.

Keywords: generating the terahertz waves, high temperature superconductor, continuous terahertz waves, large-scale simulation

1. Introduction

Terahertz wave exists in a band between micro wave and infrared light. The wave ranging from 0.3 to 10 terahertz has been targeted by many researchers because the waves are able to resonate with vibration of molecule of cells and to penetrate into various chemical or anatomy. These characteristics solicit them to utilize the targeted terahertz wave for advanced sensor technologies for the nano- or bio-science & technology and security measures to counterterrorism as shown in Fig. 1.

The targeted terahertz waves are classified into two categories; pulse waves and continuous waves. The pulsed waves are usually generated by the laser systems with the organic nonlinear optical crystals or p-type germanium (p-Ge) lasers. There is however still shortfall in the output power of the pulse waves for practical use due to the broad range spectrum of pulse waves. In order to cover the shortfall of the pulse wave, the continuous terahertz wave has been focused because of the expected high output-power and the controllability for the practical application. Thus, the quantum cascade laser, backward-wave oscillator (BWO) and laser mixing methods have been developed so far in USA, Europe and Japan. However these methods have failed to gain the required power level in the most profitable frequency band ranging from 1 to 4 THz as shown in Fig. 2.

For this situation, Tachiki et al. have proposed a unique theory [1] that shows a possibility that the targeted continuous terahertz waves can be generated in a high-temperature superconductor(HTC) placed in a magnetic field and impressed with direct currents, as a device shown in Fig. 3. In the superconductor, a superconducting layer of CuO_2 and insulating layer of $Bi_2Sr_2Ca\ Cu_2O_{8+\delta}$, with the thickness of 3Å and 12Å, are alternatively stacked along the c-axis(z-axis). These layers form a naturally multiconnected Josephson junction as called the intrinsic Josephson junction (IJJ). In the junction, it is well known that there appears the excitation wave as called the Josephson plasma. Its frequency is in the range of terahertz. Tachiki's theory is based on the dynamics equations of the Josephson plasma, showing intense nonlinearity in interaction between superconductor current and electro magnetic field. Thus some experimentalists aiming at generating of the targeted terahertz wave have faced severe

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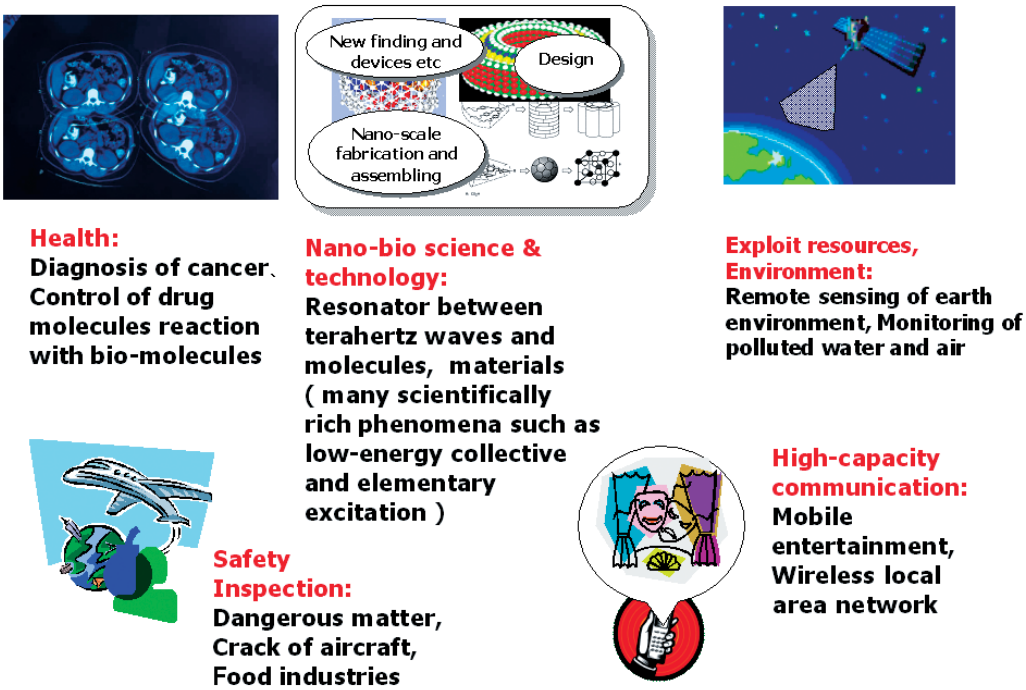

Fig. 1 Applications of terahertz waves.

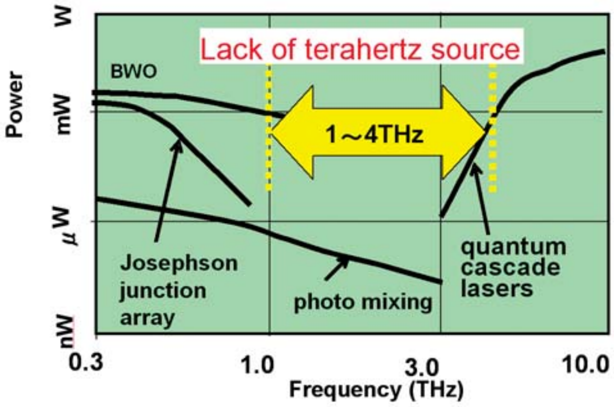

Fig. 2 Relation of terahertz waves frequency and power by conventional terahertz waves generating technology. Practical technology of generating terahertz waves is needed.

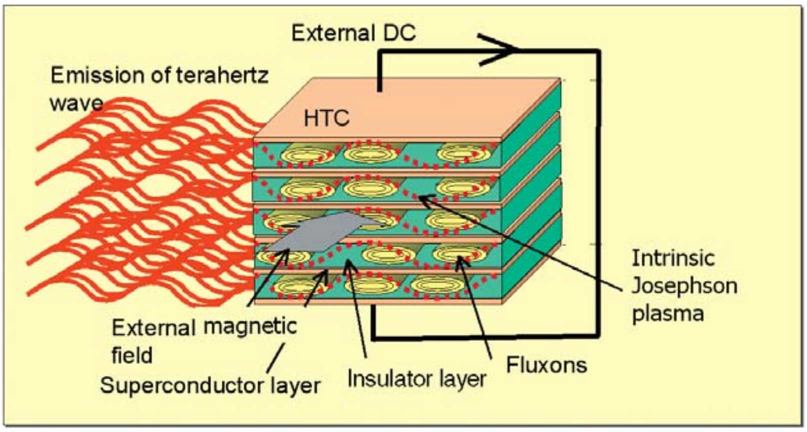

Fig. 3 High-temperature-superconductor (HTC): naturally multi-connected Josephson junction called intrinsic Josephson junction (IJJ).

work for searching their optimum device design, depending on their experimental ways. If they tried to get their optimum parameters through appropriate simulation by using their computers, the capability and capacity of the computers in those days were so limited and insufficient for revealing the complex system of the Josephson plasma dynamics in the high-temperature superconductor device. As an example, R. Kleiner[2] predicted the stable coherent motion of regular lattice of moving fluxons with standing wave in the electric field, by simulating his model based on a theory similar to Tachiki's. Machida et. al.[3] simulated only the structural transitions and stable regular lattice of fluxons accompanied by traveling electro-magnetic wave with the same velocity as that of the plasma wave. Then they simulated Tachiki's theory by using the finite difference method in space, Runge-kutta method in time and periodic boundary along x-axis. For Kleiner and Machida cases, the analysis region was limited to narrow space where the length in the x-axis direction was from 10 to 30 μm, the number of layer in the c-axis direction was from 20 to 40 compared with the experimental region where the length in the x-axis direction is 5 to 200 μm, the number of layer in the c-axis direction was from 5 to 1000. Their analysis conditions were also insufficient to reveal the mechanism of complex and nonlinear dynamics of Josephson plasma. In order for researchers to solve the mechanism systematically, it is needed to set the space and time fully, vary parameters widely, model device structure and boundary conditions realistically and run many simulation cases, through conserving physical values accurately over the phenomena.

The appearance of the Earth Simulator in 2002 enabled us to challenge a large- and multi-scale simulation covering the scale in space from 10Å to hundreds of μm and in time from 10 atto-second to several nano-second with 10^8 time steps and millions of cells, as shown in Fig. 4.

2. Simulation model

In this research, we have conducted a system simulation dealing with the resonance of Josephson plasma and generation of the targeted terahertz waves from the device.

As for the basic device design, we assumed a configuration as shown in Fig. 4. The generation of the terahertz waves is modeled by the equations describing dynamics of the Josephson plasma in the high-temperature-superconductor device and Maxwell's equations describing propagation of the terahertz to the external space. In the device, the equations are as follows [1, 4, 5];

$$\begin{aligned}&\left(1-\frac{\lambda_{ab}^{2}}{sD}\Delta^{(2)}\right)\left[\frac{\partial^{2}\varphi_{k}}{\partial t'^{2}}+\beta\frac{\partial\varphi_{k}}{\partial t'}+sin(\varphi_{k})+\right.\\&\left.s'\frac{\varepsilon\mu^{2}}{sD}\left(\Delta^{(1)}\frac{\partial\rho'_{k}}{\partial t'}+\beta\Delta^{(1)}\rho'_{k}\right)\right]=\frac{\partial^{2}\varphi_{k}}{\partial x'^{2}}+\frac{\partial^{2}\varphi_{k}}{\partial y'^{2}},\end{aligned}\tag{1}$$

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

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

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

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

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

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

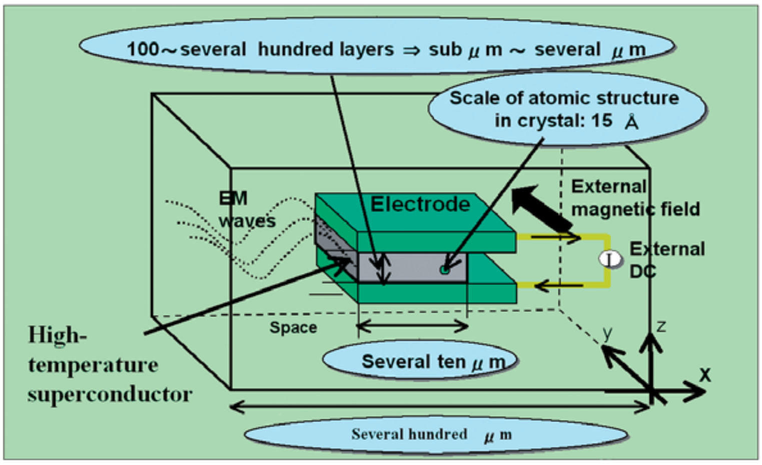

Fig. 4 Space-time scale of generating terahertz waves using HTC device.

Using these equations, we solve gauge-invariant phase difference, charge, electric and magnetic field. The gauge-invariant phase difference is defined between superconducting layer l+1 and l. It gives the Josephson's superconducting current. In the outside space of high-temperature-superconductor device, Maxwell equation is presented as follows;

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

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

In theses equations, $\Delta^{(2)} A_k$ is $A_{k+1}-2A_k+A_{k-1}$, k: the numbers of insulator layer between superconducting layer l and l+1, φ_k gauge-invariant phase difference in insulator layer k, $\rho'_{k+1/2}$: normalized charge density in superconducting layer in k+1/2, E'^{z}_{k}: normalized electric field in z direction at insulator layer k, B'^{y}_{k}: normalized magnetic field in y direction at insulator layer k, Φ_O: flux unit, Jc: critical current density, s, D: superconducting and insulating layer thickness, μ: the Debye length, λab: penetration depth in the ab-plane, $\lambda_c = \sqrt{\frac{c\Phi_0}{8\pi^2 DJ_c}}$: penetration depth in the bc-plane, $\beta = \frac{4\pi\sigma\lambda_c}{\sqrt{\varepsilon}\, c}$: normalized conductivity of the quasi-particles, σ: conductivity of the quasi-particles along c-axis, ε: dielectric constant of the insulating layers, $\omega_p = \frac{c}{\sqrt{\varepsilon}\,\lambda_c}$: Josephson plasma frequency, $t' = \omega_p t$: normalized time, $x' = x/\lambda c$: normalized coordinate in x direction, $\rho' = \rho\lambda c\omega_p/Jc$: normalized charge density, $\mathbf{E}' = \mathbf{E}/ (2\pi cD/\Phi 0\omega p)$: normalized electric field vector, $\mathbf{B}' = \mathbf{B}/ (2\Phi 0\omega p/cD)$: normalized magnetic field vector, $J' = J/Jc$.

The equation of gauge invariant phase difference forms sin-Goldon equations for each set of insulating and superconducting layer. The sin-Goldon equations on all of set in the super-conductor are solved through the coupling variables as follows; Josephson current $\sin \varphi_k$, normal current $\beta E'^{z}$ and displace current dE'^{z}/dt'. The system of these equations behave nonlinearly because of the term of $\sin \varphi_k$.

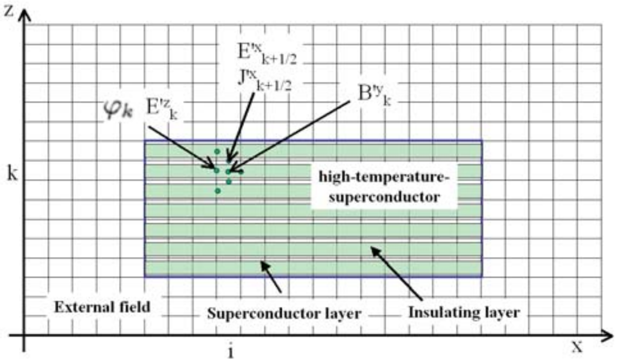

Fig. 5 FDM mesh and variables allocations.

These equations are solved numerically by Time-Dependent Finite Difference Method (TDFDM). Variables of φ_k, $E'^{z}_{k,}$ $E'^{x}_{k+1/2}$ and $J'^{x}_{k+1/2}$ are allocated on an edge of cell, variable of B'^{y}_{k} is allocated on the center of cell and variable of $\rho'_{k+1/2}$ is allocated on the corner of cell as shown in Fig. 5.

We have conducted the large-scale simulations in order to search the optimum conditions generating terahertz waves by using the Earth Simulator with the conditions of Table 1.

3. Simulation results [6, 7]

The simulation has shown that the device of the intrinsic Josephson junction works as a cavity for resonance. The Josephson plasma appears as standing wave when interval of the center of AC Josephson currents, i.e. clusters of disordered fluxons, coincides with the electromagnetic waves lengths of cavity resonance as shown in Fig. 6. In the multilayer case, fluxons do not always position regularly in each layers. When one looks down upon the fluxon distribution over a superconductor, one can find that fluxons form clusters along the c-axis as shown in Fig. 7. Then the clusters of fluxons resonate with electromagnetic waves, changing their width and intervals of clusters. Therefore, the Josephson plasma holds excita-

Table 1

Material properties	Spatial dimension	External condition
$\lambda ab = 0.4\mu m$, $\lambda c = 100 \sim 200\mu m$, s = 3Å, D = 12Å, μ = 0.6 Å, $\beta = 0.01 \sim 0.05$, dielectric constants along the z-axis in the IJJ and the dielectric constant of MgO to be ε = 10.	number of layers = 20 ~ 1000, device length along x-axis = 50 ~ 200μm.	magnetic field along the y-axis = 0.5 ~ 2 Tesla, normalized external current J'^{z} from 0.0 to 1.5 in steps of 0.0125.

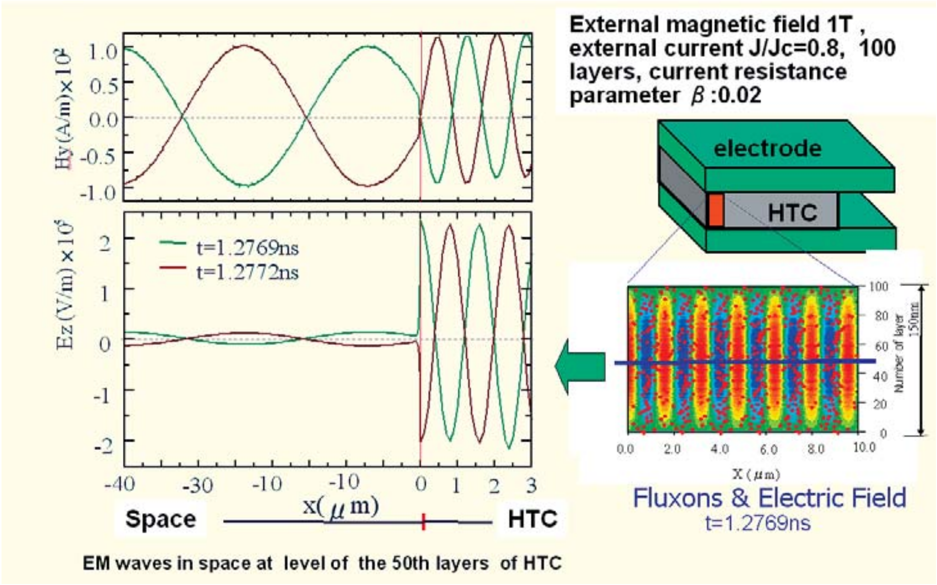

Fig. 6 Novel mechanism of terahertz emission (A). Ez, Hy plots show a snapshot of the electric and magnetic fields of the standing wave at the 50th insulating layer from the bottom surface in the direction of the z axis. The device works as a cavity, and the input energy is stored in a form of standing wave of the excited Josephson plasma. A part of the energy is emitted as terahertz waves.

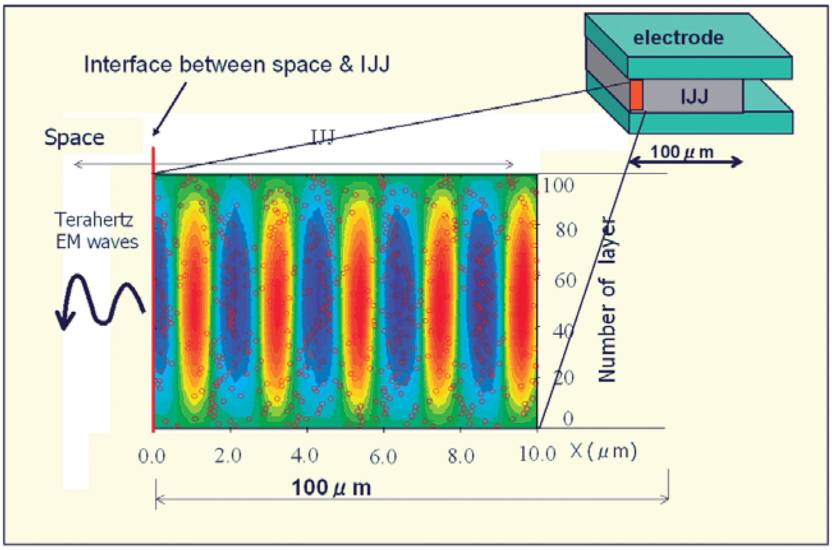

Fig. 7 Novel mechanism of terahertz emission (B). The red circles show the centers of fluxons. A disordered distribution of fluxons in HTC engages in the terahertz oscillation. The fluxons form a triangle lattice at zero external currents. When an external current is applied, the lattice moves with a small oscillation of fluxons. When the current exceeds a critical value, clusters are formed with disordered fluxons.

tion continuously and accumulates energy in the cavity. A certain part of the accumulated energy is emitted as continuous terahertz waves as shown in Fig 6, 7. The terahertz waves are emitted from the surface of the device continuously with a power of 2000 W/cm2 and the frequency of 2.2–3.0THz corresponding to the external direct current $J^{'z}$ of 0.9–1.2 as shown in Fig. 8 (left). By changing the external direct current and the voltage, the frequency of the emitted terahertz waves varies continuously as shown in Fig. 8 (right). The simulation also shows a possibility of generation of the targeted continuous terahertz waves through the Josephson plasma excited resonantly with the Josephson current under the magnetic field, as predicted by Tachiki theory. These results

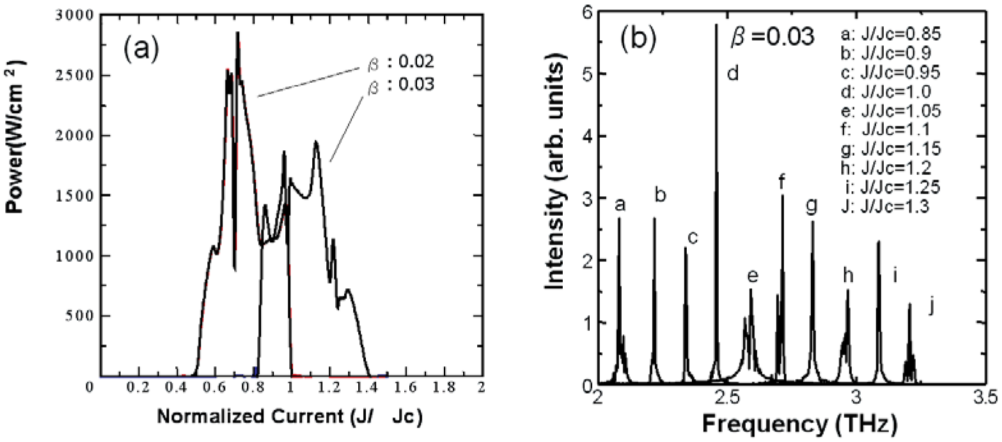

Fig. 8 Novel mechanism of terahertz emission (C). (a) Power distribution of emitted terahertz waves from HTC device. (b) Frequency spectrum of emitted terahertz waves from HTC device.

suggest that, by simulation, we can control the generation of terahertz waves and design the optimum device for application.

4. Effects of the Earth Simulator on analysis

As for the nonlinear phenomena generating terahertz waves from the device, many researchers have conducted so far their analyses by their computers as personal computers or clusters with less capability than supercomputers. The less computing capability could only allow them to model their device within the limited spaces of several ten layers along c-axis, 10 μm in length and 0.1 nano-second in time with cyclic boundary conditions. The approaches forced them to solve nonlinear dynamics of the Josephson plasma by introducing linear approximations in the infinite or semi-finite region. Then their methods were insufficient to reveal the nonlinear and systematic mechanics of generating the terahertz waves.

Fortunately, by taking advantage of high capability of the Earth Simulator, we carried out a large-scale and integrated system simulation for analyzing generation of terahertz waves. We could totally deal with the complex relations among the Josephson plasma, the supplied voltage, currents and the device configuration, including a surrounding space where terahertz waves propagate. Our approach led us to design a realistic device which is composed of the hundreds of layers of the Josephson junction, ranged from 50 to 200 μm of the length, and connected to the outer space through the edge surface. The time step was limited to 10 atto-second by courant condition dt = dx/c regarding atomistic spatial scale of 10Å. The simulation time was determined as 10 nano-second by the condition that system attains to meta-stable state. Our simulation steps reached to several hundred million time steps.

For TDFDM, we adopted a central finite difference method for discrete space and time. This is because the

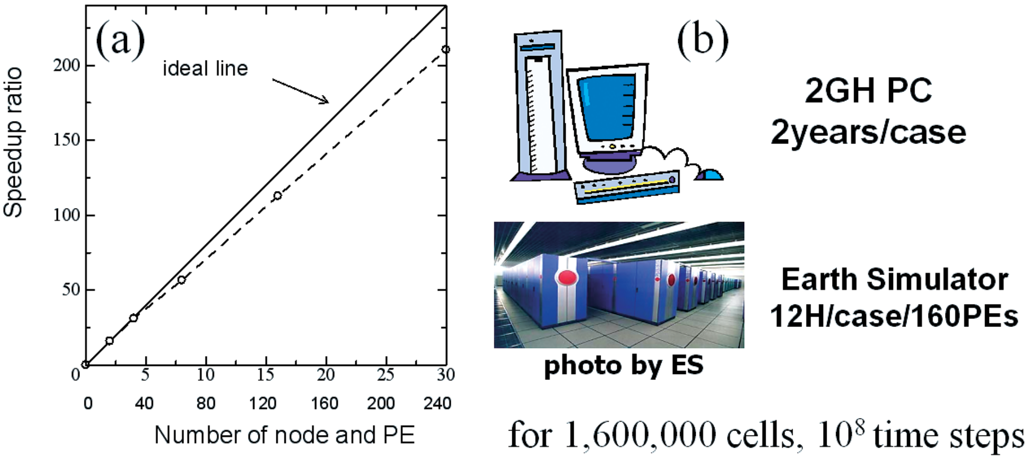

Fig. 9 Performance of simulation for a terahertz oscillating superconductor device on Earth Simulator. (a) scale of performance, (b) example of performance.

method enables us to calculate efficiently the large number of mesh on space and time, conserving physical values and reducing computing load. The effective performance on the Earth Simulator reached up to about 20% of the peak speed with 160 vector processors of 20 nodes on the Earth Simulator. It allows us to reduce the time to solution to 12 hours for a single case of parametric simulation and helps us to design the device system efficiently, while it was estimated for a personal computer of 2 GHz to take a couple of years to perform only a single simulation (see Fig. 9). By utilizing the capacity of the Earth Simulator effectively, we could carry out many cases at once.

Our example shows that the capability and capacity of the computer for researchers might be very important factors for their discoveries.

5. Summary

The large-scale simulations supported by the high-performance computing of the Erath Simulator, have been carried out in order to design the high-temperature superconductor device generating the continuous terahertz waves. The simulation revealed that there exists the complex mechanism emitting the continuous terahertz waves under some optimum conditions; fluxons dynamics, configuration of device, the supplied direct current and magnetic fields. The capability and capacity of the Earth Simulator could expand the searching space and parameters for finding optimum device design and generating terahertz wave. It led us to reach to the solution with short time period. 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.

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