Simulations of Transition Radiation from a Flat Target using CST Particle Studio

K V Lekomtsev¹, A S Aryshev¹, P V Karataev², M V Shevelev¹, A A Tishchenko³ and J Urakawa¹

¹High Energy Accelerator Research Organization (KEK), 1-1 Oho, Tsukuba, Ibaraki, 305-0801, Japan
²John Adams Institute at Royal Holloway University of London, Egham, Surrey, TW20 0EX, UK
³National Research Nuclear University “MEPhI”, Kashirskoe shosse 31, Moscow, 115409, Russia

E-mail: konstlek@post.kek.jp

Abstract. Numerical simulations of Backward Transition Radiation originating from a flat ideally conducting target inclined at 45 degrees with respect to a charge propagation direction are presented in this paper. The simulation results are compared with the theory for the wave and pre-wave zones. The main characteristics of the simulated radiation distributions are discussed in detail.

1. Introduction

In accelerator physics research various target geometries such as screens and gratings can be used as sources of radiation [1 - 4] and for beam diagnostics [5, 6]. Most of the target geometries have well developed analytical models describing characteristics of the radiation processes such as Transition, Diffraction and Smith – Purcell radiation [7]. However, these models are usually idealised and have applicability limitations when compared with experimental data. Advanced electromagnetic simulations provide an opportunity to perform simulations describing a real experiment in a more efficient manner, e.g. to take into account surrounding hardware of an experimental setup and, for example, identify potential sources of backgrounds.

Computer Simulation Technology (CST) Particle Studio (PS) is a specialist tool for a fast and accurate analysis of charged particle dynamics in 3D electromagnetic fields [8, 9]. The time domain particle-in-cell (PIC) solver of CST PS can perform a fully consistent simulation of particles and electromagnetic fields. It is based on the Finite Integration Method which adopts a self-consistent algorithm combining full Maxwell’s equations along with the classical and relativistic equations of motion.

The main goal of this study is to establish a certain level of confidence in the simulations by calculating well understood phenomenon such as Transition Radiation (TR) in CST PS and comparing it with the theory. Once a good agreement is achieved the radiation characteristics for more complex target geometries and radiation phenomena may be considered [4, 10]. In this report we present initial
simulations of Backward Transition Radiation (BTR) originating from a flat target positioned at 45 degrees with respect to a charge propagation direction. The calculations are performed for the millimetre wavelength range and a relativistic beam of electrons consisting of a single bunch.

2. PIC solver

In this section we will introduce the key concepts of the field calculation in the CST PS. The PIC solver calculates the development of the fields generated by a charged particle at discrete time samples. The fields are estimated at discrete points whereas the particles are tracked in continuous phase space. The field calculation is performed by the “Leap Frog” updating scheme. This method remains stable if the integration time step does not overcome the maximum usable time step which is related to the minimum mesh step used in the discretization of the considered geometry. The PIC solver is a self-consistent simulation method for particle tracking, therefore it is necessary to interpolate fields to provide feedback on the particle motion and calculate particle currents for the fields computation [8].

2.1 Finite Integration Theory

The PIC solver is based on MAFIA4, which is a general purpose electromagnetic simulation software package. It is based on the Finite Integration Theory [11]. This theory is a discretisation scheme which defines Maxwell’s equations in integral form on a dual non-co-ordinate grid doublet \( \{G,G'\} \). The non-co-ordinate discretisation scheme was introduced as an extension of the standard co-ordinate scheme in order to improve the capability of the grid to approximate curved boundaries. A discretisation of \( R^3 \) space into the doublet \( \{G,G'\} \) results in the so-called Maxwell’s Grid Equations [12]:

\[
\begin{align*}
\frac{\partial}{\partial t} \mathbf{b} &= \mathbf{C e} \\
\frac{\partial}{\partial t} \mathbf{d} &= \mathbf{C' h} \\
\mathbf{S_b} &= 0 \\
\mathbf{S'} \mathbf{d} &= \mathbf{q}
\end{align*}
\] (1)

where \( \mathbf{e} \) and \( \mathbf{h} \) are electric and magnetic grid voltage vectors, \( \mathbf{d}, \mathbf{j} \) and \( \mathbf{b} \) are the corresponding facet flux vectors. Discrete permeability, permittivity and conductivity are defined as:

\[
\begin{align*}
\mathbf{b} &= \mathbf{D_b h} \\
\mathbf{d} &= \mathbf{D_d e} \\
\mathbf{j} &= \mathbf{D_j e}
\end{align*}
\] (2)

The material matrices \( \mathbf{D_b}, \mathbf{D_d} \) and \( \mathbf{D_j} \) are sparse for a generalised case and diagonal for the dual orthogonal grid-doublet.

3. Problem definition.

A description of the considered geometry is presented in figure 1. In the top view one may see that a bunch of electrons enters the calculation domain along axis \( z \), it travels all the way to the target, hits the target surface and as a consequence BTR is generated in the direction of specular reflection. All planes confining the calculation domain act as free spaces, so the radiation leaves the domain without any additional reflections. The fields are calculated in the spherical wave approximation, i.e. the distance from the radiation source to the observation plane is larger compared to the considered wavelength. It is important to point out the difference between the pre-wave zone \( (\gamma^2 \lambda > d >> \gamma \lambda) \) and the wave zone \( (d >> \gamma^2 \lambda) \) of the radiation formation, where \( d \) is the distance between the target centre and the observation plane. In case of the wave zone the radiation source is point-like and the radiation wave may be considered as a plane wave. In case of the pre-wave zone the radiation source cannot be represented as point-like any more, because one has to consider the interference between the spherical waves emitted from individual points on the target surface. In the CST context for relativistic and
ultra-relativistic beam energies the spherical wave approximation is more applicable for the field calculations in the pre-wave zone, rather than the wave-zone. The BTR distributions are derived from the field intensities calculated at the observation plane for individual mesh cells.

![Figure 1. Schematic view of the considered geometry.](image)

The parameters used in the simulation are shown in table 1. The target is made of perfect electric conductor and positioned in vacuum at 45 degrees with respect to the beam propagation direction. Electron bunch is point-like in the transverse plane (size of the source is much smaller than the considered wavelength and the other characteristic dimensions). Longitudinally the charge is distributed over Gaussian with \( \sigma \) shown in table 1. The characteristic dimensions of the target (height and width) are larger than \( 2.5 \times \gamma \lambda \) for the radiation considered in the pre-wave zone and \( 5 \times \gamma \lambda \) for the radiation in the wave zone. This should limit the edge effects in the simulated radiation distributions [13, 14], especially for the wave zone due to the fact that the Fourier components of the transverse particle field are spatially limited within a circle of the radius \( \gamma \lambda \) [15].

Table 1. Model parameters.

| Parameter                                    | Value, units                          |
|----------------------------------------------|---------------------------------------|
| Beam energy (\( \gamma \))                  | 5 (wave zone) / 10 (pre-wave zone)    |
| Wavelength (\( \lambda \))                  | 10 – 12 mm                            |
| Target dimensions                            | 300 x 300 x 1 mm                      |
| Target material                              | Perfect Electric Conductor            |
| Calculation domain material                  | Vacuum                                |
| Target inclination angle                     | 45 deg.                               |
| Dimensions of the integration domain         | (1125/625/500/375) x 310 x 250 mm     |
| Target centre – observ. plane dist. (d)      | 1000/500/375/250 mm                   |
| \( \sigma \) of longitudinal charge distr. (\( \sigma_{\text{bunch}} \)) | 0.03 mm                               |
| Bunch charge (\( Q_{\text{bunch}} \))       | 0.5 nC                                |
4. Simulation results

In this chapter test simulations of the BTR in the wave and pre-wave zones of radiation formation will be compared with the existing theories. Firstly we shall consider the pre-wave zone. For comparison with the simulation results we shall use the theory developed in [16] using the Kirchhoff’s method for a flat target. In this paper analytical distribution of BTR from a finite ideally conducting target inclined at arbitrary angle to a charge trajectory was obtained for the distances from the target $\gamma^2 \lambda > d \gg \gamma \lambda$.

The CST radiation distributions are calculated at the observation plane and then may be plotted as 2D or 3D graphs. In order to identify the key properties of the BTR in the pre-wave zone three different volumes (calculation domains) were chosen. Each volume corresponded to a certain distance, $d$, from the target centre to the observation plane.

The radiation distributions plotted for three different distances from the target to the observation plane and the wavelength of 12 mm are shown in figure 2. According to the theory the radiation distribution in the Oxz plane has to demonstrate an asymmetry between peaks [7]. From figure 2 one may conclude that there is a clear asymmetry, well reproduced by the simulations for the distances 125 and 250 mm, also the larger the distance $d$ the smaller the distance between peaks. The latter is in agreement with the theory which states that for the TR distribution in the pre-wave zone the distance between peaks is larger compared to the wave zone [7].

Figures 3, 4 and 5 show a direct comparison between the simulated BTR distributions and the theoretical ones. For the distances $d = 125$ mm and $d = 250$ mm (figure 3 and 4) the asymmetry is in agreement with the theory, however the positions of the left hand side peaks are slightly shifted away from the centre of the distribution. The simulated curves are confined within the theoretical envelopes, but their overall shape is rather approximate. For the distance $d = 375$ mm the simulation demonstrates large intensity variation, which causes the disagreement in terms of peaks asymmetry as well as overall integrated intensity.

There might be several factors which cause this type of disagreement between the theory and the simulations. The most obvious one may appear due to incorrect meshing. It is important to point out that the CST automatic meshing tool should provide a reasonable result already at the first meshing iteration, especially for such simple geometries. The target edge effects may also contribute in the approximate shape of the simulated BTR distributions. More detailed studies will be required to investigate these issues.
$Q^2$ dependence, where $Q$ is the bunch charge, shall be tested since in this paper we consider coherent radiation which is observed when the radiation wavelength much larger than the bunch length and as a result radiation intensity is proportional to the number of electrons in the bunch squared [7]. Figure 6 shows the TR intensity distribution corresponding to four different bunch charges and normalised by the maximum value of the radiation distribution corresponding to the bunch charge of 2 nC. The shape remains the same for all radiation distributions; there is only change in the maximum intensity. By averaging the distributions in figure 6 over the range of angles from 45 to 135 deg. and normalising obtained values by the value corresponding to the average TR intensity for the bunch charge of 0.5 nC; one may obtain the intensity dependence as a function of a bunch charge. The $Q^2$ dependence is shown in figure 7, it is confirmed for four values of a bunch charge.

Now we shall move on to the study for the wave zone and consider larger vacuum cube corresponding to the distance $d = 1$ m from the target to the observation plane. The theory developed by Ter-Mikaelian within macroscopic approach in the wave zone for an inclined ideally conducting plate of a limited thickness was used for comparison with the simulations [15, p.223, eq. (25.27)-(25.28)]. Three chosen wavelengths in combination with the electron beam energy of $\gamma = 5$ satisfy the condition for the wave zone $d \gg \gamma^2 \lambda$. Figure 8 demonstrates the comparison of the theory with the simulation for the wavelength of 12 mm. The distribution within the angular region of 60 to 90 degrees demonstrates an oscillating shape confined within the theoretical envelope. By slightly
changing the wavelength to 11 mm (figure 9) we observe the change in the simulated radiation distribution. The dash-dot curve reproduces the asymmetry of the distribution, but the shape of the distribution is very approximate in relation to the theoretical curve with a large intensity variation. At the wavelength of 10 mm (figure 10) the simulated radiation distribution demonstrates less oscillating shape, but the left peak is much narrower compared to the theoretical curve.

Figure 8. BTR distributions in Oxz plane for $d = 1\, m$, $\gamma = 5$ and $\lambda = 12\, mm$ in the wave zone.

Figure 9. BTR distributions in Oxz plane for $d = 1\, m$, $\gamma = 5$ and $\lambda = 11\, mm$ in the wave zone.

Figure 10. BTR distributions in Oxz plane for $d = 1\, m$, $\gamma = 5$ and $\lambda = 10\, mm$ in the wave zone.

Figure 11. Shift of the simulated radiation distributions in figures 8 – 10.

5. Discussion and conclusions
The BTR from ideally conducting target was simulated and compared with the theory for the wave and the pre-wave zones. A reasonable qualitative agreement is achieved for the radiation distributions in the pre-wave zone. The asymmetry between peaks is in agreement with the theory; however calculation uncertainties or possibly target edge effects cause oscillating behaviour in the obtained distributions. Evaluation of the target edge effects in the wave zone will require additional studies.

The major issues that have to be addressed in the future work are the following. For the simulation results, especially in the wave zone, the distribution shapes are rather approximate and not in full agreement with the theory. The peaks asymmetry in the wave zone is not consistent for all frequencies.
Providing that the identified issues are resolved, this work may be considered to be the first step towards the usage of CST PS for simulations of other phenomena such as Diffraction radiation and Smith - Purcell radiation. This will be very important for the THz program at LUCX facility at KEK [17], where SPR gratings and other more advanced structures for THz radiation generation will be studied experimentally [3, 4].

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References

[1] Smirnov A V 2008 A high performance, fir radiator based on laser driven e-gun (In: Photonics Research Developments, ed V.P. Nilsson, Nova Science Publishers)
[2] Bashmakov Y A, Bondarenko T V, Komarov D A, Polozov S M, Rashchikov V I, Shchedrin I S, Smirnov A V, Voronkov A V and Tishchenko A A 2012 Problems of Atomic Science and Technology 79 (№3) 92
[3] Konoplev I, Aryshev A, Urakawa J, Lekomtsev K, Shevelev M and Seryi A 2013 Linac based broadband source of THz coherent Smith-Purcell radiation Proc. 38th International Conference IRMMW - THz (Mainz, Germany)
[4] Ponomarenko A A, Ryazanov M I, Strikhanov M N and Tishchenko A A 2013 NIM B 309 223
[5] Muto T, Araki S, Hamamatsu R, Hayano H, Hirose T, Karataev P, Naumenko G, Potylitsyn A and Urakawa J 2003 Phys. Rev. Lett. 90 104801
[6] Doucas G, Blackmore V, Ottewell, Perry C, Huggard P, Castro-Camus E, Johnston M, Lloyd Hughes J, Kimmitt M, Redlich B and Van der Meer A 2006 Phys. Rev. STAB 9 092801
[7] Potylitsyn A P, Ryazanov M I, Strikhanov M N and Tishchenko A A 2011 Diffraction radiation from relativistic particles (Springer)
[8] http://www.cst.com/Content/Products/PS/Overview.aspx
[9] Clemens M, Drobny S, Kruger S, Pinder P, Podebrad O, Schillinger B, Trapp B, Weiland T, Wilke M, Bartsch M, Becker U and Zhang M 1999 The electromagnetic simulation package MAFIA 4 Proc. ICCEA'99 pp 565 - 568
[10] Lekomtsev K V, Strikhanov M N and Tishchenko A A 2010 J. Phys.: Conf. Ser. 236 012023
[11] Weiland T 1977 Electronics and Communication (AEU) 31 116
[12] Weiland T 1996 Time domain electromagnetic field computation with finite difference methods International Journal of numerical modelling: electronic networks, devices and fields 9 295
[13] Shul’ga N F and Dobrovol’skii S N 2000 JETP 90 579
[14] Tishchenko A A, Strikhanov M N and Potylitsyn A P 2005 NIM B 227 63
[15] Ter-Mikaelian M L 1972 High-energy electromagnetic processes in condensed media (Wiley-Interscience)
[16] Karlovets D V and Potylitsyn A P 2008 NIM B 266 3738
[17] Aryshev A, Araki S, Fukuda M, Lekomtsev K, Shevelev M, Urakawa J, Potylitsyn A and Sakaue K 2013 Development of Advanced THz Generation Schemes at KEK LUCX Facility Proc. Particle Accelerator Society of Japan (Nagoya, Japan)