

Modeling of Bound Electron Effects in Particle-in-Cell Simulation

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Abstract. To include the bound electron effects in particle-in-cell (PIC) simulation, we propose a model in which the response of the dipole components of partially ionized ions to external electromagnetic fields can be included. Instead of treating the macro-ion particle as a single particle without an internal structure, the ions are considered to have a structure composed of a central nucleus and a bounded electron cloud in our model. The two parts experience the interactions of both the external electromagnetic fields and the internal Coulomb fields. In this way, the laser scattering effects by a partially ionized medium can be modeled properly in the PIC simulation. The laser propagation in a neutral medium and the Bragg scattering of the laser in crystal structure have been simulated with a PIC code modified based on our model as the benchmark. Our model may find applications to study some interesting problems, such as the x-ray laser-driven wakefield acceleration in crystals, the x-ray laser-driven high energy density physics, and intense laser propagation in partially ionized nonlinear optical materials, etc.

AMS subject classifications: 65Z05, 65M75

Key words: Particle-in-cell simulation, bound electrons, x-rays, crystals.

1 Introduction

Particle-in-cell (PIC) codes are widely used in plasma physics, especially in the simulation of laser-plasma interaction [1], such as in inertial confinement fusion [2], laser wakefield acceleration [3, 4], high order harmonics generation [5] and so on. However,

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the usual PIC codes only consider the electric currents contributed by free electrons and ions. These charged particles are modeled by particle clouds with special shapes and finite size, *i.e.* macro-particles. They are accelerated by external electromagnetic (EM) fields which are calculated from the Maxwell equations with source terms contributed by the charged particles. The internal EM properties of some particles, such as the dipole components contributed by the bound electrons and the central nucleus, are neglected. For particles with the same charge to mass ratio, their trajectories would be identical once their initial positions and velocities are the same. For example, the dynamical evolutions of a proton and a He^+ ion in normal PIC simulation are the same although there is one bound electron in the He^+ ion. Even though the ionization process is included in some PIC codes [6,7], the effects of the bound electrons of the ions are still neglected, where only the free electrons which are ionized will respond to the external EM fields.

On the other hand, in some applications, where the laser fields are not high enough to ionize all the electrons of the ions and the electromagnetic response of the bound electrons cannot be neglected, the usual PIC codes will be inadequate. In the wakefield acceleration by x-ray pulses in crystal [8], nanotubes, and dense plasmas [9–12], for example, although the x-ray propagation and the following wakefield acceleration have been numerically studied and even the radiation reaction and the collision have also been included [13], the response of the internal bound electrons has not been included. Some researchers have placed the ions periodically in space to simulate the crystals effect [14] and the fine modulation of the wake was observed in the simulations [15]. However, the laser diffraction by the crystal structure cannot be properly simulated since this effect is related to the response of the internal bound electrons.

In this paper, we extend the usual PIC algorithm to include the effects of the bound electrons. The ions that are not fully ionized are considered a two-body macro-particle. The Coulomb interaction connects the two bodies. Since one macro-particle in the PIC codes represents many real particles with similar trajectories in the phase space. To extend this model to the bound electrons, some limitations should be satisfied for specific applications. Otherwise, the effect of the bound electrons may be amplified due to the artificial coherence induced by the macro-particle. As long as the size of the macro-particles (λ_{pseu} , usually characterized by the grid resolution dx) is much smaller than the character scale length of the concerned problem (λ_c , usually characterized by the laser wavelength λ_0 , radiation wavelength or the plasma wavelength), the macro-particle can be used not only to represent the trajectory of the represented particles; but also to correctly handle the coherent synthesis effects of these particles. In this case, although the electrons are combined to different ions, their responses to the external EM fields can be coherent since $\lambda_{pseu} < \lambda_c$. The artificial coherence embedded in the macro-particle model correctly represents the real physical effect. Another issue is the different responses of each bound electron in the same ion. Usually, the bound electrons are in different quantum states. The outer ones may show a stronger response to the external fields since the Coulombic force from the ion is relatively weak. However, it is impossible to include these detailed quantum responses of different bound electrons in a PIC code and it is not necessary