Theoretical model used in the PIGLET software

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Abstract. *The theoretical model which is used for developing the PIGLET software is described. We discuss the FDTD realisation which is used in the software, including contribution from the conduction-band electrons, and present the formalism used for the 3 ionization rate models which are utilized in the simulations.*

1. Theoretical model

We consider a normal incidence of linearly polarized pulse, which travel in the direction $+z$, on a multi-layer structure, with all layers parallel to each other. We write the one-dimensional Maxwell equations which governs the time evolution of electric $E_x(z,t)$ and magnetic $H_y(z,t)$ fields during the pulse propagation as follows:

$$\frac{\partial E_x(z,t)}{\partial t} = \frac{1}{\epsilon_0}\left(-\frac{\partial H_y(z,t)}{\partial z} - J_{ion}(z,t) - \frac{\partial P_x(z,t)}{\partial t}\right) \tag{1}$$

$$\frac{\partial H_y(z,t)}{\partial t} = \frac{1}{\mu_0}\frac{\partial E_x(z,t)}{\partial z}, \tag{2}$$

where $P_x(z,t)$ is the polarization and $J_{ion}(z,t)$ is the current which describes the loss due to photoionization[1]: $J_{ion}(z,t) = N_0(1-\rho(z,t))\Gamma(z,t)E_g/E_z(z,t)$, whereby N_0 is the concentration of the entities, such as atoms or molecules, which can be ionized, $\rho(z,t)$ is the relative density of the ionized entities, $\Gamma(z,t)$ is the ionization rate, E_g is the bandgap. The material response and motion of the photoionized electrons in the conduction band is described by polarization $P_x(z,t)$, which is connected to the electric field $E_x(z,t)$ in the frequency domain by

$$P_x(z,\omega) = E_x(z,\omega)\left(\epsilon_\infty - \frac{N_0\rho e^2}{\epsilon_0 m_e\omega(\omega - i\nu)}\right) \tag{3}$$

where e is the electron charge, ν is the decay rate of the electron motion, and m_e is the effective electron mass. Finally, the time evolution of the relative plasma density is described by

$$\frac{\partial\rho(z,t)}{\partial t} = [1-\rho(z,t)]\Gamma(z,t). \tag{4}$$

For the ionization rate $\Gamma(z,t)$, three formalisms are included. In the Ivanov-Yudin formalism, the cycle-resolved ionization rate is given [2] by (in atomic units, that is, with frequency ω, time t and field $\mathcal{E}$ measured in the corresponding Hartree units $\omega_a = 0.26$ rad/as, $t_a = 24.2$ as, $x_a = 0.0529$ nm, and $\mathcal{E}_a = 514.2$ V/nm):

$$\Gamma(z,t) = \frac{\pi}{\tau_T} \exp\left(-\sigma_0 \frac{\langle 2\mathcal{E}(z,t)^2\rangle}{\omega^3}\right) \left[\frac{2\kappa^3}{\sqrt{\langle 2\mathcal{E}(z,t)^2\rangle}}\right]^{2Z/\kappa} \exp\left[-\frac{\mathcal{E}(z,t)^2}{2\omega^3}\sigma_1\right]. \quad (5)$$

Here Z is the effective atomic charge, $\kappa = \sqrt{I_p/(\hbar\omega_a)}$, $\sigma_0 = \frac{1}{2}(\gamma^2 + \frac{1}{2})\ln C - \frac{1}{2}\gamma\sqrt{1+\gamma^2}$, $C = 1 + 2\gamma\sqrt{1+\gamma^2} + 2\gamma^2$, and $\sigma_1 = \ln C$-$2\gamma/\sqrt{1+\gamma^2}$. The quantity $\langle E(z,t)^2\rangle$ is the averaged value of the squared electric field over few past periods (two periods are assumed in PIGLET).

In the multiphoton formalism, the $\Gamma(z,t)$ is given (in atomic units) by

$$\Gamma(z,t) = E(z,t)^{2N_{ph}}, \quad (6)$$

where N_{ph} is the lowest number of pump pulse photons which have energy sufficient to overcome the bandgap.

Finally, in the ADK approximation[3], the ionization rate is expressed (in atomic units) as

$$\Gamma(z,t) = \left(\frac{3e'}{\pi}\right)^{3/2} \frac{1}{3n^3(2n-1)} \left(\frac{4e'}{(2n-1)|E(z,t)|}\right)^{2n-1.5} \exp\left(-\frac{2}{3n|E(z,t)|}\right), \quad (7)$$

where $e' = 2.71828\ldots$ and $n = (2E_g)^{-0.5}$.

The above models are corrected in PIGLET by a prefactor calculated from the phenomenological damage threshold. For this calculation, it is assumed that threshold occurs at the intensity for which the plasma frequency (arising from the electrons in conduction band) is equal to the pump frequency[4].

2. Numerical realisation

The pulse propagation is described using the standard Yee-cell one-dimensional FDTD approach[5]. The initial condition approach was utilized, with unidirectional pulse (travelling from the lower values of z to higher values of z) determining the electric $E_x(z,0)$ and magnetic $H_y(z,0)$ fields for zero time. The absorbing boundary conditions at boundaries $z = 0$ and $z = z_{max}$ are given by

$$c\frac{\partial E_x(0,t)}{\partial z} = \frac{\partial E_x(0,t)}{\partial t} \quad (8)$$

$$c\frac{\partial E_x(z_{max},t)}{\partial z} = -\sqrt{\epsilon(z_{max},t)}\frac{\partial E_x(z_{max},t)}{\partial t}. \quad (9)$$

Finally, the implementation of Eq. (3) in the time domain is based on the following discretization scheme [6] which provides the values of $E_x(z, t + dt)$ and $P_x(z, t + dt)$:

$$P_x(z,t+dt) - P_x(z,t) + \frac{1}{2}\nu dt(P_x(z,t+dt) + P_x(z,t)) =$$
$$-\frac{\omega_p^2}{2\nu}dt(E_x(z,t) + E_x(z,t+dt)), \tag{10}$$
$$\epsilon_\infty(E_x(z,t+dt) - E_x(z,t)) + P_x(z,t+dt) - P_x(z,t) =$$
$$\frac{dt}{\epsilon_0}(-H_y(z+dz,t) + H_y(z,t) - 0.5\sigma(E_x(z,t) + E_x(z,t+dt)), \tag{11}$$

where dt is the time step, $\omega_p^2 = N_0 e^2 \rho/(\epsilon_0 m_e)$ and $\sigma = \epsilon_0 \omega_p^2/\nu$.

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