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Laser induced electronic acceleration process in nano dot

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ABSTRACT

A physical model of the laser induced electron transport in dielectric with small size is discussed. The model assumes that free electrons are originally existent or produced by impact detrapping. The free electrons transporting in low dimensional dielectrics interact with phonons and surface. When the laser electric field strength is high enough, the inelastic electron scattering such as impact ionization and cascade processes will play important roles. A small size effect has been found in electron absorbing laser energy under the conditions that the laser wavelength is in near infrared zone and the material has size in nanometer level. This is a very significative effect to enlighten us on preparing ultrahigh threshold laser films with new nano-structure.

1. Introduction

The process of dielectrics absorbing laser energy is relevant to electron acceleration when the laser wavelength is in visible or near infrared zone and the power density is in GW/cm^2 level [1,2]. The initial seed electrons will be accelerated in laser field and transfer the absorbed energy to lattice. As a result, the dielectrics will be damaged subsequently. In order to investigate the detailed damage mechanism, the electron transporting process should be studied.

The Boltzmann transport equation provides a comprehensive description of the carrier transport dynamics under semi-classical conditions [3,4]. Given the general complexity of the Boltzmann equation, one of the more useful approaches for its solution is the numerical Monte Carlo method [5,6]. The Monte Carlo method provides a direct solution of the Boltzmann equation through microscopic simulation of the trajectories of particles subjected to the band structure, scattering mechanisms, applied fields, as well as device geometries, if applicable [7]. Although other techniques have been used to solve the Boltzmann equation [8–10], the Monte Carlo solution is the most common one. Its ease of use and overall simplicity help make it the tool of choice.

The Monte Carlo method has been successfully employed to investigate a great variety of transport properties in semiconductors [11]. Subjected to the force of applied external fields, the charge carriers follow trajectories determined by Newton's law [11,12]. The drifting process is interrupted by scattering events that are considered to be local in space and instantaneous in time.

2. Basic theory

The model has been developed for calculating the electron transport in dielectrics exposed to laser irradiation which has power density in GW/cm^2 level. The size of dielectrics is in nanometer level which is corresponding to the nano-structure of porous laser films. The detrapped electrons can be accelerated or decelerated in laser field [13,14]. Electrons drifting in the dielectrics are scattered by ions, acoustic or optical phonons, and surface depending on their energy [15,16]; they also participate in processes of impact ionization and cascading. Trapped electrons can only be detrapped by impacting with electrons which have energy beyond band gap energy. For laser pulse with power density of GW/cm^2 and wavelength in near infrared band, the tunneling effect and photoionization can be ignored. When the temperature of dielectrics is low, thermo-ionization can be ignored as well.

The first step deals with the calculation of the laser electromagnetic field. A Gaussian laser electric field which is $\boldsymbol{x}$ direction linearly polarized and propagates along the $\boldsymbol{z}$ axis is considered. The detail expression of electromagnetic field can be obtained from ref. [17].

Secondly, it is a step to deal with the calculation of the electron band structure of the dielectrics under investigation. The band structure can be obtained either via empirical or ab-initio techniques. The former requires experimental information that is not always available for emerging materials. This information becomes more critical as the need to optimize the band structure increases [18]. Often, when it is not at all possible to obtain information to produce a reliable empirical band structure, the application of ab-initio methods makes it possible to calculate, at the least, a basic set of data that can be used as a starting point for empirical methods [19].

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If a free electron shifts in a laser filed without any scattering, it is difficult for it to absorb laser energy. Scattering can disturb the regularity of the force that an electron endured in laser field, hence the electron can absorb laser energy efficiently [20].

To investigate the transport properties of a material, it is necessary to describe the interaction between carriers and the lattice. Techniques of different levels of sophistication can be employed to perform this task. Lattice dynamics, which describes the phonons, can be evaluated either analytically or numerically. The knowledge of the electron band structure and the lattice dynamics allows the carrier–phonon interaction to be determined [21,22].

Among the various scattering mechanisms that control the transport of carriers in a solid, only the electron–phonon and electron-surface interactions have been taken into account in the description. The electron–electron scattering is negligible because of the very low concentration of carriers present in the conduction band of dielectrics. The scattering with impurities, defects and interface can be treated as elastic scattering and can be significant. However, the investigations on experiments [23] showed that the average energies are influenced little by these scattering sources when they have low concentration. For this reason, the impurity and interface scattering mechanisms have not been included in this manuscript.

Some materials, such as SiO_2, exhibit a mixed bonding character [24]: both the polar and nonpolar interactions are relevant to energy loss process. The latter is dominant in covalent materials, whereas the former is the main scattering event in ionic materials. In order to describe the electronic energy and velocity distributions, both scattering mechanisms should be analyzed.

The nonpolar interaction is treated within the deformation potential approximation. Electrons interact with longitudinal acoustic and transversal optical phonons, and such interactions are dominant at high energies. The local deformation of a crystal lattice due to an acoustic vibration is associated with a shift of the band edges. As for the interaction of electrons and optical phonons, it may occur though intravalley or intervalley scattering between equivalent minima.

In ionic insulators, the strong interaction between electrons and the polar molecular of dielectric is due to the polarization field of ions. The coupling between electron and the polar phonon is very effective for electron energies comparable with the energy of the phonon modes. This interaction is particularly strong in the case of longitudinal–optical phonons. Besides, the piezoelectric polarization cause by acoustics phonons has been included also.

In the energy-conserving delta function, the energy of the acoustic phonon has been assumed small compared to the initial and final energies, and in this approximation, the acoustic phonon scattering is quasi-elastic.

The electron-surface scattering cannot be neglected if the device is very small. In nano-materials, this kind of scattering will be dominant when its size is near or smaller than the electron mean free path. Here the surface scattering is treated as an elastic process and a simple mirror reflection mechanism is adopted.

The electron-ion scattering is important when electron energy is high, but it is also not significant because of low concentration of charged ions in dielectrics such as SiO_2.

All the formulations used to evaluate different kinds of scattering rates are given in refs. [25] and [26].

The probable ionization mechanisms include: Thermo-ionization which happens in the condition of high temperature appears between neutral atoms; Strong field ionization occurs in the case of laser pulse with high electric field; photon ionization occurs in the case of laser irradiation with short wavelength. These three ionization mechanisms are ignored when material with low temperature is exposed to laser irradiation with power density of GW/cm^2 and wavelength in near infrared zone [27].

The other kind of ionization mechanism, impact ionization event, occurs when a high-energy carrier impacts with the lattice. During this collision, the initial, high-energy carrier transfers some portion of its kinetic energy to a bound electron. This transfer of energy may be sufficient to liberate the bound carrier, thereby creating a secondary electron-hole pair. In order for the initiating carrier to free a bound carrier, the energy of the initiating carrier must be equal to or greater than the band gap.

The study of the electronic transport properties of dielectrics cannot proceed without an accurate description of the impact ionization process. Impact ionization will limit the maximum operating laser power density of some optical components because avalanche breakdown may harm the components or alter its performance.

The formulation used for evaluate ionization rate can be obtained from ref. [26].

To describe broadly the Mont Carlo bulk simulator, it could be stated that the simulator consists of two basic mechanisms: drifting and scattering. Each simulated particle drifts due to the applied field, and if a carrier–phonon or carrier-surface interaction occurs, the particle is scattered. Statistics are collected along the way.

The particle drifts according to Newton's Law of motion, by updating the energy and wave vector. Carrier value that affects the global statistics such as average energy change per drift can be updated before moving to the next phase of the transport process. After a given particle drifts and its kinetic energy is updated, a random number is generated to determine if a carrier will scatter, based on the total scattering rate at the carrier energy.

In the trivial case where no scattering event occurs, the simulator considers the next carrier. However, if it is determined that a carrier will scatter, another random number is generated to determine the particular scattering mechanism. A random number r_m will be generated, and if it meets the relationship of $F_{j-1}<r_m<F_j$, the jth scattering mechanism is selected. $F_i = \sum_{i=1}^{j} P_i$ and $P_i=\lambda_i/\lambda$, where λ_i, λ are the scattering rate of the ith scattering mechanism, and the total scattering rate respectively. For the case of the phonon scattering events, each mechanism consists of two possibilities, absorption and emission.

Once a scattering mechanism is chosen, it is then necessary to determine the carrier's final state. Based on the type of mechanism, and whether the process is one of absorption or emission, the final carrier energy can be decided since the phonon energies are assumed constant. What is unknown, however, is the new carrier wave vector. The determination of the new carrier wave vector is the primary role of the final state selection algorithms. The final state selection employed in the Monte Carlo simulator is similar to, and based on, the work by Fischetti and Laux [28].

After the scattering process is complete, the simulation statistics are again updated. The drift-scatter process repeats for the pre-determined simulation time.

3. Theoretical results and discussions

Silicon dioxide is the most commonly used insulator in laser films. Since the reliability problems is related to the absorption, it is crucial to achieve a correct physical description of carrier transport in SiO_2. The sketch of simulation model is shown in Fig. 1.

The parameters used in simulation [29,30]: laser wavelength is 1064 nm; laser pulse width is 1.0 ps; laser beam waist is 0.1 mm; laser power density is 1 GW/cm^2. The lattice temperature is 573 K; The band gap of SiO_2 is 9 eV; The density of SiO_2 is 2200 kg/m^3; The refractivity of SiO_2 is 1.46. The deformation potential of acoustic wave is 6 eV; the piezoelectric coefficient is 0.3 C/m^2; the relative dielectric constant is 3.9; the sound velocity is 6000 m/s; The optical phonon energy is 0.063 eV and 0.152 eV; The initial ion density is 10 mm^{-3}; The initial coordinate of free electron is $(0.25, 0.25, 0.25)$ L, where L is the size of simulation unit in square shape.