Application of the Fokker Planck approach for modelling of nano-structural defects in fusion materials

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Abstract. The materials used in the first wall of ITER and fusion power plants will be required to withstand neutron bombardment produced in fusion plasmas. The development of models describing the structural defects in fusion materials has become an important element in the development of a prototype of a fusion power reactor. Modeling of structural defects requires new modeling approaches giving theoretical predictions that could be experimentally validated. In this review paper, we propose the Fokker-Planck kinetic equation for modeling of nanovacancies, nanovoids and dislocation loops in fusion materials under cascade producing irradiation. It will be shown that in the simplest approximation that includes the effects of the statistical and cascade induced fluctuations, the kinetics of the evolution of the nanostructural defects can be described by the Fokker-Planck equation for the defect size distribution function. The proposed model can be applied to fusion materials under irradiation conditions that represent those of the first wall of a fusion reactor.

1. Introduction

In the Brownian motion case the complete solution of a macroscopic system would consist in solving all the microscopic equations of the system. Since this cannot be done in general a stochastic description is used instead – the system is described by macroscopic variables which fluctuate in a stochastic way.

The Fokker-Planck equation is an equation of motion for the distribution function of fluctuating microscopic variables. For a deterministic treatment the fluctuations of the macroscopic variables are neglected. By solving the Fokker-Planck equation one obtains distribution function from which any averages of microscopic variables are obtained by integration. Since the application of the Fokker-Planck equation is not restricted to systems near thermal equilibrium, we may apply it to systems far from thermal equilibrium, for instance, solids under intense laser or neutron radiation. Moreover, the Fokker-Planck equation not only describes stationary properties, but also the dynamics of systems, if the appropriate time-dependent solution is used.

The Fokker-Planck theory has been widely applied in the studies of laser interaction with dielectric and semiconducting materials. It was demonstrated [1] that when the same model system was considered in calculations using the Fokker-Planck approach (FPA) and the Boltzmann transport equation (BTE) by means of the Monte Carlo method, the results of both approaches showed good agreement in the high laser field regime. The FPA considers transport as a certain diffusive-drifting “motion” of the carriers in the energy space. An electron in the CB of a dielectric or a semiconductor
can continuously gain or lose energy through interaction with phonons and the incident laser field. In this picture, the energy change of electrons is small if the laser field is not extremely strong, and the electron energy displacements are random with time. This is reminiscent of the Brownian motion of conduction electrons in energy space and Uhlenbeck and Ornstein [2] proposed a Fokker–Planck equation and applied it to the time evolution of the electron distribution function, where an assumption that electron energy does not change significantly over many collisions was introduced. The FPA method is semi-classical by nature and applicable when the average electron energy is much larger than the exchanged energy with phonons. The FPA has the advantage of being analytical, saves computational time and allows a more transparent physical interpretation.

Modeling the nanostructure evolution of materials driven far from equilibrium by intense neutron irradiation has recently become important for the development of a prototype fusion power station. Cascade irradiation produces small mobile and immobile vacancy and interstitial clusters. Recognizing the importance of stochastic fluctuations a nanostructure evolution theory can be formulated using the Fokker–Planck equation, to take into account the stochastic effects of the fluxes of mobile defects, arising from the random nature of diffusion jumps and cascade initiation.

The goal of this paper is to illustrate the successful application of the Fokker–Planck theory approach for describing the microscopic processes in dielectrics and semiconductors under laser field irradiation and to demonstrate how this theory may be used for modeling of structural defects in fusion materials under cascade producing irradiation.

2. Fokker–Planck approach for short pulse laser interaction with dielectric and semiconductor materials

Previously we have performed theoretical investigations of picosecond-to-femtosecond laser pulse interaction with selected dielectrics and semiconductors.

The Fokker–Planck quantum dynamical theory is a first-order approximation of a general semi-classical Boltzmann theory. We derive the kinetic Fokker–Planck-type equation for excited conduction electrons in bulk semiconductors systematically in the presence of a pulsed laser beyond the classical limit. We start with the total Hamiltonian of the electron–phonon system irradiated by a pulsed laser field in second quantization [3]. Initially using Fermi’s Golden Rule we obtain a dynamic equation by including only the electron–phonon interaction within the first order perturbation theory. Limiting ourselves to the diffusive limit, we expand the electron distribution function and get the Fokker–Planck equation for the thermal motion of electrons in energy space. The intraband transitions of conduction electrons cannot optically respond to the spatially uniform laser field due to the impossibility of conserving energy and momentum simultaneously during the absorption of a photon by an electron, and the effect of the laser field treated classically is included in the equation using the following considerations: (a) after the laser field is applied there is no net momentum change of electrons within an interval of collision time \( \tau_p \) (many time periods of the oscillating laser field) over which two successive collisions with phonons occur, and this is different from the case with a dc electric field; (b) electrons will gain net power from the laser field. In the presence of the laser field, a drift in energy space is obtained which is described by

\[
\frac{\partial f^e_i}{\partial t} = \lim_{\lambda \to 0} \frac{1}{\lambda} \left[ f^e_i(E^e_i, t) - f^e_i(E^e_i, t) \right] - \frac{dE^e_i}{dt} \frac{\partial f^e_i}{\partial E^e_i}.
\]

Since the time period of the laser field \( 2\pi/\Omega_L \) is much shorter than \( \tau_p \), a time average is taken of the Fokker–Planck-type equation over many periods of the laser field, an averaged fluctuation which represents the average energy gained by electrons by absorbing the laser power \( E_p = \langle \Delta E^e_i \rangle = \int dE^e_i \langle \Delta E^e_i(t) \rangle f^e_i \) is introduced and for \( E_p \ll E^e_i \) the expansion
The function $f_{\epsilon_k}(E^\epsilon_k, E^\epsilon_k) = f_{\epsilon_k}(E^\epsilon_k) - E^\epsilon_k \frac{\partial f_{\epsilon_k}}{\partial E^\epsilon_k}$ is used. Finally, we obtain the generalized Fokker–Planck-type equation [3]:

$$\frac{\partial f^\epsilon_k}{\partial t} + V^\epsilon_k \frac{\partial f^\epsilon_k}{\partial E^\epsilon_k} - D^\epsilon_k \frac{\partial^2 f^\epsilon_k}{\partial (E^\epsilon_k)^2} = A_k f^\epsilon_k + S_k$$

(1)

In equation (1) we have included the coupling of the energy drift of electrons in the presence of the laser field to the phonon-assisted intraband electron transitions which gives an additional anti-diffusion current and have given analytical expressions for all the source terms up to second order perturbation theory, including single-photon absorption, impact ionization due to Coulomb interaction between electrons and holes, and non-radiative recombination due to a phonon-mediated interaction. We calculate numerically the hot electron distribution function which can be used to evaluate the electron number density, the average electron energy, and the non-equilibrium electron temperature. The magnitude of the distribution function becomes very large at high intensity $I_L$ of the incident laser field because of the large optical absorption proportional to $I_L$. The increased absorption directly leads to a larger electron number density (solid curve) in figure 1. The shifted up peak of the electron distribution function in energy produces a larger average electron kinetic energy when the laser intensity becomes strong as can be seen in figure 2.

**Figure 1.** Comparison of the electron number density as a function of the scaled time with higher or lower laser intensity.

**Figure 2.** Comparison of the scaled average electron energy as a function of the scaled time with higher or lower laser intensity.

In addition, we have developed a model for electrons in a bulk semiconductor material interacting with an infrared laser field and an applied strong dc electric field. In the model we couple the first order force balance equation for the slow center-of-mass motion of electrons and the Fokker–Planck-type equation for the ultrafast relative scattering motion of the excited electrons beyond the relaxation-time approximation. The Fokker–Planck type equation obtained is an approximation to the Boltzmann scattering equation which we systematically derive when the Fermi energy of the electrons is much larger than the phonon and photon energies and the drift energy of the electrons [4].

We find that the drift velocity of electrons increases with the amplitude of the infrared laser field when its polarization is parallel to the dc field due to a suppression of momentum relaxation as seen in
figure 3 but decreases with the infrared field amplitude for the perpendicular polarization (figure 4) due to an enhancement of momentum relaxation. The heating of electrons is described beyond the first order energy balance equation. For both cases the non-equilibrium electron temperature increases with increasing of the infrared field amplitude due to the increase of the average kinetic energy of electrons by power absorption from the applied infrared laser field [4].

![Figure 3](image1.png)  
**Figure 3.** Calculated drift velocity and nonequilibrium electron temperature as functions of the amplitude of the incident infrared field when it is parallel to the dc field.

![Figure 4](image2.png)  
**Figure 4.** Calculated drift velocity and nonequilibrium electron temperature as functions of the amplitude of the incident infrared field when it is perpendicular to the dc field.

3. Nanostructure defect evolution under cascade-damage irradiation

A basic assumption implicit in the conventional theory of nanostructure evolution in irradiated materials based on the chemical reaction rate theory is that the defects (vacancies and interstitials, etc.) are produced continuously and uniformly in time and space at some appropriate mean value. In contrast, under cascade damage conditions, point defects are produced in discrete packages, randomly in time and space so the conventional picture of point-defect production is not appropriate for irradiation by neutrons and heavy ions, where point defects are produced in cascades in a highly localized and segregated fashion. Because of the random nature of both the diffusing jumps and the cascade occurrence, point defect arrival rates at sinks are also probabilistic and fluctuate all the time.

The nanostructure evolution under nonequilibrium irradiation involves random aggregation or absorption of mobile point defects plus the formation of vacancies. It can be described by the theory of stochastic processes which starting point is a master equation (e.g. Smoluchowsky–Chapman –Kolmogorov equation for a Markovian process) for the distribution of defect sizes. The master equation can be reduced to a deterministic rate equation for the concentration of specific defects if the transition probabilities in the equation are replaced by reaction rates. This mean-field approximation does not take into account the statistical nature of defect production, cascade effects, and the arrival and absorption of defects at defect clusters. One unique feature of nanostructure evolution under
irradiation is that the size of atomic transitions is generally smaller than the defect cluster size and the mobility of large defect clusters is negligible, and, hence, one can derive a Fokker–Planck equation as an approximation to the master equation.

In the simplest approximation, within which the stochastic effects due to the random nature of both the point-defect migratory jumps and cascade initiation can be included, the kinetic equation for the void evolution takes the form of the Fokker–Planck equation [5]:

$$\frac{\partial f(n,t)}{\partial t} + \frac{\partial}{\partial n} \left[ V(n,t) - \frac{\partial D(n,t)}{\partial n} \right] f(n,t) = j_0.$$  \hspace{1cm} (2)

Here $f(n,t)$ is the defect density distribution function in the space of defect sizes at time $t$. The drift term on the right hand side the Fokker–Planck equation describes the mean defect growth rate defined by the time-averaged fluxes of free vacancies and interstitials towards the defect cluster. The diffusivity term governs the stochastic spread of the defect size distribution function by taking into account the stochastic fluctuations in defect cluster sizes initiated by the cascades. It is related to the average point-defect fluxes and cascade properties. The last two terms in the equation are source and sink terms. They describe, respectively, the production rate of small interstitial defect clusters by cascades or by random jumps, and the rate of their removal by absorption at dislocation network and interstitial loops by sweeping.

$$V(n) = \frac{3n^{\frac{3}{2}}}{4\pi} \left[ D_1 C_v - D_2 C_i - D_3 C^*,(n) \right]$$

is the defect growth rate defined by the mean field theory. The parameters are as follows: $a = \left[3\Omega/4\pi \right]^\frac{1}{2}$ where $\Omega$ is the atomic volume, $C_j$ is the concentration of defects, $D_j$ is the defects diffusion coefficient $(j = i,v)$ being the indices for voids and interstitials. $C^*,(n) = C_e \exp \left\{ \frac{2\gamma \Omega}{kTR_c} \right\} \approx C_e \left[ 1 + \frac{2\gamma \Omega}{kTR_c} \right] \cdot$ is the equilibrium concentration of defects in a neighborhood of a void with radius $R_c(n) = an^{\frac{1}{2}}$, $C_e$ is the equilibrium vacancy concentration; $\gamma$ is the surface tension coefficient, $k$ and $T$ are the Boltzmann constant and absolute temperature respectively.

In the equation (2)

$$D(n) = D^d(n) + D^j(n) + D^c(n)$$

is the “diffusivity” that describes the diffusive spread of the defect size distribution in time due to the stochastic fluctuations of point defect fluxes.

$$D^d(n) = \frac{3n^{\frac{3}{2}}}{2a^2} \left[ D_1 \left\{ C_v - C^*,(n) \right\} + D_2 C_i \right]$$

is the contribution to the diffusivity due to the random migratory jumps;

$$D^j(n) = \frac{3n^{\frac{3}{2}}}{4a} \left[ G_v \left\{ \langle N^2_{d} \rangle \right\} + G_i \left\{ \langle N^2_{s} \rangle \right\} \right]$$

is the contribution to the diffusivity due to random cascade initiation;

$$D^c(n) = \frac{9n^{\frac{3}{2}} D C_s(n)}{2a^2}$$

is the contribution to the diffusivity due to random emission of point defects. In the expressions above $N_{d}$ is the average number of point defects, $\langle N^2_{s} \rangle$ is the average square number of point defects and $k_j^2$ is the total sink strength for point defects of type $j$ [6].
The term on the right hand side of the Fokker–Planck equation describes the rate of production of small interstitial clusters by cascades and the rate of their removal by absorption at dislocation network and interstitial loops by sweeping. For simplicity it is assumed that the initial sizes of the defects are the same ( \( n_0 \) being the initial number of defects) which is reflected in the \( \delta \) function:

\[
\frac{\delta}{n_0} j_0 = \frac{\varepsilon_i G}{n_0} \delta(n - n_0) - \left( \rho_N + \rho_l \right) WF(n, t),
\]

where \( \varepsilon_i \) is the fraction of point defects immobilized in primary clusters, \( G = Q \Omega N_d \) is effective generation rate of free point defects ( \( Q \) – mean number of cascades per unit volume per unit time, \( N_d \) – average number of free point defects), \( \rho_N \) and \( \rho_l \) are the dislocation densities for the network and the interstitial loops, respectively, and \( W \) is the reaction constant between the primary clusters and the sweeping dislocations [7].

Vacancy clusters consisting of several vacancies are mobile and a void shrinking below a minimum size \( n_{\text{min}} \) can no longer be treated as a void. In this case, the left boundary condition of the Fokker–Planck equation should be a vanishing size distribution function at any time and for defect size equal to the minimum one: \( f(n = n_{\text{min}}, t) = 0 \).

To ensure a finite total defect number density the right boundary condition of the Fokker–Planck kinetic equation should be a vanishing size distribution function at any time and for defect size equal to infinity [8]: \( f(n \rightarrow \infty, t) \rightarrow 0 \).

4. Conclusions

On the basis of the Fokker–Planck approach (FPA) used for describing the microscopic processes in dielectric and semiconductor materials irradiated by short pulsed laser we demonstrate that FPA can be applied for studying nanostructural defect evolution under cascade-damage irradiation in different ITER fusion materials.

The FPA can be used as an alternative method to Density functional (DFT) method for describing the defect evolution in fusion materials. The numerical results of the two methods can be compared.

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