Simulation of Ultra-Intense Laser Irradiation Induced Electronic Excitation of Bandgap Materials

T. Apostolova [1], **P. Detistov**[2], **M.V.Ivanov**[1], **A. Rivera**[2], **J.M. Perlado**[2]

[1]Institute for Nuclear Research and Nuclear Energy, Sofia, Bulgaria
[2]Instituto de Física Nuclear, Madrid, Spain

A quantum kinetic approach based on the Boltzmann equation is employed to describe the response of dielectric and semiconductor materials to high excitation laser irradiation from the initial photo-ionization inter-band processes through free carrier absorption inducing additional impact ionization to the final heat up by electron-phonon coupling. Swift thermalization through electron-electron scattering, auger recombinatation and formation of free excitons and their self-trapping accompanied by generation of simple point defects in materials will also be included. The energy exchange between the electrons and phonons will given by a separate equation for the lattice temperature where the rate of energy transfer from the electrons to the lattice per unit volume will be defined quantum mechanically. In addition, the kinetic model will be coupled to a molecular dynamics code. This model will allow to follow the evolution of the electron system and couple it realistically to lattice modification. As a result of our calculations the electron energy distribution function, average kinetic energy of the electron system and electron density will be obtained as a function of laser intensity, laser photon energy (wavelenght) and laser pulse duration. In addition we will obtain the change of lattice temperature. Thus it is expected the calculations to demonstrate that for low densities processes such as defect generation, amorphization or densification occur. On the other hand high densities lead to permanent optical damage and eventually to surface ablation with severe consequences for the integrity of the material. Adapting the same theoretical formalism it will be possible explore a number of aspects related to the modification of plasmonic systems (metallic nanoparticles in dielectric medium) by means of high electronic excitation caused by the intense ultra short laser pulses.