Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

First-principles calculation for electron dynamics in dielectrics induced by intense laser pulses SHUNSUKE A. SATO, KAZUHIRO YABANA, University of Tsukuba, YASUSHI SHINOHARA, Max Planck Institute, KYUNG-MIN LEE, Center for Relativistic Laser Science, TOMOHITO OTOBE, Japan Atomic Energy Agency, GEORGE F. BERTSCH, University of Washington — We have been developing a theoretical and computational method to describe electron dynamics in crystalline solids irradiated by laser pulses. Our method is based on the time-dependent density functional theory (TDDFT), which enables us to treat quantum electron dynamics in the first principles level. By solving the time-dependent Kohn-Sham equation in real-time, it is possible to describe nonperturbative nonlinear electron dynamics induced by intense laser fields. We further combine the electron dynamics calculation in the TDDFT with the Maxwell's equation for electromagnetic fields so as to achieve simultaneous descriptions of both micro-meter-scale laser-field propagation and nanometer-scale electron dynamics induced by the fields. We call it "Maxwell + TDDFT multiscale simulation." As an application of the method, we show calculated transferred energy distribution from a laser pulse to a bulk SiO2 sample. We evaluated the laser damage threshold and the ablation depth from the distribution. We found that the calculation nicely reproduced measured results of both threshold and depth.

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Date submitted: 13 Nov 2014

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