Seminario

Grupo de Procesado por Láser

Instituto de Óptica, CSIC

JUEVES 6 DE OCTUBRE 2023

10:00 HORAS

SALA DE CONFERENCIAS

CALLE SERRANO 121, MADRID

Programa:

10:00 - 10:45. **Jörn Bonse** – BAM – Berlin, Alemania

Probing laser-driven structure formation at extreme scales in space and time

10:45 - 11:15. Pausa

11:15 - 12:00. **Thibault J-Y. Derrien** – HiLASE- Praga, República Checa

First-principle simulations for ultrashort laser processing of solids and nanomaterials

Los resúmenes de las presentaciones se encuentran en la siguiente hoja

Seminario organizado en el marco del proyecto ILINK22056 "UnderControl: Understanding and controlling volumetric laser-induced modifications in materials for advanced photonic applications" del programa i-LINK 2022

Probing laser-driven structure formation at extreme scales in space and time

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Irradiation of solid surfaces with intense ultrashort laser pulses represents a unique way of depositing energy into materials. It allows to realize states of extreme electronic excitation and/or very high temperature and pressure and to drive materials close to and beyond fundamental stability limits. As a consequence, structural changes and phase transitions often occur along unusual pathways and under strongly nonequilibrium conditions. Due to the inherent multiscale nature — both temporally and spatially—of these irreversible processes, their direct experimental observation requires techniques that combine high temporal resolution with the appropriate spatial resolution and the capability to obtain good quality data on a single pulse/event basis. In this respect, fourth-generation light sources, namely, short wavelength and short pulse free electron lasers (FELs), are offering new and fascinating possibilities. As an example, this talk will discuss the results of scattering experiments carried out at the FLASH free electron laser at DESY (Hamburg, Germany), which allowed us to resolve laser-induced structure formation at surfaces on the nanometer to submicron length scale and in temporal regimes ranging from picoseconds to several nanoseconds with sub-picosecond resolution [1]. The current status and future perspectives in this field via exploiting the unique possibilities of these 4th-generation light sources will be discussed [2].

[1] https://doi.org/10.1007/978-3-031-14752-4_6

[2] http://doi.org/10.48550/arXiv.2309.02971

First-principle simulations for ultrashort laser processing of solids and nanomaterials

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Processing solids using ultrashort laser pulses triggers a wide range of phenomena from the electron excitation to the modification of atomic bonds in the laser field [1]. By modifying the space charge distribution of a solid, an intense laser excitation of the electrons can trigger the motion of the materials structure, resulting in a strongly anisotrope electron-phonon interaction.

To avoid such complexity, working with laser pulses shorter than the electron-phonon coupling time (ranging from 10 to 1,000 fs depending on the chosen material) offers an excellent opportunity for benchmarking the available first-principle simulation methods such as the time-dependent density functional theory (TDDFT). For such regime where material heating is limited [2], it was found that TDDFT is able to provide relevant predictions of the electron excitation in various experimental conditions, particularly in the case where the strong laser field subsequently leads to materials' modification.

In this seminar, by relying on Top500 supercomputing facilities, we demonstrate that the TDDFT is a highly valuable tool (i) to identify the validity range of established simplified models of interaction [3], (ii) to predict the spectra of harmonics emitted by laser-irradiated crystals [4]. We also demonstrate that (iii) TDDFT can help to identify new parameters, e.g., for controlling the amount of laser energy absorbed by the irradiated sample. To support the latter, in-house experiments have revealed the possibility to modify the single-pulse damage threshold on a range of +/- 10% for silicon simply by acting on the crystal orientation [5].

Overall, our results demonstrate how non-equilibrium condensed matter simulation and high-power computations can help to reach new degrees of precision for the laser processing of solids. Perspectives for predicting the behavior of nanomaterials in the laser field will also be provided.

[1] Derrien, T. J.-Y.; Levy, Y. & Bulgakova, N. M. Insights into laser-matter interaction from inside: wealth of processes, multiplicity of mechanisms and possible roadmaps for energy localization. *Ultrafast Laser Nanostructuring - The Pursuit of Extreme Scales (Eds. Razvan Stoian and Jörn Bonse), Springer,* 2023

[2] Bonse, J.; Baudach, S.; Krüger, J.; Kautek, W. & Lenzner, M. Femtosecond laser ablation of silicon □“ modification thresholds and morphology *Appl. Phys. A,* 2002, 74, 19-25

[3] Derrien, T. J.-Y.; Tancogne-Dejean, N.; Zhukov, V.; Appel, H.; Rubio, A. & Bulgakova, N. M. Photoionization and transient Wannier-Stark ladder in silicon: First principle simulations versus Keldysh theory. *Phys. Rev. B,* 2021, 104, L241201

[4] Suthar, P.; Trojánek, F.; Malý, P.; Derrien, T. J.-Y. & Kozák, M. Role of Van Hove singularities and effective mass anisotropy in polarization-resolved high harmonic spectroscopy of silicon. *Commun Phys,* 2022, 5, 288.

[5] Sládek, J.; Levy, Y.; Bonse, J.; Bulgakova, N. M. & Derrien, T. J.-Y. Polarization-dependent damage threshold of Si (100) upon femtosecond and picosecond laser irradiation. In preparation.