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Sub-Picosecond Non-Equilibrium States in the Amorphous Phase of GeTe

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The sub-picosecond response of amorphous Germanium Telluride 500 nm thin film to a 30 femtosecond laser excitation is investigated using time-resolved 2 colors frequency domain interferometry (FDI) at the Aurore laser facility in University of Bordeaux [1]. The time-resolved measurements of surface dynamics, for impinging fluences ranging from F = 16 to 80 mJ/cm², reveals a dielectric response faster than 300 fs (Figure 1). For F≥26 mJ.cm², a shrinkage of the surface is observed and assigned to the propagation of a melted layer of a liquid phase that is confirmed by post-irradiation analysis [2]. The systematic *ab initio* molecular dynamics (AIMD) simulations in non-equilibrium conditions (Figure 1) allow us to retrieve the atomic configurations for ionic temperature (T_i) from 300 K to 1100 K and width of the electron distribution from 0.001 eV to 1.0 eV (T_e). Local order of the structures is characterized by in-depth analysis of the angle distribution, phonon modes and pair distribution function which evidence a transition towards a new amorphous electronic excited state close in bonding/structure to the liquid state. Our results shed a new light on the optically highly excited states in chalcogenide materials involved in both important processes in non-equilibrium conditions: phase-change materials in memory device and Ovonic threshold switching phenomenon induced by static field [3].

[1] N. Fedorov *et al.*, Review of Scientific Instruments 91, 105104 (2020)
[2] P. Martinez *et al.*, Adv. Mater., 32, 2003032 (2020)
[3] P. Noé *et al.*, Science Advances, 6, 9 eaay 2830 (2020)

Figure 1: *Left panel : Relative variation of the real part of the dielectric constant of GeTe films as a function of time for increasing laser fluences. Right panel - top: Angular limited three-body correlation (ALTBC) map of the AIMD simulation at T_i=600 K, T_e = 0.3 eV - Bottom: Corresponding structure, Ge and Te atoms depicted in red and blue respectively.*