Formation of a cylindrical cavity in LiF crystal by X-ray pulse

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Volumetric modification of materials requires lasers with X-ray emission. It was demonstrated [1] that a free-electron laser with a single X-ray pulse of 9 keV photons can form a long cylindrical cavity in LiF crystal. The plasma channel created by such a pulse generates a divergent cylindrical shock wave (SW) with a pressure of $\sim$ 1TPa, which can lead to damage, melting, and polymorphic transformations in materials under study.

We analyzed the formation and propagation of pressure waves in LiF using continuum smoothed particle method (SPH) and molecular dynamics (MD) simulations. A sequence of processes leading to formation of a long cavity with a flat bottom has been identified. At high energy density near the sample surface, SPH and MD simulations both show the formation of an initial channel of low-density hot fluid due to radial material movement in a divergent plastic SW. After reaching the maximum size, the radius of the channel remains practically unchanged. At lower density of energy deposited in the depth of material, the channel is filled with dense melt, in which tensile stresses arise by heat conduction to surrounding cold material. MD simulation shows that a flat bottom of cylindrical cavity is formed due to the stop of propagation of cavitation bubble nucleation front when it meets a crystallization front in the melt [2].

[1] Makarov S, Grigoryev S, Inogamov N and et al 2023 *Opt. Express* **31** 26383

[2] Makarov S, Grigoryev S, Zhakhovsky V and et al 2024 Formation of high-aspect-ratio nanocavity in LiF crystal using a femtosecond of X-ray FEL pulse (*Preprint* `arXiv:2409.03625`)