

Damage processes in ruthenium thin films induced by XUV and x-ray free electron lasers

Survivability of optical elements exposed to high doses of laser radiation is an important issue in the context of rapidly developing x-ray free-electron laser (XFEL) light sources. In order to prevent optics from being damaged the fundamental mechanisms governing the material response to ultrashort high peak power XFEL pulses must be identified and examined.

We present a computational study of the interaction of femtosecond XUV and x-ray laser pulses with ruthenium (Ru) thin films designed for x-ray grazing incidence optics. Our hybrid model consists of three parts: (i) the photoabsorption and non-equilibrium electron kinetics are modelled with the event-by-event Monte Carlo code XCASCADE(3D) [1]; (ii) after the cascading is over, the diffusion of thermalized electrons, heating of the lattice via electron-phonon interaction and hydrodynamical movement of the material in the two-temperature regime are modelled with the two-temperature hydrodynamics code [2]; (iii) after the thermal equilibrium between electrons and the lattice is reached, the classical molecular dynamics approach [3] is used to simulate the lattice evolution. The calculations show that the mechanism responsible for the ablation of Ru is thermo-mechanical spallation.

The results of our simulations are compared with single-shot damage experiments where 50 nm thick Ru films were exposed to XFEL laser pulses at different photon energies, namely 92, 7000 and 12000 eV [4,5]. The similarities in damage mechanisms between XUV and hard x-rays are illustrated. The comparison of the calculated damage threshold values with experimental results lead to reasonable agreement.

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[2] N. A. Inogamov et al., "Two-temperature relaxation and melting after absorption of femtosecond laser pulse," *Appl. Surf. Sci.*, vol. 255, no. 24, pp. 9712–9716, 2009.

[3] V. Zhakhovskii et al., "A new dynamical domain decomposition method for parallel molecular dynamics simulation," in *Cluster Computing and the Grid*, 2005. CCGrid 2005. IEEE International Symposium on, 2005, vol. 2, pp. 848–854.

[4] I. Milov et al. "Mechanism of single-shot damage of Ru thin films irradiated by femtosecond extreme UV free-electron laser." *Optics express* 26.15 (2018): 19665-19685.

[5] A. Aquila et al. "Fluence thresholds for grazing incidence hard x-ray mirrors." *Applied physics letters* 106.24 (2015): 241905.