Combining Finite-Element and Molecular Dynamic Calculations for LIPSS (Laser Induced Periodic Surface Structures) formation during ultra short laser ablation

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Irradiation of many surfaces materials by ultra-short laser radiation, typically wth pulsewidths of 10-300fs, result in the development of Laser-induced self-organized periodic surface structures (ripples). The periodicity of these structures range from the wavelength λ of the laser to well below λ. Structures down to a few tens of nm can be observed. However, the existence and form of the LiPSS critically depends on the the intensity, fluence, wavelength and pulsewidth of the laser light as well as on the number of laser pulses and, not to forget, the material properties [1].

The development of the LiPSS structure can be regarded as a complex interplay between the electric field on the surfaces (including surface plasmon-polaritons) [2] and the ultra-short-laser-ablation dynamics [3]. Since the formation of LIPSS in most cases requires multiple laser pulses, the surface topography and hence the electric field distribution will change from shot to shot. Only the resulting feedback allows for the development of the LIPSS.

The present paper discusses a new approach to simulate the physics described above by calculating the electric field on and below the surface after each laser pulse for the newly developed surface topology with COMSOL Multiphysics (finite element method). This information of this field distribution, which should incorporate all possible plasmons etc., is then transferred to the irradiated material (various possibilities according to the wealth of physical processes in laser ablation [3] are evaluated) as a starting point for Molecular Dynamic (MD) simulations (LAMMPS) in order to obtain the new surface topology. The real challenge in the realization of the simulation is twofold: a) The calculation of the electric field (Fig, 1) and the MD simulation in a volume, where at least 2-3 ripples are observed approaches the possible limits with respect to memory and calculation times of COMSOL and LAMMPS. b) The data exchange between COMSOL and LAMMPS is not trivial and required a quite complicated and time consuming interface. First results have been obtained on the VSC3 cluster.

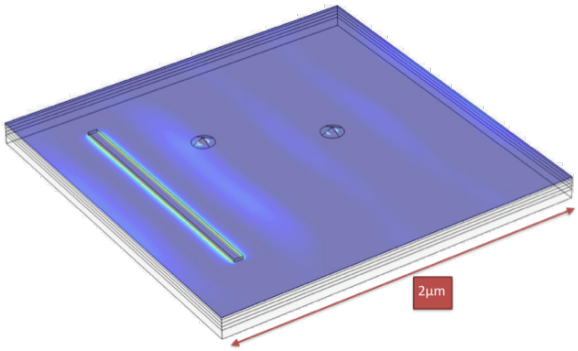

Fig. 1: Result from a COMSOL simulation of the square of the electric field for a $2\mu m$ by $2\mu m$ Ti surface with a thin oxide over-layer irradiated with a constant laser intensity.

References

[1] Nathala, C. S. R., A. Ajami, A. A. Ionin, S. I. Kudryashov, S. V. Makarov, T. Ganz, A. Assion and W. Husinsky, Optics Express **23(5)**, 5915 (2015).

[2] Kudryashov, S. I., S. V. Makarov, A. A. Ionin, C. S. R. Nathala, A. Ajami, T. Ganz, A. Assion and W. Husinsky, OPtics Letters **40(21)**, 4967 (2015).

[3] Dachraoui, H. and W. Husinsky., Applied Physics Letters **89(10)**, 4102 (2006).