Thin Films and Interfaces group, special seminar
April 8th, Monday at 16:00 in room OFLG/402

Generation of crystal defects in ultrashort pulse laser processing of surfaces and nanoparticles: Large-scale atomistic modelling and practical implications

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Abstract

The ultrashort (femtosecond and picosecond) pulse laser processing of materials offers unique opportunities for surface modification with high accuracy and spatial resolution. The shallow depths of the laser energy deposition and steep temperature gradients, produced by the ultrashort pulse laser irradiation, can lead to the cooling rates in excess of 1012 K/s. Resolidification of a transiently melted surface region, occurring under conditions of rapid quenching and dynamic relaxation of laser-induced stresses, creates the conditions for generation of highly nonequilibrium densities and configurations of crystal defects, which can drastically alter the physical, chemical, and mechanical properties of surface layers processed by ultrashort laser pulses [1]. The high densities of crystal defects are also found in nanoparticles produced by laser ablation in liquid environment. The defects, attributed to the highly nonequilibrium synthesis conditions, are found to strongly enhance the catalytic activity of the nanoparticles [2].

The understanding of the mechanisms and driving forces responsible for laser-induced generation of crystal defects is important for the advancement of laser processing applications aimed at tuning the properties of surfaces or nanoparticles to the needs of practical applications. Large-scale atomistic modeling can help in physical interpretation of experimental results and may facilitate the development of laser-enabled techniques for a localized or large-area defect engineering integrated into manufacturing processes. Several examples of the applications of atomistic modeling to investigation of the generation of crystal defects in ultrashort pulse laser processing [3-7] are illustrated in Figure 1 and will be discussed in the presentation. The computational predictions will be related to the results of time resolved optical and X-ray probing of laser-induced processes, as well as ex-situ nanoscale characterisation of surface microstructure.

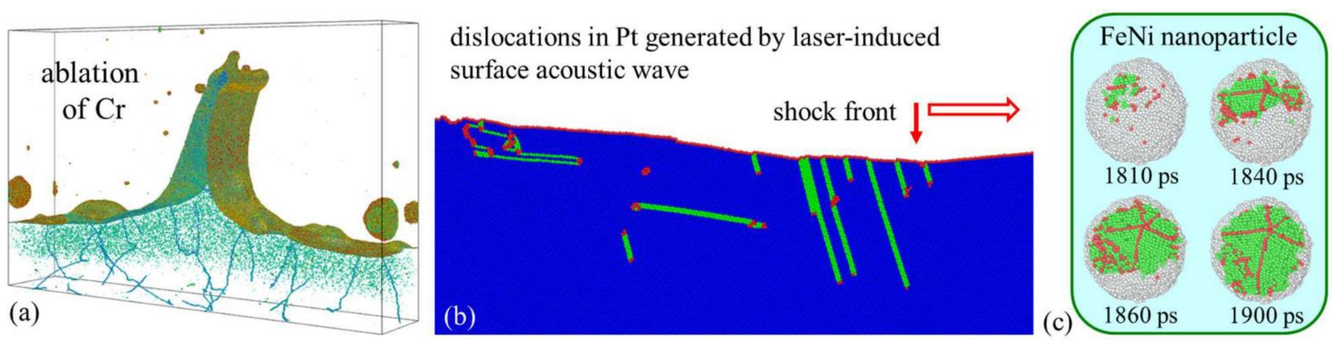

Figure 1. Examples of the generation of crystal defects predicted in large-scale atomistic simulations: (a) Dislocations and vacancy clusters present in and below the frozen protrusions generated in simulations of spatially-modulated laser ablation of Cr targets [3], (b) Emission of dislocations in a Pt (111) substrate during the nonlinear propagation and sharpening of a laser-induced surface acoustic wave, and (c) Generation of twins (red atomic planes separating fcc crystallites colored green) during the crystallization in a nanoparticle generated in pulsed laser ablation of FeNi target in a liquid environment [6].

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