WS101-7: Computer simulation of possible materials modification effects by very high-flux accelerated ions

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Ion implantation is a widely used tool in materials research and industry. For instance, doping of semiconductors is routinely carried out by ion implantation, making the field essentially a multi-billion dollar industry. In this talk, I focus on comparing the differences between laser-driven and conventional ion acceleration with respect to the physics of ion irradiation of materials. Laser ion acceleration essentially opens up a new regime of peak fluxes for materials modification, one where the ion-induced collision cascades can overlap in both space and time, something which essentially never occurs during use of conventional ion accelerators. This flux regime is, however, not entirely unprecedented: during electrical arc discharges, similar fluxes are present, in a limited time and space domain [1]. The laser ion irradiation involves a very wide energy range, which also differs strongly from the conventional accelerator condition.

Thanks to these differences, laser-driven ion acceleration would open up several new interesting physics regimes for exploration. The much wider energy spread of laser-driven ion bunches compared to conventional ion irradiation may actually offer advantages of practical value. In fact, in modern materials processing quite often “box-like” ion implantation depth profiles are desired, and to achieve these, the implantation is split up into several stages that utilize different ion energies. Laser acceleration could at least in principle achieve the same goal with a single “shot” – although this would require achieving a fairly well-defined, controllable ion energy profile with the laser-driven scheme.

Comparison with the arc plasma modification, on the other hand, indicates that laser-driven acceleration with similarly high fluxes could open up a new materials modification regime. The laser-acceleration could have the advantage over arcing that one could use any ion-material combination – arcing is limited to using the same material for both the implanted ions and the material to be implanted. Moreover, the laser acceleration would be more controllable and the ion flux densities could be better tuned. Also a regime slightly below the “heat spike overlap” regime could be very interesting from a basic science point of view, as it would allow studying materials modification in a regime where there is very little time for thermally driven defect migration. The combination of very high flux density and little time for defect migration could allow for making new kinds of metastable thin films.

[1] Timko H, Djurabekova F, Costelle L, Nordlund K, Matyash K, Schneider R, Toerklep A, Arnau-Izquierdo G, Descoeudres A, Calatroni S, Taborelli M, and Wuensch W. Mechanism of surface modification from the arc plasma-surface interaction in Cu. *Phys. Rev. B,* **81**:184109, 2010.