Direct Simulation Monte Carlo simulations of laser-produced plasma expansion using SPARTA

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In laser machining, when the incident pulsed laser is strong enough to remove layers from the material target, a laser-produced plasma (LPP) forms, which is widely applied from material characterization to thin film deposition. LPP has been used in pulsed laser deposition to grow complex films with good stoichiometry [1]. A good model of the plasma expansion dynamics allows us to better predict the thickness distribution of the resulting film, especially considering the inherently narrow angular distribution of typical LPPs.

We model the LPP expansion using Direct Simulation Monte Carlo method [2], which treats the plasma constituents as representative particles and evaluates the particle interactions stochastically–in contrast with the deterministic modelling in molecular dynamics. We used SPARTA (Stochastic Parallel Rarefied-gas Time-accurate Analyzer) [3], which is an open-source code, to implement the expansion of the LPP from a copper target to a model substrate. The ablation is assumed to be caused by a nanosecond pulsed laser with a rectangular beam spot, and the particle emission input for SPARTA consists of copper atoms with a shifted Maxwellian velocity distribution [4].

We validated the model by demonstrating the flip-over effect, which is known as the apparent rotation of the plume aspect ratio as it propagates away from the target. By assuming the particle flux over a plane as representative of the film thickness distribution, we demonstrated the 90° flipping of the film distribution. This effect has also been experimentally observed in numerous studies and is considered a qualitative validation of LPP expansion models [5–6]. Modelling of LPP with DSMC paves the way for a facile and low-cost optimization of pulsed laser deposition, such as using mechanical filters of various geometries and exploring different deposition geometries, towards a more uniform film thickness distribution.

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