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Fundamental mechanisms of accelerated and plasma ion interactions with materials: insights from atomistic simulations

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In this talk, I will overview how atomistic computer simulations carried out over the last about 30 years, have enabled a much improved understanding of how ions accelerated in a vacuum interact with materials. Molecular dynamics simulations have enabled a good understanding of heat spikes, in which damage production mechanisms are fundamentally different from those predicted by traditional binary collision-based theories. Heat spikes can lead to direct production of large damage clusters and sputtering of atom clusters. Most recently, joint experimental and theoretical efforts have shown that in nanoclusters and nanowires, heat spikes can lead to huge sputtering yields exceeding 1000 atoms and major modification of the entire structure. I will also present a new systematic approach to analyze ion channeling. The results show that for typical ion implantation conditions, a large fraction (20-60%) of all crystal directions are channeling. Due to this, even when irradiating polycrystalline materials, one cannot a priori assume channeling effects are negligible.

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