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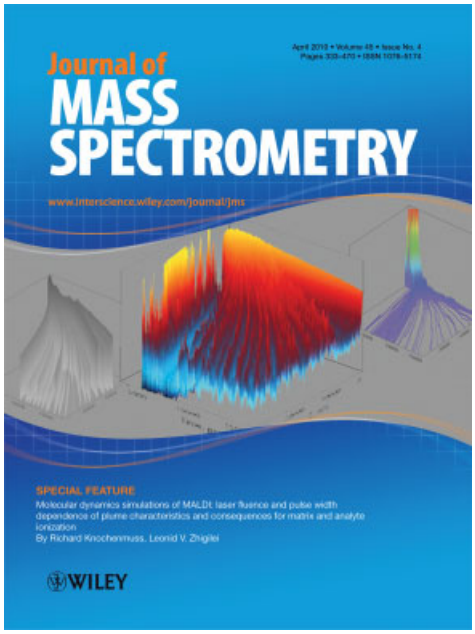
This month's special feature tutorial authored by Richard Knochenmuss and Leonid V. Zhigilei is entitled 'Molecular Dynamics Simulations of MALDI: Laser Fluence and Pulse Width Dependence of Plume Characteristics and Consequences for Matrix and Analyte Ionization. The cover image shows three aspects of a molecular dynamics simulation of a MALDI ablation event, as a function of time and position above the original surface. The left image shows the density of the ablated material. Clusters and droplets appear as curved surfaces, with low density gas between. As they evaporate, the heights of the surfaces decrease. The central image shows the temperature. As the ensemble expands, the gas cools faster than the entrained clusters. The right image shows the density of laser-generated ions. Evident is a very high initial spike during the laser pulse, followed by rapid recombination as the material disintegrates and ions become mobile. Only a few ions survive to reach the detector.



Molecular dynamics simulations of MALDI: laser fluence and pulse width dependence of plume characteristics and consequences for matrix and analyte ionization

Richard Knochenmuss* and Leonid V. Zhigilei

Molecular dynamics simulations of matrix-assisted laser desorption/ionization were carried out to investigate laser pulse width and fluence effects on primary and secondary ionization process. At the same fluence, short (35 or 350 ps) pulses lead to much higher initial pressures and ion concentrations than longer ones (3 ns), but these differences do not persist because the system relaxes toward local thermal equilibrium on a nanosecond timescale. Higher fluences accentuate the initial disparities, but downstream differences are not substantial. Axial velocities of ions and neutrals are found to span a wide range, and be fluence dependent. Total ion yield is only weakly dependent on pulse width, and consistent with experimental estimates. Secondary reactions of matrix cations with analyte neutrals are efficient even though analyte ions are ablated in clusters of matrix.

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