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Dynamic coupling between particle-in-cell and atomistic simulations

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We propose a method to directly couple molecular dynamics, finite element method and particle-in-cell techniques, to simulate response of a metal surface to high electric fields. We use this method to simulate the evolution of a field emitting tip under thermal runaway, by fully including the 3D space-charge effects. We also present a comparison of the runaway process between two tip geometries of different widths. The results show with high statistical significance, that in case of sufficiently narrow field emitters, the thermal runaway occurs in cycles where intensive neutral evaporation alternates with cooling periods. The comparison with previous works shows, that the evaporation rate in the regime of intensive evaporation is sufficient to ignite a plasma arc above the simulated field emitters.

The proposed method, which is under constant development, forms the basis for fully simulating the processes that lead from thermal runaway of intensively field emitting nanotips tips to full arc plasma onset. By introducing and handling new particle species such as neutrals and ions, we aspire to bridge the gap of understanding between the dark current and the vacuum arc ignition. This understanding is becoming increasingly important, in view of recent developments in the analysis of the dependence of the breakdown rate to the available electromagnetic power.

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