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Improving 1-D TD-DFT Simulations of Optical Field Emission from Nanopatterned Cathodes

Nanopatterned cathodes, operating under the strong optical field emission regime, are promising candidates for high brightness electron beam generation. Previous theoretical studies have indicated that brightness monotonically increases with the enhanced laser intensity, provoking the thermomechanical studies to determine the cathodes'limits. We present an in-progress ab initio calculation of the dominant heating process, vacuum heating, within a one-dimensional time-dependent density-functional theory framework. The Hartree potential embodies the mixed geometry of the chosen system, the nanoblade, where the vacuum region is treated with cylindrical symmetry and the bulk region with planar symmetry. Additionally, with the goal of improving backscatter current yields, we present progress in improving these rescattering simulations by developing an effective one-dimensional surface potential which adheres to reflection probabilities as calculated via density-functional theory. For all these efforts, numerical solution stability remains problematic.

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