

Physics and Applications of High Brightness Beams



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Modeling field electron emission from a flat Au(100) surface with density-functional theory

Field electron emission, or electron tunneling through a potential barrier under a strong electrostatic field, is of broad interest to the accelerator physics community. For example, it is the source of undesirable dark currents in resonant cavities, providing a limit to high-field operation. The classical approach to field electron emission is the Fowler-Nordheim framework, which incorporates a simplistic surface potential to compute the electron transmission coefficient. We build a more realistic model using a density-functional theory (DFT) calculation. We use the potential and charge densities from an Au(100) surface to construct an improved one-dimensional potential barrier. This potential is used under the Wentzel–Kramers–Brillouin (WKB) approximation to find the electron transmission coefficient and emission current densities. Moving beyond the WKB approximation, we numerically solve Schrödinger’s equation using the transfer matrix technique. Our results indicate that the WKB approximation is inaccurate for surface fields exceeding 10 V/nm as has been achieved in laser-field emission experiments.

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