First-Principles Calculations of Field Evaporation in Atom Probe Tomography

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Atom probe tomography (APT) has developed into a key technique for studying 3D element distribution in complex microstructures at near- atomic resolution. At the heart of the technique is the evaporation of single atoms from a very sharp tip exposed to huge electric fields (10^{11}V/m). However, commonly used geometric reconstruction algorithms fail to take into account any details of the evaporation mechanism, such as differences in evaporation between chemical species or from different sites. To shed light on the factors influencing eld evaporation, we study desorption from various sites (ad-atom, steps, kinks) on prototypical metal surfaces by means of density-functional theory calculations. From these calculations, we obtain electric-field-dependent evaporation barriers, which will be used in subsequent APT simulations. We also find evidence for the roll-over effect at steps, that has been proposed to explain orientational bias in evaporation trajectories.