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Induced changes in surface bonding by Electric Field: Integrating First Principles and Atom Probe Tomography JOAQUIN PERALTA, CLAUDIA LOYOLA, Departamento de Física, Universidad Andrés Bello, República 220, Santiago, Chile, SCOTT BRODERICK, KRISHNA RAJAN, Department of Materials Science and Engineering, Iowa State University, 2220 Hoover Hall, Ames, IA 50011-2230, USA — Evaporation field is a phenomenon that occurs when surface atoms start to evaporate with the presence of a strong electric field. This is utilized in Atom Probe Tomography (APT), by a voltage over a specimen tip. The evaporation of these ionized atoms allow us to generate a three dimensional reconstruction of the specimen. Despite the big amount of information extracted from APT, the phenomenology of the process in an atomic level has not been widely studied. In this work we investigate the evaporation process on an Al_3Sc surface under the presence of a strong electric field by using DFT with Quantum-Espresso software. The chosen surface contains a slab of 80 atoms of Al_3Sc in the $< 111 >$ direction along the z-axis. The calculations were performed with four different configuration of ad-atoms on the surface: Al, Sc, Al–Al, Al–Sc. The electric field is applied slowly to the surface up to 36 V/nm. The distance of the ad-atom or dimer to the surface is not modified during the simulation. The charge density between these and the surface is determined. This work describes an exhaustive analysis of the charge bonding of the ad-atoms and the surface with the presence of a strong electric field. Variations of the bonding are clearly observed and related to detected ions in APT.

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