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First Principles Modeling Studies of Field Evaporation: Preliminary Studies Relevant to the Atomscope

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The design and construction of an integrated instrument, that combines atom probe tomography (APT) and scanning transmission electron microscopy (STEM), the proposed *Atomscope* [1], poses not only design challenges but also the need to link the physics of image formation and chemical analysis in the APT with the imaging and microanalysis in the STEM. The development of meaningful correlations between APT and STEM modalities requires a detailed understanding of the impact of specimen chemistry and specimen geometry on evaporation mechanisms [2]. This study provides some of the initial [3] first principles modeling findings of parallel studies exploring the energetics of i) preferential evaporation (relevant to multicomponent systems) and ii) evaporation based on the role of tip shape. The computations are based on Quantum-Espresso (QE) codes [4]. QE is an integrated suite of computer codes for electronic-structure calculations and materials modeling at the nano-scale. It is based on Density Functional Theory (DFT), plane waves and pseudo-potentials (norm-conserving, ultra-soft and the projector augmented wave method (PAW)).

The field evaporation on the surface of Al_3Sc, was studied with ab-initio techniques for two kinds of different atomic configurations of ad-atoms on this surface: single atom evaporation (Sc and Al evaporation) and two atom evaporation (Sc-Al and Al-Al dimer evaporation). A general structure of this surface is shown in Fig. 1. The study was developed using the QE code that allows the application of high electric fields to slab geometry. The evaporation fields registered by the simulations are in good agreement with experimental results, Fig. 2. The polarization effects will also be studied for the ad-atoms species considering charge density of different configurations for systems under different electric fields. At the same time, the goal is show the variation of the bond nature with increasing electric fields. Ab-initio techniques have been used to explore the response of tip shape to different electrical fields. Some representative results for a hemispherical tip under different field strengths are shown in Fig. 3. It is noteworthy that the close-packed {111} Al plane exhibits systematically lower hump energies, consistent with the proposal [5] that the deeper potential wells in the more close-packed planes facilitating a higher spatial resolution in the direction of these plane-normals. [6]

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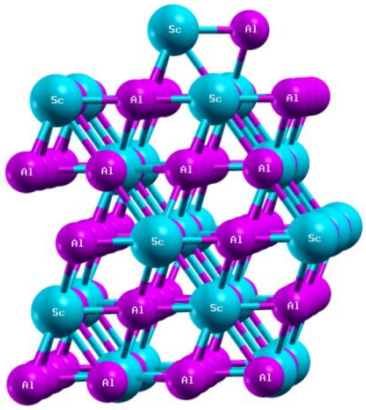

FIG. 1: A structure of Al_3Sc composed of 5 layers and 2 ad-atoms in the surface (Al-Sc).

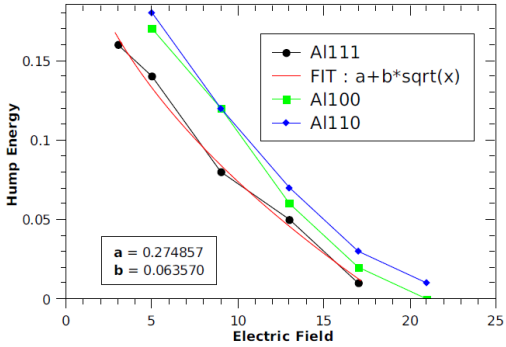

FIG. 2: Results of field evaporation for different Al surfaces <111>, <110> and <100>. This result demonstrates how the field evaporation changes for different kinds of surface configurations.

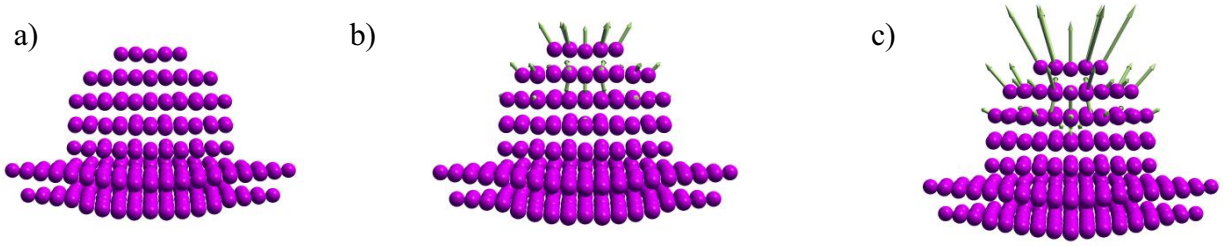

FIG. 3: Simulation of the effect of different electrical fields on hemispherical tip shape: a) no field, b) 13 V/nm, and c) 15 V/nm

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