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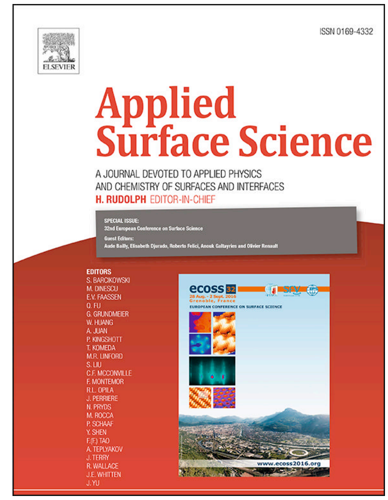


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# $Ba_xSc_yO_z$ on W (001), (110), and (112) in Scandate Cathodes: Connecting to Experiment via $\mu_O$ and Equilibrium Crystal Shape

Qunfei Zhou[a], Xiaotao Liu[a], Tyler Maxwell[a], Bernard Vancil[c], T. John Balk[a,b], Matthew J. Beck[a,*]

[a]*Department of Chemical and Materials Engineering, University of Kentucky, Lexington, KY, USA*
[b]*Electron Microscopy Center, University of Kentucky, Lexington, KY 40506, USA*
[c]*E-beam Incorporated, Beaverton, 97007, Oregon, USA*

**Abstract**

Quantum mechanical calculations of the structure and properties of a range of $Ba_xSc_yO_z$ adsorbate layers on W (001), (110), and (112) surfaces reveal the importance of O chemical potential in controlling the surface structure, surface energy, equilibrium crystal shape, and work function of W particles in Sc-containing (scandate) cathodes. Using the experimentally observed shape of W particles present in a high-emission scandate cathodes as a constraint, screening of ~2000 possible combinations of surface configurations reveals that the observed W grains are terminated with $Ba_{0.50}O/W_{(001)}$, $Ba_{0.25}O/W_{(110)}$ and $Ba_{0.50}O/W_{(112)}$ surfaces, and were equilibrated in an O-poor environment with $\mu_O$ between ~-8.5 and -8.0 eV/at. Examination of the surface structures studied reveals that competing Ba-O and O-W interactions control the net surface dipole and that this dipole directly correlates with computed work functions, implying that the surface dipole alone is sufficient to explain low work functions observed for scandate cathodes. Analysis of the present results suggests that the role of Sc in scandate cathodes is to tune $\mu_O$ and that difficulties in manufacturing scandate cathodes likely arises from variability in the availability of O at the cathode surface during activation and operation.

*Keywords:* thermionic cathodes; tungsten surfaces; scandate cathodes; work function; density functional theory; equilibrium crystal shape

## 1. Introduction

Electron emitting thermionic cathodes are key components in a range of vacuum electronic devices, including traveling wave tubes for RF amplification, microwave devices, thermionic energy converters, and more[1, 2]. Ongoing efforts to improve performance of thermionic cathodes focus on increasing the emitted current density at fixed temperature,

*Corresponding author
*Email address:* m.beck@uky.edu (Matthew J. Beck)