First-Principles Model of Miram Curve from Polycrystalline Tungsten Cathodes

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Abstract: *Previously, we constructed a first-principles statistical model to predict the non-uniform emission from polycrystalline tungsten cathodes, which incorporated microstructure characterization results, crystallographic-orientation-specific work function values via density functional theory (DFT), and temperature-limited (TL) emission physics. This previous model could only predict the TL region of the Miram curve and not the transition between TL and full-space-charge-limited (FSCL) regions. In this work, we have expanded our model to predict emission along the entire Miram curve, including the transition from TL to FSCL regions, without any empirical assumptions on work function distribution or empirical emission equations. This more advanced model provides a pathway to understanding the complex physics of emission from heterogeneous cathode surfaces, which is a key issue for the commercial production and use of thermionic cathodes in vacuum electronic devices.*

Keywords: Miram curve; impregnated cathode; thermionic emission; non-uniform emission.

Thermionic electron emission cathodes comprised of porous, polycrystalline tungsten bodies impregnated with an oxide mixture of CaO-Al_2O_3-BaO (B-type cathodes), and cathodes impregnated with the prior oxide mixture and containing an Os-Ru layer (M-type cathodes) have been widely used as electron sources in commercial high power vacuum electronic devices (VEDs) for many years. In addition, recent studies of scandate cathodes have propelled them close to commercial viability [1]. Previous works have demonstrated the work functions of tungsten-based cathodes vary with the facet orientation [2] and that tungsten-based cathodes have spatially non-uniform emission [3].

The well-known Richardson-Laue-Dushman thermionic emission equation and more generalized emission equations, such as Jensen's combined thermal-field-photoemission equation [4] can accurately predict the uniform emission from a homogenous cathode with a single work function. However, real cathodes have rough morphologies and contain many emitting surfaces with emitted currents which vary as a function of position on the cathode surface and over time. These complex surface physics make it challenging to predict the Miram curves for polycrystalline cathodes from a first-principles theoretical physics basis.

Our previous work [5], [6] provided an approach to predict the two-dimensional (2-D) work function map by combining the crystallographic orientation distribution via electron backscatter diffraction (EBSD) and DFT-calculated work function values to model the physics of non-uniform emission in the TL region from cathodes with multiple work functions. Fig. 1 shows the 2-D work function map of a representative sample of a commercial B-type cathode from L3 Technologies. The work function values are discretely distributed and range from 1.9 eV to 2.6 eV [2], [7], which is quite different from the simplified continuous work function distribution assumptions made in some previous studies of Miram curves [8].

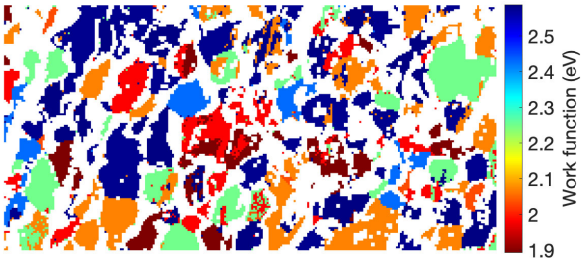

Figure 1. Work function map of a commercial B-type cathode sample. Areas where the grain orientations are unrecognized by electron backscatter diffraction (EBSD) are plotted in white.

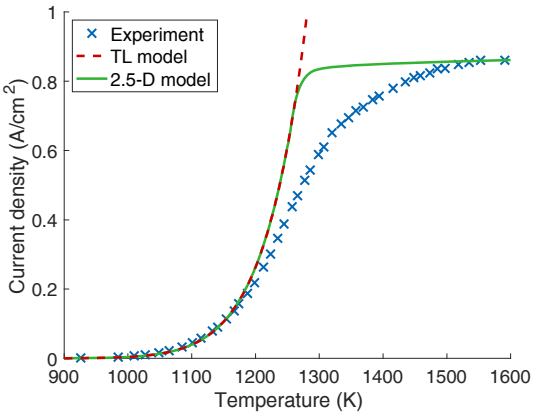

Figure 2. Predicted Miram curves using the work function map of the B-type cathode sample shown in Fig. 1. The previous temperature-limited (TL) model is shown as a dashed line, the 2.5-D model from this work is shown as a solid line, and the experimental emission data shown as '×' symbols, all for the same B-type cathode.

Fig. 2 contains experimental emission data from the same cathode depicted in Fig. 1, together with predicted Miram curves from our previous and present models. The dashed curve in Fig. 2 shows the predicted Miram curve using our previous model and the work function distribution of Fig. 1. Under the assumption that each work function patch emits independently, this previous model works only in the TL region [6] and cannot predict the transition region (sharp or rounded) between TL and full-space-charge-limited (FSCL) emission in the Miram curve.

An advanced first-principles model to compute the entire Miram curve, especially the transition region between TL and FSCL regions, would be beneficial as one could use this model to predict the electron emission, including the knee temperature, based on the microstructure of real cathodes and the geometry of the device in which it is used (e.g. electrode positions and distances, applied potentials, etc.). This knowledge would provide insight on the impact of cathode microstructure and morphology on the emission and improve models used to design VEDs.

Recent studies [9], [10] have illustrated that the interaction of emitted electrons originating from different work function patches has a considerable effect on the predicted Miram curve. Further, these studies verified that the Miram curves computed under infinite-*B* (magnetic field) assumption (1.5-D model) and under zero-*B* assumption (MICHELLE) agree with each other for cathodes with 1-D variation of the work function, e.g. as a series of stripes of alternating work function. To simplify the calculation of the Miram curve from a cathode with a 2-D spatial distribution of work function, the infinite-*B* assumption was used in this work, which forces the electrons to only travel along the cathode-anode direction (i.e. the electrons have no transverse velocity). In this work, a 2.5-D model, which was made by adding an additional dimension to the 1.5-D model used in previous studies [9], [10], was used to solve the emission from the 2-D work function map shown in Fig. 1 with periodic boundary conditions. This 2.5-D model includes the interaction of different work function patches on a 2-D surface. The only fitting parameter in this 2.5-D model is the cathode-anode distance $d_{\text{A-K}}$, which was obtained by fitting the emission current at the FSCL region. The value of $d_{\text{A-K}}$ was fit rather than measured because its value is expected to change slightly, but non-negligibly, as a function of temperature due to thermal expansion effects.

The solid curve in Fig. 2 illustrates the Miram curve predicted by the 2.5-D model. The 2.5-D model overlaps with the previous TL model in the TL region but has a smooth transition between the TL and FSCL regions. However, the experiment displays a significantly larger degree of rounding between the TL and FSCL regions than the 2.5-D model. Research is ongoing to understand the origin of this discrepancy.

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References

[1] D. M. Kirkwood et al., "Frontiers in Thermionic Cathode Research," IEEE Trans. Electron Devices, vol. 65, no. 6, pp. 2061–2071, Jun. 2018.

[2] R. Jacobs, D. Morgan, and J. Booske, "Work function and surface stability of tungsten-based thermionic electron emission cathodes," APL Mater., vol. 5, no. 11, p. 116105, Nov. 2017.

[3] C. Wan, J. M. Vaughn, J. T. Sadowski, and M. E. Kordesch, "Scandium oxide coated polycrystalline tungsten studied using emission microscopy and photoelectron spectroscopy," Ultramicroscopy, vol. 119, pp. 106–110, Aug. 2012.

[4] K. L. Jensen, Introduction to the Physics of Electron Emission. Wiley, 2017.

[5] D. Chen, R. Jacobs, V. Vlahos, K. L. Jensen, D. Morgan, and J. Booske, "Combining theory and experiment to model electron emission from polycrystalline tungsten cathode surfaces," in 2018 IEEE International Vacuum Electronics Conference (IVEC), 2018, pp. 39–40.

[6] D. Chen, R. Jacobs, V. Vlahos, D. Morvan, and J. Booske, "Statistical Model of Non-Uniform Emission/rom Polycrystalline Tungsten Cathodes," in 2019 International Vacuum Electronics Conference (IVEC), 2019, pp. 1–2.

[7] S. De Waele, K. Lejaeghere, M. Sluydts, and S. Cottenier, "Error estimates for density-functional theory predictions of surface energy and work function," Phys. Rev. B, vol. 94, no. 23, p. 235418, Dec. 2016.

[8] J. C. Tonnerre, D. Brion, P. Palluel, and A. M. Shroff, "Evaluation of the work function distribution of impregnated cathodes," Appl. Surf. Sci., vol. 16, no. 1–2, pp. 238–249, May 1983.

[9] D. Chernin, Y. Y. Lau, J. J. Petillo, S. Ovtchinnikov, D. Chen, A. Jassem, R. Jacobs, D. Morgan, J. Booske, "Effect of non-uniform emission on Miram curves," IEEE Trans. Plasma Sci., vol. 48, no. 1, pp. 146–155, Jan. 2020.

[10] J. Petillo, S. Ovtchinnikov, D. Chernin, A. Jassem, Y. Y. Lau, D. Chen, R. Jacobs, D. Morgan, and J. Booske, "Investigations Into The Physics Of Miram Curves," in 2020 IEEE International Vacuum Electronics Conference (IVEC), 2020. [Submitted]