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More precise determination of work function based on Fermi–Dirac distribution and Fowler formula

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ABSTRACT

More precise numerical method to simulate current–voltage of metal at fixed temperature is presented in this paper. The new algorithm for the simulation has been developed via Fermi–Dirac distribution step by step. These calculated characteristics are shown to remain in excellent agreement with the experimental ones, taken for a range of different metals, which strong supports the validity of the model. It is also shown that based on the Fowler formula, higher precise work function can be determined.

1. Introduction

Although the purely thermal electron emission was not originally developed for the sake of interpreting the work function of metal [1–3], the work functions of many metals have been detected via thermal electron emission [4–12]. Thermionic emission is important in the context of development of cathodes [13] and has been investigated extensively for variety of applications such as X-ray tubes, high power microwave device, cathode ray tubes, and fluorescent lamps [14,15]. Historically, there are many applications of electric arcs in industrial processing of materials, for example in welding, cutting, thermal spraying, heating, surface treatment and chemical vapor deposition (CVD) [16,17]. In general, thermonic electron emission from the cathode surface is a function of both the cathode temperature and the work function of the electrode materials, which is today known as the Richardson–Dushman equation. Since thermonic emission requires a very high surface temperature close to the melting point of metal, energy transfer from the free-burning arc to the cathode electrode is necessary for maintaining this high surface temperature. For example, ions accelerated by the electric field between anode and cathode fall zone.

More precise measuring the work function of metals would be extremely helpful for a better understanding of the physical behavior in the electrode region, which would contribute to developments of advanced control and evaluation system for materials processing by the arcs through the prediction of properties of the total arc processing system [18]. The more precise thermonic current can be obtained, the more precise work function of metals may be calculated, and the behavior of the emitted current depends on the strength of the electric field applied to remove and detect the emitted electrons. At low field strengths which refer to voltage is lower than 25 V, experimental plot $I(V,T)$ against $I(0,T)\exp(p_1\sqrt{V/T})$ cannot explain the experimental curve constructed via I and V since the electrons are not removed rapidly enough and their repulsive charge distribution slows the rate at which electrons can actually reach the detector. When the applied electric field strength is large which means voltage is higher than 25 V, the work function of the material is decreased, and the measured emitted current is related to the actual current by the following relation:

$$I(V,T) = I(0,T)\exp\left(\frac{p_1\sqrt{V}}{T}\right)$$

The Richardson–Dushman equation is a convenience; in practice, however, there is still a lack of practical method to determine the work function more precise than that of by Richardson–Dushman. Hence, a model is needed which would allow prediction current of metal at one temperature by voltage at the highest precise level. Such a model is developed and verified experimentally in this paper. In this article the main features of the Fowler formula on

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calculation work function are also concerned using the most precise results of thermal electron emission.

2. Mechanism between current and voltage

In the past, electron transport over the work function from the surface of metal is described by thermionic emission theory (TE) based on the Schottky effect with the expression:

$$I(V,T)=I(0,T)\exp\left(\frac{p_1\sqrt{V}}{T}\right) \tag{1}$$

where $I(V,T)$ is the current generated by both electronic field and heating, $I(0,T)$ is thermionic current, in other words, thermionic current is electron beam emission only by heating. T is absolute temperature of filament, p_1 is constant controlled by the structure of both anode and cathode, the V is the voltage between anode and cathode. One notable is that the electric potential of cathode must be lower than or equal to that of anode in function (1). For thermal electron emission, however, the nonlinearity in $Ln(I(V,T))$ against $\sqrt{V}$ cannot be interpreted via Eq. (1).

Because electron is fermions, the Fermi–Dirac distribution should apply to electron. [3,19] Fermi–Dirac distribution is usually written:

$$f(E)=\frac{1}{1+\exp((E-E_f)/kT)} \tag{2}$$

where $f(E)$ is the probability that a particle will have energy E, E_f is Fermi energy, T is Absolute temperature, k is Boltzmann constant and its value is $k=1.38\times10^{-23}$ in SI unit.

The kinetic energy of thermion electron is $eV-e\varphi-e\delta$ after it has been liberated from the metal and enter into the external electronic field with V. Where e=electron charge=1.602×10^{-19}, $e\varphi$ is the work function of the metal. $e\varphi$ is the energy you must give to an electron at the Fermi level to kick it out of the metal and turn it into a free election. An electron below the Fermi level needs more than $e\varphi$ to escape, δ is an additional contact potential because the surfaces of the anode and cathode are different. An electron now has kinetic energy $eV-e\varphi-e\delta$, thus the probability that an electron will have the kinetic energy $eV-e\varphi-e\delta$ is

$$f(E)=\frac{1}{1+\exp((E-E_f)/kT)}=\frac{1}{1+\exp((V-\delta-\phi)\cdot\frac{e}{kT})} \tag{3}$$

let

$$V_c=\delta+\varphi \tag{4}$$

$$V_0=\frac{kT}{e} \tag{5}$$

Function (3) become

$$f(E)=\frac{1}{1+\exp((V-\delta-\phi)\cdot\frac{e}{kT})}=\frac{1}{1+\exp\left(\frac{V-V_c}{V_0}\right)} \tag{6}$$

One natural conclusion is that current liberated by electric field at temperature of T, $I(V)$, is proportional to the probability, $f(E)$, that a electron will have energy $eV-e\varphi-e\delta$, in mathematical language:

$$I(V)=\frac{I_2}{1+\exp\left(\frac{V-V_c}{V_0}\right)} \tag{7}$$

But mathematical result shown that:

$$\frac{1}{1+\exp\left(\frac{V-V_c}{V_0}\right)}|_{V\to\infty}=0 \tag{8}$$

Experimental results of field emission tell that as the electric potential of cathode approaches low enough relative to anode, the anode current, $I(V)$, goes asymptotically to a constant value know as the forward saturation current, I_{max}:

$$I(V)|_{V\to\infty}=I_{max} \tag{9}$$

Boundary condition (9) predicts that the field emission current and voltage should be related as

$$I(V)=I_1+\frac{I_2}{1+\exp\left(\frac{V-V_c}{V_0}\right)} \tag{10}$$

Combining Eqs. (8), (9) and (10) yields

$$I_1=I_{max} \tag{11}$$

Substitution of Eq. (11) into Eq. (10) leads to following expressions:

$$I(V)=I_{max}+\frac{I_2}{1+\exp((V-V_c)/V_0)} \tag{12}$$

where I_{max} is the forward saturation current predicted via Eq. (12), I_2 is the current constant expected by Eq. (12), V_c is the inflection point voltage, when the voltage is less than V_c, the I–V curve is concave, while, as long as the voltage is higher than V_c, the I–V curve is large convex, meanwhile, the average value of the field emission current is fixed at V_c, the V_0 is constant of voltage. I_{max}, I_2, V_c and V_0 will be optimized.

In according to the definition of thermionic current, when there is no any accelerating field which means that the voltage between anode and cathode is zero in Eq. (12), the mechanism of the thermionic current can be read:

$$I_0(T)=I(o,T)=I_{max}+\frac{I_2}{1+\exp(-V_c/V_0)} \tag{13}$$

3. Application

The anode current against voltage curves was collected at each different temperature of tungsten as filament (cathode). Use the commercial measurement system for work function typed ZN17-SLWY-III to sweep the anode voltage from 16 V to 122 V. I–V plots of *the experimental data for* tungsten (W) are shown in Fig. 1.

In this paper, the field current curves of tungsten were analyzed at different temperatures in accordance with the above Eq. (12). Then through experimental data employed in the method of the regression analysis, the experimental curves for W at various temperatures have been simulated using the experimental data as shown in Fig. 1. Optimized parameters employed to simulate the component curves are also listed in Table 1. The modeled verification is also carried out by a comparison of modeled field current obtained by numerical integration of field current to measured field current in Fig. 1.

Although the current of Tungsten has been calculated via voltage at several temperatures, this does not give enough idea about how accuracy of the methodology suggested in this paper. To test for the determination of the field current of any kind of metal using experimental data of field current, *Experimental* I–V data of Potassium is taken from *published* paper and displayed in Fig. 2 [20]. At the same time, all of the data in Fig. 2 was fitted to the functional (12) and illustrated as cross in Fig. 2. The best parameters to obtain the best results of calculation are also listed in Table 1.