Journal of the Korean Vacuum Society
Vol. 3, No. 1, March 1994, pp. 1-7

〈연구논문〉

Energy Exchanges and Inversion Temperatures in Electron Emission at High Fields and Temperatures

M. S. Chung, I. W. Kim, J. S. Choi and J. M. Park

Department of Physics, University of Ulsan, Ulsan, Kyeognam 680-749
(Received November 2, 1993)

고전장 고온도에서 전자방출의 에너지 교환과 역온도

정문성 · 김일원 · 최점수 · 박지모

울산대학교 물리학과
(1993년 11월 2일 접수)

Abstract — A new calculation of energy exchanges and inversion temperatures in electron emission is presented. In this calculation, we introduce the tunnelling state contribution as a mechanism to vacate levels available for replacement electrons in field emission. It is found that the tunnelling contribution to the availability of vacant states is necessary to explain the replacement process occurring in the emitter region. The net energy exchange $\Delta\varepsilon$ per electron obtained as a function of both temperature and field shows much improved agreement with experimental data. The inversion temperature T_i as a function of field is now in good quantitative agreement with existing experimental data. The present results favor the argument of Fleming and Henderson in the Nottingham-Fleming and Henderson controversy concerning the average energy of the replacement electrons.

요 약 — 전자방출에서 에너지 교환과 역온도를 새롭게 계산하였다. 전자방출에서 대체전자들에 유용한 빈상태들을 만드는 요소로 터널링 효과를 이 계산에서 고려하였다. 그것은 방출부분에서 일어나는 대체과정을 설명하기 위해서는 빈상태를 만드는데 터널링 기여가 필수적이기 때문이다. 이렇게 계산하여 온도와 전장의 함수로 얻어진 전자당 에너지 교환은 실험결과와 잘 일치하였다. 또한 전장의 함수로 얻어진 역온도도 실험치와 만족할 만한 일치를 보여주었다. 이 결과는 대체전자들의 평균에너지에 대한 노팅햄-플레밍과 헨더슨의 논쟁에서 후자의 견해를 지지하는 것이다.

1. Introduction

With the advent of new emitter technologies for applications in vacuum microelectronics and electron microscopy [1, 2], there has been renewed interest in the study of thermal stability of these atomic sized tips. In particular, the energy exchange between the replacement electrons from the external circuit and the cathode becomes important at the very high emission densities present in field and thermal-field emission. This exchange process, or so-called Nottingham effect [3], is a stabilizing factor in determining the local temperature at the emitter surface [4, 5]. If the average energy $\langle\varepsilon_e\rangle$ of the emitted electrons is less than that of the replacement electrons supplied from the external circuit, $\langle\varepsilon_r\rangle$, the cathode tends to be heated during the emission; if $\langle\varepsilon_e\rangle$ is greater than $\langle\varepsilon_r\rangle$, the cathode tends to be cooled by the exchangeas predicted by Nottingham [3]. For emission at $T=0$ K, all the energy states above the Fermi energy are empty; hence, all emitted electrons have less than the Fermi energy. If $T>0$ K, the higher levels become populated and contribute preferentially to the emission, causing a decrease in the average heat transfer per emitted electron. There exists a temperature, called the inversion temperature T_i, at which the Nottingham effect changes from one of heating to one of cooling. This effect, although difficult to measure experimentally, has been observed in both normal [6-8] and superconducting metals [9].

Early theoretical studies of energy exchange by Swanson *et al.* [4] used the free electron model [10] and an equilibrium distribution for the electron gas. Subsequent work by Engle *et al.* [11, 12] included a quantum modified barrier and non-local equilibrium effects due to temperatures and fields. Although improved agreement with the experiment was obtained for the inversion temperature, there is still disagreement between the calculated and experimental values. More recently, Miskovsky *et al.* [13] demonstrated that there is a significant dependence of the inversion temperature on geometry of the microtip.

The theory of the average energy of the replacement electrons, $\langle \varepsilon_r \rangle$, has been a subject of controversy since Nottingham's assertion that $\langle \varepsilon_r \rangle$ is equal to the Fermi energy or the chemical potential μ of the emitter. This was contested by Fleming and Henderson [14] who developed a theory predicting that $\langle \varepsilon_r \rangle$ can be tens of meV's below the Fermi energy. However, although experiments and the calculations of Engle *et al.* [11, 12], Barengolts *et al.* [15], and Miskovsky *et al.* [13] are consistent with values of $\langle \varepsilon_r \rangle = \mu(1-x)$ where $x \sim 0.1$, the subject is still controversial.

In the present work we extend the heuristic arguments of Fleming and Henderson [14] and the work of Chung *et al.* [16] for the calculation of $\langle \varepsilon_r \rangle$. The determination of the replacement energy is made for a quasi-equilibrium charge carriers. In the present context, quasi-equilibrium means that the tunneling state contribution to $\langle \varepsilon_r \rangle$, which is inherently a non-equilibrium process, is taken into account using the equilibrium Fermi-Dirac distribution function. This is justified because the relaxation times for thermal equilibrium processes are much longer than tunneling times. In fact, a typical tunnelling time is around 10^{-15} sec [17] and thermal excitation or relaxation time is about $10^{-9} \sim 10^{-14}$ sec. Therefore, the distribution of replacement carriers is not expected to be in a thermal equilibrium state over a time scale of 10^{-15} sec. This analysis differs from the theory of Fleming and Henderson [14] in that we have explicitly included the tunnelling states in the calculation of $\langle \varepsilon_r \rangle$. Fleming and Henderson, on the other hand, only allow for occupancy of available states by replacement electrons as dictated by the equilibrium Fermi-Dirac distribution function. The quasi-equilibrium analysis predicts that $\langle \varepsilon_r \rangle$ depends on both the temperature and field and, in turn, reveals how the average energy exchange per electron $\Delta\varepsilon \equiv \langle \varepsilon_e \rangle - \langle \varepsilon_r \rangle$ also depends on these parameters.

In section 2, we derive an expression for the average energy including tunnelling state contribution in the replacement process. In section 3, we calculate the average energies of the emitted and replacement electrons. In section 4, the net energy exchange and the inversion temperatures are calculated within the quasi-equilibrium approximation. Conclusions are given in section 5.

2. Average Energy of Charge Carriers

Electron emission from the metal or semiconductor surface can occur via tunnelling when a strong field is applied (see Fig. 1). Under steady state conditions for each electron emitted from the cathode, a replacement electron is supplied to the system from the external wire. In this dynamic exchange, energy states in the emitter are emptied out by thermal excitation or tunnelling and are reoccupied by electrons supplied from the external reservoir. This replacement current makes possible the steady state current in the emitter region. Since the transport mechanisms (i.e., scattering) are different in each region, the average energies of charge carriers are not expected to be the same over the entire region.

In the ensuing discussion we assume a free electron model of the emitter. To calculate the average energy $\langle \varepsilon \rangle$, we use

$$\langle \varepsilon \rangle = \frac{\int \varepsilon\, j(\varepsilon)\, d\varepsilon}{\int j(\varepsilon)\, d\varepsilon}, \tag{1}$$

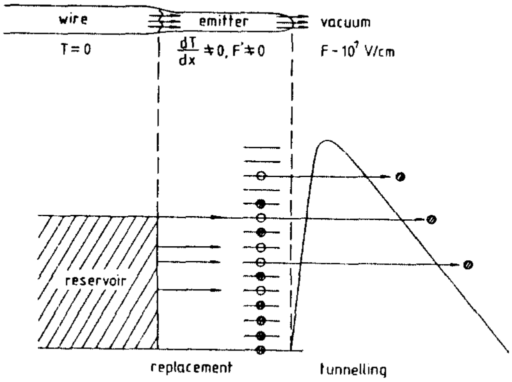

Fig. 1. Schematic of field emission tunnelling and replacement process. Empty states are produced due to thermal excitation and tunnelling. By conservation of charge, a portion of vacant states are reoccupied. The F is the applied field and F' is the field inside the metallic emitter. A vacant state in the emitter has a probability (say, A in text) to reoccupied by an electron supplied from the external reservoir (replacemet process).

where $j(\varepsilon)\,d\varepsilon$ is the current density in the energy range between ε and $\varepsilon+d\varepsilon$ and represents the particle flux. In phase space the particle density is the volume divided by the cube of Planck's constant, h^3 and by the configuration volume. Then the particle flux, Φ, moving in the positive x-direction (normal to the surface) is

$$\Phi=\frac{2}{h^3}\int d^3p\, v_x=\frac{4\pi m}{h^3}\int d\varepsilon\int d\varepsilon_x\,, \qquad (2)$$

where $\varepsilon=1/2\,mv^2$ and $\varepsilon_x=1/2\,mv_x^2$. The factor 2 is introduced due to spin. The total current density j, which is the particle number flux times the electronic charge, is given by

$$j=e\Phi=\int j(\varepsilon)\,d\varepsilon \qquad (3)$$

According to statistical mechanics, we can calculate an average energy $\langle\varepsilon\rangle$ given in the form of Eq. (1), irrespective of conduction or scattering mechanisms.

For field emission, the emitted current density j_e is due to tunnelling (see Fig. 1). Within the kinetic formalism, j_e is given by

$$j_e=\frac{4\pi me}{h^3}\int_0^\infty d\varepsilon\int_0^\infty d\varepsilon_x\, f(\varepsilon)\,D(\varepsilon)_x\,, \qquad (4)$$

where $f(\varepsilon)$ is the Fermi distribution function and $D(\varepsilon_x)$ is the transmission coefficient for an electron of normal energy ε_x.

Let the replacement current density be j_r. If the reservoir is at $T=0$ K, then the replacement electrons have energies equal to or less than the chemical potential of the reservoir μ (see Fig. 1). In the emitter at $T\geq 0$ K, the available empty states below μ are due to either thermal excitation (the Fermi factor) or tunnelling of the electrons out of the emitter. Including all available empty states, the replacement current density j_r is

$$j_r=\frac{4\pi me}{h^3}\int_0^\mu d\varepsilon\int_0^\varepsilon d\varepsilon_x[1-f(\varepsilon)+f(\varepsilon)D(\varepsilon_x)]\,A(T,\,F) \qquad (5)$$

The factor A is the fraction of the empty states which have been reoccupied by replacement electrons. Thus, A depends on temperature and field and is essentially a transmission coefficient for the interface between the cold reservoir (wire) and the emitter. The factor $1-f(\varepsilon)$ represents the probability of a level being vacant when a system is in thermal equilibrium. However, it is important to note here that the inclusion only of levels vacated by thermal excitation is not sufficient for a complete description of the replacement current in the field emission process. This can easily be seen from the following. The replacement current due to the thermal vacancies (the factor $1-f(\varepsilon)$) must be zero at absolute zero, while the field emission current is not. This is a contradiction. The physics demands that we include the tunneling states in the factor $f(\varepsilon)D(\varepsilon_x)$ which describe the additional probability for empty states produced due to tunnelling. It is precisely this factor that has not been included by Fleming and Henderson [14] although they did recognize that the replacement energy is a statistical average of the vacant states into which replacement electrons can be scattered. In the Fleming and Henderson model, only the empty states due to thermal excitation are accounted for.

Using Eqs. (1), (3), (4) and (5), the average energies for emitted and replacement electrons are given by,

$$\langle \varepsilon_e \rangle = \frac{\int_0^\infty d\varepsilon \int_0^\infty d\varepsilon_x \varepsilon f(\varepsilon) D(\varepsilon)}{\int_0^\infty d\varepsilon \int_0^\infty d\varepsilon_x f(\varepsilon) D(\varepsilon_x)}, \tag{6}$$

$$\langle \varepsilon_r \rangle = \frac{\int_0^\mu d\varepsilon \int_0^\varepsilon d\varepsilon_x \varepsilon [1-f(\varepsilon)+f(\varepsilon) D(\varepsilon_x)]}{\int_0^\mu d\varepsilon \int_0^\varepsilon d\varepsilon_x [1-f(\varepsilon)+f(\varepsilon) D(\varepsilon_x)]}. \tag{7}$$

In obtaining Eq. (7), the factor A of j_r is canceled. The average energies $\langle \varepsilon_e \rangle$ and $\langle \varepsilon_r \rangle$ can be calculated if $D(\varepsilon_x)$ is known. In the following analysis, we assume that $D(\varepsilon_x)$ is given by the WKB approximation. We will evaluate Eqs. (6) and (7) under a quasi-equilibrium approximation explained in the previous section.

3. Calculations of Average Energies

We assume a one-dimensional surface potential barrier (see Fig. 1). The transmission coefficient D is approximated by the WKB tunnelling probability [16, 18].

$$D = \exp[-c + (\varepsilon_x - \mu)/d] \tag{8}$$

where c and d are field-quantities whose values are given in Ref. [16, 18].

The average energy of emitted electrons, $\langle \varepsilon_e \rangle$, given by Eq. (6) can be obtained straightforwardly [4, 16, 18]:

$$\langle \varepsilon_e \rangle = \mu - d \frac{\pi k_B T/d}{\tan(\pi k_B T/d)}. \tag{9}$$

Here, the values of d are 0.42 eV for $F = 10^8$ V/cm and 0.5 for $F = 1.2 \times 10^8$ V/cm. The $\langle \varepsilon_e \rangle$ is shown as a function of temperature in Fig. 2 for $F = 10^8$ V/cm (a) and 1.2×10^8 V/cm (b). These results are the same as the works of Good and Muller [18] and Swanson *et al.* [4]. Similarly, we evaluate Eq. (7) to obtain [16]

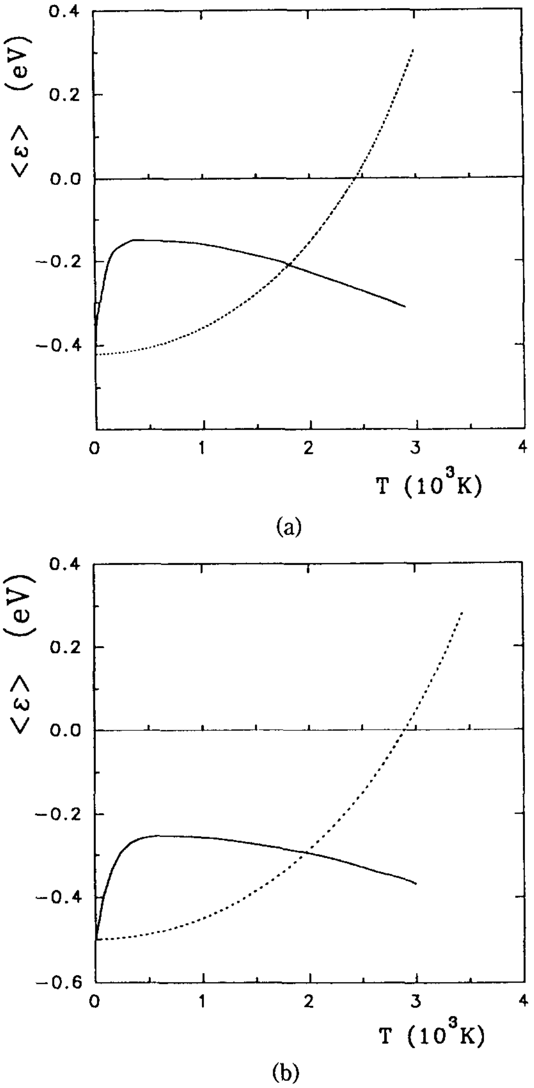

Fig. 2. Average energies of emitted (dotted line) and replacement (solid line) electrons, $\langle \varepsilon_e \rangle$ and $\langle \varepsilon_r \rangle$, respectively, for (a) $F = 1 \times 10^8$ V/cm and (b) $F = 1.2 \times 10^8$ V/cm. The two curves intersect at $T = T_i$. The difference in two curves represents the energy loss of the emitter. At $T = 0$ K, $\langle \varepsilon_e \rangle = \langle \varepsilon_r \rangle = \mu - d$, where $d = 0.42$ eV for $F = 10^8$ V/cm and $= 0.50$ eV for $F = 1.2 \times 10^8$ V/cm. For convenience, we choose $\mu = 0$.

$$\langle \varepsilon_r \rangle = \mu \frac{k_B T \ln 2\left[1 - \frac{\pi^2}{6 \ln 2} \frac{k_B T}{\mu}\right] + \frac{d^2}{\mu} e^{-c}\left[1 - \eta(1) \frac{k_B T}{d} - \frac{d}{\mu}\right]}{k_B T \ln 2\left[1 - \frac{\pi^2}{12 \ln 2} \frac{k_B T}{\mu}\right] + \frac{d^2}{\mu} e^{-c}\left[1 - \eta(1) \frac{k_B T}{d}\right]}, \tag{10}$$

where $\eta(1)=0.693$. As seen in Eq. (10), the thermal excitation contribution is dominant at high T while the tunnelling contribution dominates at low T. Thus, $\langle \varepsilon_r \rangle$ can be expressed in the following forms for different temperature regimes,

$$\langle \varepsilon_r \rangle = \mu - \frac{\pi^2}{12 \ln 2} k_B T - \frac{d^3 e^{-c}}{\mu k_B T \ln 2}, \quad T \gg T_r \quad (11)$$

$$\mu - d + \frac{\mu k_B T \ln 2}{d e^{-c}}, \quad T \ll T_{tr} \quad (12)$$

$$\mu - \frac{1}{2}\left(d + \frac{\pi^2}{12 \ln 2} k_B T\right), \quad T = T_{tr} \quad (13)$$

where $T_{tr}=d^2 e^{-c}/(\mu k_B \ln 2)$, the transition point temperature between the two dominant regions, the tunnelling and thermal excitation regions. The values of d are given just after Eq. (9). The values of e^{-c} are 0.21 for $F=10^8$ V/cm and 0.51 for $F=1.2\times10^8$ V/cm. It is worthwhile to note that the first two terms in Eq. (11) are equal to the average energy of the replacement electron obtained by Fleming and Henderson [14]. The third term in Eq. (11) is the correction due to tunnelling at high temperature. The analytic forms of Eqs. (11)~(13) make it possible to draw the whole graph of $\langle \varepsilon_r \rangle$ by interpolating into the region where the approximation is not valid. The results are shown in Fig. 2. The portion of the $\langle \varepsilon_r \rangle$ curve with positive slope represents the region where tunnelling is dominant, while the portion of the curve with negative slope is dominated by thermal excitation contribution. The intersection of the two curves represents the inversion temperature for the value of field.

In Fig. 2, T_{tr} is below $T_{max}=(12\, d^3 e^{-c}/\mu)^{1/2}/\pi k_B$ at which $\langle \varepsilon_r \rangle$ has the maximum. For $F=10^8$ V/cm, $T_{tr}=109$ K and $T_{max}=668$ K. For $F=1.2\times10^8$ V/cm, $T_{tr}=375$ K and $T_{max}=1353$ K. For $T>T_{tr}$, the tunnelling state contribution is negligible. This is usually the case when an experiment is operated. As shown in the Fig. 2, as T increases, $\langle \varepsilon_r \rangle$ increases rapidly in the region $0<T<T_{tr}$ and then decreases slowly. The reason is as follows. At $T=0$, the empty states available for replacement electrons are produced only by tunnelling. Since there are no thermal processes involved, the energy distribution of replacement electrons is exactly the same as the one of emitted electrons: $\langle \varepsilon_r \rangle = \langle \varepsilon_e \rangle = \mu - d$ at $T=0$. For $0<T<T_{tr}$, only the levels just below the Fermi energy are evacuated. These new vacancy levels ($\sim\mu$) are much higher than the average energy ($\sim\mu - d$) of replacement electrons. As T increases, the deeper levels become increasingly evacuated. Thus, $\langle \varepsilon_r \rangle$ increases rapidly for $0<T<T_{tr}$, and reaches a maximum and then decreases with T. Since the carrier population depends on field, the slope is steeper for small fields. It is important to note that $\langle \varepsilon_r \rangle < \mu$, which favors the argument of Fleming and Henderson.

4. Energy Exchanges and Inversion Temperatures

Within the quasi-equilibrium approximation, the energy exchange per electron in field emission is defined as

$$\Delta\varepsilon = \langle \varepsilon_e \rangle - \langle \varepsilon_r \rangle. \quad (14)$$

where $\langle \varepsilon_e \rangle$ is given by Eq. (9) and $\langle \varepsilon_r \rangle$ is given by Eqs. (11)~(13).

The calculated values of $\Delta\varepsilon$ are plotted as a func-

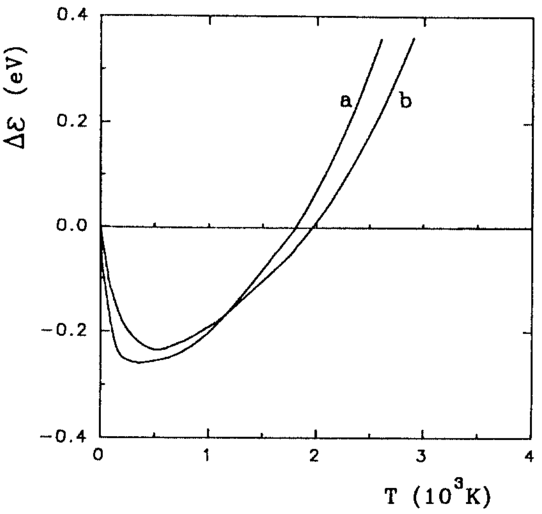

Fig. 3. Average energy exchange (or energy loss) per electron, $\Delta\varepsilon$, as a function of temperature for (a) $F=1\times10^8$ and (b) $F=1.2\times10^8$ V/cm. The value of the intersection with the x-axis defines the inversion temperature T_i.

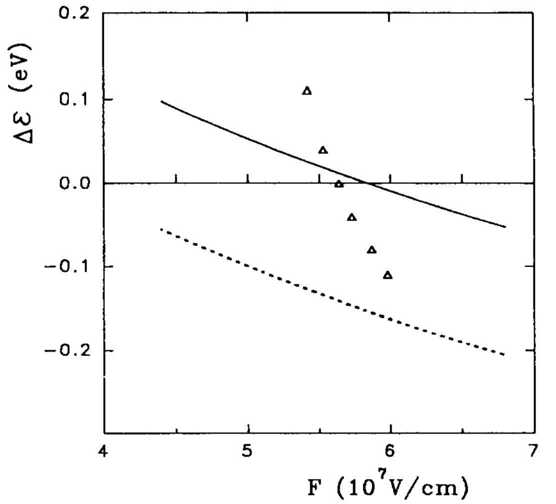

Fig. 4. Average energy exchange (or energy loss) as a function of field for T=961 K. The solid line represents the current theoretical values; the dotted line is the theoretical results of Swanson *et al* [4]; the triangles are the experimental data of Swanson *et al.* [4] for a clean tungsten surface.

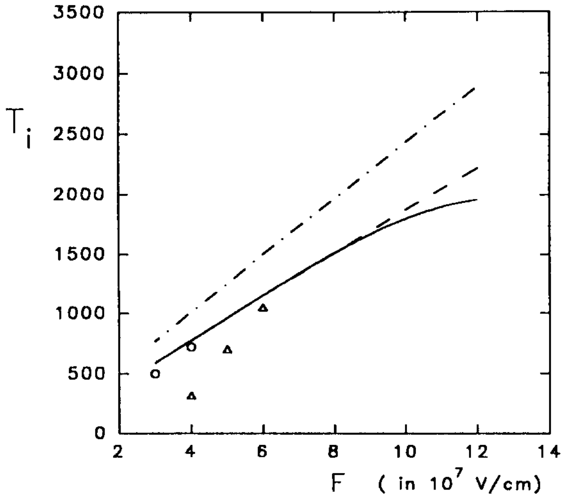

Fig. 5. Inversion temperature T_i as a function of field. The solid line represents the results for quasi-equilibrium analysis. The long dashed line are the calculated results for the equilibrium analysis without the inclusion of the available emptied tunnelling states; the dashed-dot line are the calculated theoretical results of Swanson *et al.* [4]. The two sets of experimental data are due to Swanson *et al.* (△) and Drechsler (○) [7] for a clean tungsten surface.

tion of T in Fig. 3 and as a function of F in Fig. 4. In Figs. 3 and 4, a negative value of $\Delta\varepsilon$ represents an energy gain by the emitter (heating effect); a positive value represents an energy loss (cooling effect). In Fig. 4, the calculated theoretical values of $\Delta\varepsilon$ based on the current work predicts the value of transition between heating and cooling in agreement with experiment. By contrast, calculations based upon free electron theory using Nottingham's value for there placement energy do not predict the correct crossover [4].

The inversion temperature T_i is obtained from the condition $\Delta\varepsilon=0$ and corresponds to the x-intercept in Fig. 3. Since $T_i \gg T_{tr}$, only $\langle\varepsilon_r\rangle$ given by Eq. (11) is used in the calculation of T_i. Setting $\Delta\varepsilon=0$ in Eq. (14), we obtain

$$T_i=\frac{d}{\pi k_B}\cot^{-1}\left[\frac{\pi}{12\ln 2}+\frac{d^3 e^{-c}}{\pi \ln 2\, \mu(k_B T_i)^2}\right]. \quad (15)$$

Here, the first term in the square bracket represents the equilibrium distribution (i.e., no tunnelling state contribution) and corresponds to the dashed line in Fig. 5. The second term in the square bracket is the correction term due to the inclusion of the tunnelling state in the emitter. The results obtained by including both terms is given by the solid curve in Fig. 5. In the work of Swanson *et al.* (dashed-dot line in Fig. 5), they assume $\langle\varepsilon_r\rangle=\mu$. The present calculation for T_i is found to be in good quantitative agreement with experiment [4, 7, 8] The curves in Fig. 5 are significant in that they demonstrate the importance of thermal processes in making available empty states into which replacement electrons are scattered. This is the fundamentally important idea suggested by Fleming and Henderson [14] and was ignored in subsequent free electron calculations to obtain T_i [4, 7, 8, 11]. Finally, the departure of Eq. (15) from non-linearity defines the limits of validity of the approximations made in free electron theory [4, 7, 8, 11, 12].

5. Conclusions

In this paper we have introduced the tunnelling state contribution to the replacement process in electron emission and calculated the average energy of the replacement electrons injected into the emitter. The calculated energy exchange $\Delta\varepsilon$ obtained as a function of both temperature and field shows much improved agreement with experimental data. The inversion temperature T_i as a function of field is in good quantitative agreement with existing experimental data. This result is significant because the statistical average of energies of electrons injected from the external circuit can be tens and even several hundreds of meV less than the chemical potential μ. This favors the original argument of Fleming and Henderson [14] that the replacement process involves the states in the emitter which are vacated due to thermal excitation for $\varepsilon \leq \mu$. To obtain the correct statistical average, one must include the tunnelling state contribution as described in this paper.

Acknowledgments

This work is partially supported by the Non-Directed Research Fund, Korea Research Foundation, 1992.

References

1. I. Brodie and C. A. Spindt, *Vacuum Microelectronics*, in Advances in Physics (Academic Press, NY, 1992), Vol. 83, p. 1.
2. Vu Thien Binh, S. T. Purcell, G. Gardet and N. Garcia, *Surf. Sci.* **279**, L197 (1992).
3. W. Nottingham, *Phys. Rev.* **59**, 907 (1941).
4. L. W. Swanson, L. C. Crouser and F. M. Charbonnier, *Phys. Rev.* **151**, 327 (1966) .
5. P. H. Cutler, Jun He, J. Miller, N. M. Miskovsky, B. Weiss and T. E. Sullivan, *Prog. in Surf. Sci.* **42**, 169 (1993).
6. F. M. Charbonnier, R. W. Strayer, L. W. Swanson, and E. E. Martin, *Phys. Rev. Lett.* **13**, 397 (1964).
7. Drechsler, Z. Naturforsch, **A18**, 1367 (1963).
8. F. M. Charbonnier, R. W. Strayer, L. W. Swanson, and E. E. Martin, *Phys. Rev. Lett.* **13**, 397 (1964).
9. H. Bergerot, A. Septier and M. Dreschler, *Phys. Rev.* **B31**, 149 (1985).
10. R. H. Fowler and L. Nordheim, *Proc. Roy. Soc. (London)*, **A119**, 173 (1928).
11. I. Engle and P. H. Cutler, *Surf. Sci.* **8**, 288 (1967).
12. I. Engle and P. H. Cutler, *Surf. Sci.* **12**, 208 (1968).
13. N. M. Miskovsky, S. H. Park, J. He and P. H. Cutler, *J. Vac. Sci. Technol.* **B11**, 366 (1993).
14. G. M. Fleming and Joseph E. Henderson, *Phys. Rev.* **58**, 887 (1940).
15. S. A. Barengolts, M. Yu. Kreindel and E. A. Litvinov, *Surf. Sci.* **266**, 126 (1992).
16. M. S. Chung, P. H. Cutler, N. M. Miskovsky and T. E. Sullivan, Accepted for publication in J. Vac. Sci. Technol. B.
17. H. Q. Nquyen, P. H. Cutler, T. E. Feuchtwang, Z.-H. Huang, Y. Kuk, P. J. Silverman, A. A. Lucas and T. E. Sullivan, *IEEE Trans. on Electron. Dev.* **36**, 1665(1989).
18. R. H. Good and E. W. Muller, *Field Emission*, in Handbuch der Physik ed. by S. Flugge (Springer-Verlag, Berlin, 1956), Vol. 21, p. 176.