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A model study of the role of workfunction variations in cold field emission from microstructures with inclusion of field enhancements

H Qiu\(^1\), R P Joshi\(^2\), A Neuber\(^2\) and J Dickens\(^2\)

\(^1\)Department of Electronic Engineering Technology, Fort Valley State University, Fort Valley, GA 31030, USA
\(^2\)Department of Electrical and Computer Engineering, Texas Tech University, Lubbock, TX 79409, USA

E-mail: ravi.joshi@ttu.edu

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Abstract

An analytical study of field emission from microstructures is presented that includes position-dependent electric field enhancements, quantum corrections due to electron confinement and fluctuations of the workfunction. Our calculations, applied to a ridge microstructure, predict strong field enhancements. Though quantization lowers current densities as compared to the traditional Fowler–Nordheim process, strong field emission currents can nonetheless be expected for large emitter aspect ratios. Workfunction variations arising from changes in electric field penetration at the surface, or due to interface defects or localized screening, are shown to be important in enhancing the emission currents.

Keywords: field emission, workfunction variations, model analyses, fowler nordheim, quantum confinement

(Some figures may appear in colour only in the online journal)

1. Introduction

Electron emission from cathodes can provide high current densities (several kA cm\(^{-2}\)) for a variety of applications such as high power microwave generation [1–3], free electron lasers [4], pumping of excimer lasers [5], in the plasma physics arena [6], and for surface modifications and material processing [7, 8]. Field emitters also play an important role in vacuum electronics [9], and as sources for neutron generators [10, 11]. Field emission is attractive (e.g. over the thermionic process) since no heating is required and the emission current is almost solely controlled by the external field. Cold cathode technology has employed Spindt-type field emitter arrays [12–14] or the more recent carbon fiber cathodes with CsI coating [15, 16]. The Spindt-type emitters, however, suffer from high manufacturing cost and limited lifetime, with failure often caused by ion bombardment from the residual gas species that blunt the emitter cones. Diamond emitting structures, though considered attractive in the past, are unstable at high current densities [17]. Electron field emission from carbon nanotubes (CNTs), first demonstrated in 1995 [18, 19], is becoming increasingly popular and has been studied extensively. CNTs offer advantages of nanometer-size diameter, structural integrity, high electrical and thermal conductivity, possibility of large aspect ratios, and chemical stability [20].

Field emission is often characterized by Fowler–Nordheim (FN)–type equations describing the process of electron tunneling from the conduction band in terms of the workfunction \(\phi\) and the local electric field \(E_L\), as reviewed by Gomer [21]. The local field can be significantly higher than the average externally applied field \(E_0\), and this increase is conventionally denoted by the enhancement factor \(\beta = E_L/E_0\). Several reports in the literature have presented theoretical discussions on electric field increases [22–27] using method of images or series expansion techniques to solve Laplace’s
equation for different geometries. The $\beta$ factor depends on the geometric shape \cite{28-31}, though a constant enhancement factor has often been used, or simply chosen as a fitting parameter to be extracted from experimental data. To avoid confusion, it may be mentioned that the enhancement factor alluded to here is separate from a corrective prefactor that often becomes necessary for FN field emission. Such a prefactor is associated with spatial details of potential barriers for electronic tunneling \cite{32}. On the experimental side, there have also been developments that have looked at novel ways to represent the electric field profile around sharp emitters \cite{33}. These have included general methods for mapping the equipotential profile for CNT or Spindt tip structures having high aspect ratios, to obtain the electric field enhancement factor.

A complete and accurate treatment of field emission is complicated and a variety of physics-based issues need to be considered. Emission relies on both electron tunneling through a potential barrier, which yields the escape probability, and the electron ‘supply’ function, which requires knowledge of the band structure and any defect states near the emitting surface. Typical model analyses assume: (i) negligible field penetration occurs in the cathode and so electrons inside the emitter are nearly in thermodynamic equilibrium. However, this is strictly incorrect since the very application of an electric field (especially of high magnitude) breaks the thermodynamic equilibrium to then establish an electron flow through the system; (ii) tunneling emission of electrons occurs through states near the emitter Fermi level (metals) or the conduction band edge; (iii) electron states within the cathode can essentially be treated as plane waves so that carrier confinement and effects on electron wavefunctions can be neglected; (iv) the workfunction and barrier height are constant and independent of either position or external field.

Yet another simplification often used is near-triangular barrier potentials \cite{34} that ignore corrections to the simple shape \cite{32, 35, 36} including dipole and image potentials, and exchange-correlation effects \cite{37}. In addition, the role of space-charge created by electron emission \cite{38} or the effects of incoming ions that might distort the local fields \cite{39} are usually overlooked. More complicated situations can arise in the case of multiple field-emitting arrays \cite{40, 41} for which the different local field enhancement factors as well as screening effects become operative \cite{42-44}. The interplay between field enhancements and screening for emitter arrays depends on the degree of charge sharing. For example, a fixed charge density associated with the emitter side of an emitting array has to be collectively shared between individual emitters. Sharing between a large number of emitters per unit area results in low field enhancement, whereas sharing between a small number of emitters per unit area yields much stronger field enhancement factors.

From the above, it is clear that the physical details associated with field emission are quite complex and many processes are at work. Many of the complexities have already been analyzed in the literature, though only a few important contributions have been cited. Here, we attempt to focus on a relatively modest aspect that, though known, has not been explicitly evaluated to the best of our knowledge. The role of spatial variation and fluctuations of the workfunction are examined here through numerical simulations for nanoscale ridge emitters. These variations are included in calculations of the field emission currents. For completeness, the electric field enhancements as a function of position and emitter aspect ratio are probed analytically based on conformal mapping techniques. Quantum corrections to the electron current arising from reductions in the emitter width are included along with workfunction variability.

\subsection*{1.1. Workfunction variability in field emitters}

The original FN approach modeled field emission as one-electron tunneling through a one-dimensional triangular potential barrier. This picture was subsequently modified to include an ‘image-force’ correction to account for the electrostatic effect of the tunneling electron that lead to a ‘rounding’ of the triangular barrier \cite{45, 46}. The image correction, however, represents an idealization, introducing an unbounded force close to the surface and overemphasizing the electrostatic effect. As is well known, conduction electrons from the emitter can quantum mechanically spillover into the vacuum up to very short distances, producing Freidel oscillations \cite{47, 48}. In the immediate vicinity of the surface, the spillover electrons have been shown to create an interface dipole barrier that influences the local workfunction \cite{49} and modifies the surface field. In addition, penetration of the electric field into the metal can also change the effective workfunction \cite{50}, alter the potential and modify electron density at the surface. The change in the workfunction for a metal was roughly given to be \cite{50}: $0.5qF_0\lambda/[[1 - qF_0\lambda/(6E_F)]\{1 - qF_0\lambda/(3E_F)\}]^{0.5}$, with $\lambda = (E_F/(6\pi^2n_0)^{3/2})$, $E_F$ denoting the Fermi level, $F_0$ the electric field and $n_0$ the free electron density. For metal electrodes with electron density $n_0$ on the order of $8 \times 10^{28} \text{m}^{-3}$ (e.g. copper) and a Fermi level of $\sim 6.8 \text{eV}$, calculations yield $\lambda = 0.89 \text{Å}$ and can result in a workfunction change above $0.5 \text{eV}$ at fields of $10^9 \text{V m}^{-1}$ or higher. However, in practical situations involving substantially lower fields, changes on the order of 0.15 eV have been reported \cite{51, 52}. In the general case of an emitter, the free electron density at the surface could also be spatially nonuniform along the lateral plane due to traps or material inhomogeneities. Furthermore, the electron field at the surface could vary across microstructures due to sharp or pointed geometries, changes in the enhancement factor, or differences in plasma densities near the emitter. Hence, the workfunction would be nonuniform, and this represents a complicated problem that is also expected to be dynamic. Thus, the usual assumption of a uniform and constant workfunction is not physically correct. Variation of workfunction has been explored to some extent in the past using inhomogeneous barrier height and patch-field models \cite{53-56} that also probe barrier heights and ideality factors \cite{57, 58}. Here, for simplicity the workfunction is simply treated as a random variable about a mean value $\phi_m$. Effects of barrier height fluctuations have previously been probed in the context of Schottky diodes \cite{59}. Since the fluctuations are the
The cathode ridge structure. (a) Schematic in the real $z (\equiv x, y)$-plane with the electric field lines shown as a guide, and (b) a conformal map of the ridge structure in the complex $w (\equiv u, v)$-plane.

integration from $(0, 0)$ to $C'$ (in the $w$-plane) yields

$$h = K \int_{u_0}^{1} dw \sqrt{\frac{w^2 - u_0^2}{1 - w^2}}. \quad (2a)$$

$$a = K \int_{0}^{u_0} dw \sqrt{\frac{u_0^2 - w^2}{1 - w^2}}. \quad (2b)$$

Dividing equation (2a) by (2b) then leads to

$$\frac{h}{a} = \frac{\int_{u_0}^{1} dw \sqrt{\frac{w^2 - u_0^2}{1 - w^2}}}{\int_{0}^{u_0} dw \sqrt{\frac{u_0^2 - w^2}{1 - w^2}}} \equiv \frac{N(u_0)}{D(u_0)}. \quad (3)$$

The numerator $N(u_0)$ in the above equation can be evaluated as

$$N(u_0) = \int_{u_0}^{1} dw \sqrt{\frac{w^2 - u_0^2}{1 - w^2}} = E\left(\frac{\pi}{2}, \sqrt{1 - u_0^2}\right)$$

$$- u_0 F\left(\frac{\pi}{2}, \sqrt{1 - u_0^2}\right). \quad (4a)$$

where $E\left(\frac{\pi}{2}, \sqrt{1 - u_0^2}\right)$ is the complete elliptic integral of the second kind. Similarly, the integration of the denominator $D(u_0)$ works out to be

$$D(u_0) = \int_{0}^{u_0} dw \sqrt{\frac{u_0^2 - w^2}{1 - w^2}} = E\left(\frac{\pi}{2}, u_0\right)$$

$$- \left(1 - u_0^2\right) F\left(\frac{\pi}{2}, u_0\right). \quad (4b)$$

1.2. Model analyses of field enhancement in an emitting ridge microstructure

In the context of a protruding ridge as shown schematically in figure 1, the field enhancement factor can easily be obtained through conformal mapping techniques. The protrusion is assumed to have a total width ($x$-axis) of $2a$ units, and a height ($y$-axis) of $h$ units. Transforming the structure from the $z (\equiv x, y)$-plane onto the $w (\equiv u, v)$-plane with the vertices $A$, $B$, $C$ and $D$ mapping onto $A'$, $B'$, $C'$ and $D'$, the Schwarz–Christoffel mapping is given by [61–63]

$$\frac{dz}{dw} = K \sqrt{\frac{w^2 - u_0^2}{w^2 - 1}}, \quad (1a)$$

with, $K = a / \int_{0}^{u_0} dw \sqrt{\frac{u_0^2 - w^2}{1 - w^2}}. \quad (1b)$

Integrating from $D$ to $C$ ($z$-plane) with a corresponding integration from $C'$ to $D'$ ($w$-plane), and similarly integrating from $(0, 0)$ to $C$ (in the $z$-plane) with a corresponding
where $F(x, a)$ is the complete elliptic integral of the first kind. Both the complete elliptic integrals in equation (4a) can conveniently be expressed in terms of polynomials [64] for ease of computational evaluation. The plot of figure 2 shows the variation of the parameter $u_0$ with the aspect ratio $h/a$ for the ridge emitter. For large aspect ratios, the value of $u_0$ is predicted to approach zero, while in the extreme limit of $a \to \infty$, the value of $u_0$ tends to unity.

The value of the electric fields in the vicinity of the ridge can now be easily determined. Considering the complex electrostatic potential $\phi_w = jF_0w$, the field $F_z$ can be expressed as

$$F_z = -jF_0 \sqrt{\frac{w^2 - 1}{w^2 - u_0^2}}. \tag{5}$$

Hence, on the top surface $BC$, the electric field works out to be $F_x + j F_y = -j F_0 [(1 - u^2)/(u_0^2 - u^2)]^{1/2}$, i.e. $F_x = -F_0 [(1 - u^2)/(u_0^2 - u^2)]^{1/2}$ for $u_0 < u < u_0$. Based on this, the field enhancement factor $\beta$ is given as

$$\beta \equiv |F|/F_0 = \left[\left(1 - u^2\right)/(u_0^2 - u^2)\right]^{1/2}. \tag{6}$$

Thus, as $u$ approaches $u_0$ (i.e. one is at the corners $C$ or $C'$) or $u_0 \to 0$, the magnitude of the normal electric field rapidly increases.

1.3. Quantum corrections to field emission

Figure 3 shows a three-dimensional schematic of a ridge emitter. Downscaling of the emitter width confines electrons in one of the transverse dimensions, thereby affecting their energies and momentum. This alteration in the characteristics of the emitter’s electronic reservoir changes the selection rules and leads to reductions in the current relative to the conventional FN current densities. Here, electrons in a Sommerfeld-type [65] metallic cathode are assumed, but with confinement along the $x$-direction and an electric field applied along the $y$-direction (normal to the emitting surface). The emitted current density $J_n(F_z)$ from the $n$th quantized level is proportional to the product of a supply function $N_v(E_v, E_m)$ and the transmission probability function $D_n(E_v, E_m, F_z)$ as discussed by Qin et al [66]. Thus,

$$J_n(F_z) = q \int D_n(E_v, E_m, F_z)N_v(E_v, E_m) \times dE_v, \tag{7}$$

where $F_z$ is the local electric field at the emitting surface and $q$ the electronic charge. In the context of the discussion of the previous section, the actual local field $F_z$ in equation (7) in the vicinity of a ridge emitter would need to be evaluated from equation (6). The emission current density for a triangular barrier $J_n(F_z)$ then works out to be

$$J_n(F_z) = \left[\frac{q/(h^2a)}{(8\pi^3)}\right]^{1/2} \times \left[\frac{(qF_0)}{(8m_0(\phi + E_m))^{1/2}}\right]^{3/2} \times \exp\left[-\left(32m_0\phi^{3/2}/(3qF_z)\right)\right], \tag{8}$$

where $E_m = n^2\hbar^2p^2/16m_0^2$. The total current density $J(F_L)$ is then a summation over all the occupied subbands, i.e. $J(F_L) = \Sigma_n J_n(F_z)$. In comparison, the FN expression for electron emission current density $J_{Fn}(F_z)$ from a bulk cathode without confinement is given as [35, 67, 68]

$$J_{Fn}(F_z) = \left[\left(qF_0^2\right)/\left(16\pi^2\hbar \phi^2(y)\right)\right] \times \exp\left[-4(2m_0)^{1/2}v(y)\phi^{3/2}/(3qF_z)\right], \tag{9}$$

where $v(y) = 0.95-y^2$ and $\gamma^2(y) \sim 1.1$, with $y = 3.79x10^{-5} F_L^{3/2}/\phi$.

Equation (9) does include image charge effects for calculations of tunneling, with the potential energy barrier $V(z)$ taken to be $q\phi-q^2/16\pi^2z^2\sim qF_z z$. If the same potential energy with image charge effects is taken into account for the two-dimensional case, rather than using a triangular potential barrier, then equation (8) is modified to

$$J_n(F_z) = \left[\frac{q/(h^2a)}{(8\pi^3)}\right]^{1/2} \times \left[\frac{(qF_0)}{(8m_0(\phi + E_m))^{1/2}}\right]^{3/2} \times \exp\left[-\left(8qF_0m_0v^{3/2}/\hbar\right)\right], \tag{10a}$$

where $G = \left[2(3)/(x_2)\right]^{1/2} \times \left[\left(\phi + E_m\right)/(qF_0)\right] \times E\left\{\pi/2, (1 - x_2/x_2)^{1/2}\right\}$

$$- 2x_2 F_1\left\{\pi/2, (1 - x_1/x_2)^{1/2}\right\}, \tag{10b}$$

and $x_{1,2} = (\phi + E_m)/(2qF_0) \pm \left[\left(\phi + E_m\right)/(2qF_0)\right]^2$

$$- q/(16\pi\phi F_z)^{1/2}. \tag{10c}$$

Here, $x_{1,2}$ are the roots of the quadratic $(\phi + E_m)x - qF_1x^2 - q^2/(16\pi\phi_0) = 0$, with $x_1 < x_2$, and arise from the use of the
Wentzel–Kramers–Brillouin (WKB) approximation [69] for evaluating the tunneling probability. Also, in the above expression, $F_l = 2\pi/2,\ (1-x_1/x_2)^{1/2}$ and $E_l = 2\pi/2,\ (1-x_1/x_2)^{1/2}$ are the complete elliptic integrals of the first and second kind, respectively.

With quantum confinement, the energy available for mobile electrons is reduced by the quantized energy $E_n$ for the $n$th subband. This effective decrease in the emission current appears through the exponential dependence on $E_n$ as given in equation (8). Thus, with downscaling of the emitter width there would be the effect of electric field enhancement leading to a stronger driver for electron emission. However, reductions in transmission coefficient reduce the actual throughput.

Finally, taking account of the workfunction variations due to charge, electric field variability, surface traps and defects, or simply due to surface erosion from repetitive device operation, the current density $J_n$ as given by the Gaussian probability density function becomes

$$J_n = \left[ \int J_n(F_{1r} \cdot \phi) p(\phi) \, d\phi \right] \sqrt{\int p(\phi) \, d\phi}.$$  \hspace{1cm} (11a)

where, $p(\phi) = \{2\pi\sigma^2\}^{-1/2} \exp \left[ -\left( \phi - \phi_0 \right)^2 / (2\pi\sigma^2) \right]$.

$$= \left[ \int J_n(F_{1r} \cdot \phi) p(\phi) \, d\phi \right] \sqrt{\int p(\phi) \, d\phi}.$$  \hspace{1cm} (11b)

In the above, $J_n(F_{1r} \cdot \phi)$ represents the current density as given in equation (11).

For completeness, it may be mentioned that strictly speaking the application of an electric field (particularly one of a large magnitude) would perturb the energy levels, wavefunctions and carrier densities in the vicinity of the emitting surface. As a result the number of energy subbands contributing to electron emission would change depending on the local electric field magnitude. This aspect have been probed and discussed in the literature [70], and shown to lead to interesting step-like current-voltage characteristics. However, such details have been ignored here for simplicity.

2. Results and discussion

The enhancement factor $\beta \equiv [F]/F_0$, was first evaluated for the ridge structure of figure 1(a). The results of the calculation showing the electric field enhancement factor as a function of the spatial distance along the ridge perimeter are given in figure 4. The three curves were obtained for an emitter height $h = 10 \mu m$, but with three different aspect ratios $h/a$ of 10, 100, and 500, respectively. The sharp peak in all three cases is at $u = u_0$ and coincides with the corner point $C$ in figure 1(a). The result underscores the potential for strong electric fields and, hence, high emission currents for narrow emitter structures. Though the surface area for emission does reduce with the half-width $a$, the exponentially dependent nonlinear enhancements in emission current density at the smaller half-widths would work to produce higher currents overall. The enhancement factor is predicted to dip well below unity for the $h/a = 10$ curve of figure 4, in the neighborhood of point $D$ which is at $u = 3u_0$. Physically, this represents an effective electric field screening due to the convergence of electric field lines at the corner $C$. Quite simply, the strong field enhancement at the corner increases the local charge density and works to draw down the electronic charge from nearby regions around point $D$.

Next, the two-dimensional current density, as given in equations (10), was obtained as a function of the local electric field. Emitters with the same $10 \mu m$ height but different half-widths of 0.5 nm, 2 nm and 10 nm were used for the calculations. The results are shown in figure 5. For comparison, the current density from bulk FN emission, as computed from equation (9) is also plotted. As evident from figure 5, the bulk formulation yields the highest current density values. The appearance of lower current density in figure 5 at higher values of emitter half-width is not counterintuitive, since the overall current which scales with emitter width is indeed higher for a wider emitter. Strictly speaking, a staircase-like structure with increasing field, as discussed by Filip et al [70], due to progressive additive contributions from the various subbands occurs. However, this aspect which depends on both the emitter dimensions and electric field is not seen on the linear scale and was not the focus of the present study.

The two-dimensional quantization aspect was next combined with the electric field enhancement to obtain a comprehensive assessment of the electron emission. The current density across the top emitting surface $B$-$C$ of the ridge emitter (figure 1(a)) as a function of position is shown in figures 6(a) and (b) for half-widths of 5 nm and 20 nm, respectively. The emitter height was maintained at $10 \mu m$ in each case. Large current increases are predicted near the
emitter corner, with the largest densities predicted for the narrowest emitter. For these evaluations, the background field \( F_0 \) (i.e. the background value far away from the emitter structure) was taken to be \( 10^7 \text{ V m}^{-1} \). For completeness it may be mentioned that the FN current densities at this constant \( F_0 \) value would be negligible.

Finally, the role of workfunction fluctuations was analyzed based on a Gaussian distribution as highlighted in equation (11). Such variations would be associated with the spatial variations in the electric field, and discrete nature of defects and/or charge near the surface. Simulation results of the current density as a function of the surface electric field are shown in figure 7 with workfunction variability taken into account. Values of the variance \( \sigma \) were taken to be 0.05 eV, 0.25 eV and 1.15 eV. Enhancements in emission current are predicted in figure 7 with corresponding increases in the variance parameter. Thus, in addition to field enhancements typically associated with localized geometry, the role of workfunction fluctuations could well remain an important yet latent and/or overlooked contribution to high field emission. Since the fluctuations depend on the local electric field and its shielding, such ‘patchwork’ emission is likely to also add a dynamic feedback process. The latter could even conceivably give rise to noisy emission currents, periodic disruption in the electron emission flux with time due to space-charge effects associated with the emission, and varying bright spots at the emitting surface. However, such details are beyond the present scope. The increase in figure 7 follows directly from the nonlinear dependence of the current on the workfunction. Physically, electrons would be emitted from localized spots having a low workfunction, possibly leading to disproportionately nonuniform current densities and even filamentary emission. As an extreme example of the latter, explosive emission in a highly localized manner as has been observed [71, 72] in high current cathodes could occur, and the workfunction fluctuations studied here could well have a contribution. However, in this context other inherent mechanisms would need to be considered in the context of localized emission. These would include localized heating

Figure 5. Current density as a function of the electric field. Results from the two-dimensional formulation for emitters of height 10 \( \mu \text{m} \) and half-widths of 0.5 nm, 2 nm and 10 nm are shown, along with the current density from bulk FN emission.

Figure 6. Calculations of the current density across the top emitting surface B-C of the ridge emitter shown in figure 1(a). The spatially varying field enhancement factor was coupled with the two-dimensional current density to yield a comprehensive assessment of the electron emission. For a constant 10 \( \mu \text{m} \) height, emitter half-widths of (a) 5 nm and (b) 20 nm were used.
3. Conclusions

Cold field emission from microstructures has been studied in this contribution with an emphasis on three distinct aspects, namely: (i) the position-dependent electric field enhancements; (ii) the role of quantum corrections to electronic field emission; and (iii) the role of probabilistic variations in the workfunction for nanoscale emitters. These variations were included through a simple Gaussian probability function. Due to the strongly nonlinear dependence of electron emission on the workfunction, significant current enhancements and non-uniformity can result. However, in the literature only the geometric enhancement factor has been attributed to this phenomenon. For completeness, the electric field enhancements as a function of position and emitter aspect ratio were also probed based on conformal mapping techniques. Quantum corrections to the electron current arising from reductions in the emitter width were also included in the field emission formulation with workfunction variability. Our results show that variations in workfunction are important in enhancing the emission currents, and could well play a role in initiating explosive emission from surface protrusions.

Results of the present study could easily be extended to other geometries and emitter tip configurations, such as the Lorentzian [26] or hyperboloid [74] shapes often discussed in the context of field emitters. As a final comment, the possibility of localized cathode heating, or material ejection that might dynamically alter the emitter aspect ratio, was ignored since our calculations apply to a shorter temporal regime and/or less intense emission currents. A more complete and rigorous analysis would require the self-consistent and time-dependent inclusion of electrothermal aspects. For example, the possibility of material vaporization from cathode tips has been reported in the literature [75, 76]. From a theoretical standpoint, this is a dynamical energy-flow process with the electrons transferring energy gained from the field to the lattice via electron–phonon interactions. This in turn, gives rise to nonequilibrium phonons with effective phonon temperatures dictated by wavevector-dependent, coupled electron–phonon and anharmonic phonon–phonon relaxation processes. At high currents, one can then have the possibility of localized melting as phonon effective temperatures exceed the melting point. However, such aspects are beyond the present scope.

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