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TOWARDS THE ULTIMATE SCANNING ELECTRON MICROSCOPE

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Abstract

An analysis of all the factors which contribute to the electron probe size in a scanning electron microscope and of the correct method of combining those effects to give optimum performance. Assuming perfect specimen preparation the only other factors are the non-local nature of the basic electron interactions and the nature of the display system.

Keywords: Scanning Electron Microscopy, Scanning Transmission Electron Microscopy, Conventional Transmission Electron Microscopy, Electron Optics, Resolution, Electron Probe Size, Electron Probe Current, Chromatic Aberration, Spherical Aberration, Diffraction, Electron Sources

Introduction

The scanning electron microscope (SEM) has been with us now for about two decades, quite long enough to have acquired some degree of maturity and quite long enough for the user community to become acquainted with its potential. In spite of this, one can easily note that there still exists a great deal of confusion with regard to the respective merits of various instruments. The manufacturers of the instruments are not at all reticent about taking advantage of this confusion and they even encourage it by contributing their own additions.

Some of you might dispute the content of my remarks so let me give a few examples. For one thing there is still no accepted or acceptable definition of resolution, something which would not be tolerated, even by the same users, in the conventional transmission electron microscope (CTEM) market. The result is that some manufacturers get away with outrageous claims while the more conservative ones suffer. There is even confusion over the difference between magnification and resolution, a difference akin to that between the top speed of an automobile and the maximum printed label on the speedometer. Another example would be that of the display system. Does it really matter that one system may have 2000 lines while another may only have 500? If 2000 is better than 500, then why not 5000? Who optimizes this number? What is it optimized for, maximum performance or maximum dollar return?

These are just a few of the many examples that I can think of but they are surely enough to justify a careful look at the whole problem of SEM performance. In this paper I cannot examine every nook and cranny of this problem, nor can I report on each of the many machines available for purchase. What I can do, however, is to look at--and look for--the ultimate instrument. The one which would incorporate the best of everything as now conceived. I will, of course, ignore all the factors akin to chromium plating and concentrate on the essential physics of the problem, the irreducible minima and maxima. In doing this I hope to be able to point the way to higher performance and perhaps provide the user with some ammunition that he or she might use in dealing with suppliers. If, in doing this I can help just one of you in your choice then it will be worthwhile. If I can induce more realism and more honesty in the information and claims of the manufacturers then I will be happy indeed.

The Electron Probe

The resolution of a SEM can never be greater than that given by the size of the electron probe itself. In practice there are many factors which could degrade the resolution well below this figure, for example the thickness of a coating. Therefore it would seem

reasonable to study the problem of electron probe formation separately from specimen preparation. It would also seem logical to specify the size and shape of the electron probe when designing or buying or selling a microscope. It is not at all difficult to measure the size and shape, all that is required is some form of transmission detector and a thin film to use as a specimen. I would make the strong recommendation that the user community insist upon having this information and using it as a proof of performance because nothing less will do.

Let me now take a look at the physics of probe formation and dispel a few of the myths which have developed even here.

The Elements of the Probe Size

One essential element of any SEM is the electron probe itself. We must generate the electrons in a source and focus them into a small probe and there must be a large enough electron current in the probe to allow the formation of an image in a reasonable time. As a general problem these considerations could lead to a very extensive discussion but here we will concentrate on instruments with the very highest resolution and this translates into the smallest probe size. This means that we can concentrate on only those solutions which can lead to this desired goal.

We begin with the most important factors in probe formation. These are spherical aberration, chromatic aberration, diffraction, source size, and probe current.

Spherical Aberration

The normal definition of the spherical aberration coefficient of a lens is derived from concepts in geometrical optics.

We consider a ray entering the lens which is parallel to the axis of symmetry, a distance r_0 from that axis. This ray will not pass through the focal point but instead will have some amplitude in the focal plane which is proportional to r_0^3. By definition we write this amplitude as:

$$\delta_s = C_s \alpha^3 \tag{1}$$

where α is the convergence angle $(-r_0/f)$ and C_s is the coefficient of spherical aberration. There is no confusion in this definition so long as $\delta_s << r_0$.

By sketching a series of such rays it will be found that there is an optimum focus at a distance $3/4$ of the way between the paraxial focus and the extreme focus. The radius of the circle of confusion at this axial position is $\delta_s/4$.

One should note the strictly geometrical nature of the description above. For example there are *no* rays with a deviation $>\delta_s/4$ in the disk of confusion. We must therefore expect to be forced to modify this description when we consider the wave nature of the electrons since sharp edges such as this cannot exist.

We should also note that for the lenses which we use in microscopy the sign of C_s is such that δ_s is always negative or alternatively the extreme focus is always closer to the lens than the paraxial focus. This is the famous Scherzer Theorem[7].

Chromatic Aberration

For magnetic or electrostatic lenses it is necessarily true that the focal length depends upon the electron energy. If we consider two electrons which have been accelerated to potentials V and $V + \Delta V$ respectively then there will be a difference in the paraxial focus and the radial distance between them at the focal plane is defined to be:

$$\delta_c = C_c \alpha \Delta V / V \tag{2}$$

where C_c is the coefficient of chromatic aberration.

We can note that δ_c has the same absolute value for either sign of ΔV and therefore it is convenient to refer our origin to some central or average potential V and consider the spread of potential as $\pm\Delta V$. The dimension δ_c is a measure of the radius of the disk of minimum confusion in the plane of the paraxial focus of electrons of potential V.

This is not the same plane as the plane of the disk of confusion for the case of spherical aberration.

Diffraction

To a good approximation we may consider the incident beam of electrons to be a plane wave so that in the absence of chromatic effects and spherical aberration the electrons are diffracted by the aperture. At the position of the paraxial focus we will not obtain a point focus but instead we will see a circular symmetric pattern which is the well-known Airy disc. This consists of a strong central peak surrounded by rings of every decreasing intensity with zeroes in between. The radius to the first zero corresponds to the Rayleigh criterion for resolution. This is:

$$\delta_d = 0.61\lambda / \alpha \tag{3}$$

Parenthetically we might note that there need not be a physical aperture in the final probe-forming lens. If there are several lenses in the system the defining aperture may be placed at any pont along the optic axis and it should have a radius corresponding to the geometrical envelope desired. Wherever it is placed the resolution will be that given above. The best place for the aperture is in the electron gun itself because scattered electrons from the edge of the aperture will be out of focus at the image and will not contribute to the contrast.

Source Size

It would appear at first sight that if we have an electron source which has a finite size (radius) ρ then the image size at the final focus would be $\delta_{ss} = M_t \rho$ where M_t is the total transverse magnification of the optical column.

This relationship is correct but it is deceptively simple since the transverse magnification is related to the change in potential and may be difficult to determine.

This can be illustrated by using the very general expression for the product of the transverse linear magnification M_t and the angular magnification M_α

$$M_t M_\alpha = \left(\frac{V_e}{V}\right)^{1/2} \tag{4}$$

where V_e is the emission voltage. This expression is based upon very fundamental results in classical mechanics. For our purpose we can rewrite it as:

$$M_t^2 = \frac{\pi \alpha_e^2 V_e}{\pi \alpha^2 V} \tag{5}$$

where α_e is the emission angle from the source. Difficulties now arise because α_e can take any value from zero to $\pm\pi/2$ ($\pi\alpha_e^2 = 2\pi$ radians) and V_e can assume any value from zero to some maximum value which is determined by the source temperature or quantum mechanical effects. M_t is therefore undetermined and so is δ_{ss}.

Probe Current

In order to conserve electrons it is necessary that:

$$B = \frac{I}{(\pi\delta^2)(\pi\alpha^2)V} = constant. \tag{6}$$

B is called the brightness and is a quantity whose value is conserved at all foci.

We can therefore write our probe current at the final focus in terms of the brightness of the electron beam:

$$I_p = B\pi^2(M_r\rho)^2\alpha^2 V \tag{7}$$

or alternatively as:

$$I_p = B\pi^2\alpha^2 V\delta_d^2\left(\frac{M_r\rho}{\delta_d}\right)^2 \tag{8}$$

where we can note that the product $\alpha^2 V\delta_d^2$ is a universal constant. We then obtain the final equation for the probe current:

$$I_p = KI_T\left(\frac{\delta_{ss}}{\delta_d}\right)^2 \tag{9}$$

where K is a constant for any particular type of source.

It is now apparent that the quantity $M_r\rho$ which was required above for the determination of the source size can be obtained simply by measuring the ratio of the probe current for a diffraction limited probe to the total emission current of the source.

We conclude that for our purposes we can say that the factor K is the most important property of an electron source. All other parameters which are commonly given, such as brightness or current density, have no particular meaning since other assumptions must be made in order to obtain numbers of any practical importance.

Note that K is dimensionless and we will simply call it the source parameter.

In the case of a cold field emission source our own data indicate that $K \sim 10^{-3}$. Much smaller values would be expected for other types of electron source.

Combining the Effects

We must now combine the various elements which contribute to the probe size in some way. Some authors have proposed using an R.M.S. value $\sqrt{(\delta_s^2 + \delta_c^2 + \delta_d^2 + \delta_{ss}^2)}$ but this is patently incorrect since the effects are not statistically independent and are based upon different concepts, ranging from geometrical optics to wave optics.

Since we are interested in obtaining the highest resolution, that is the smallest probe size, we must necessarily be concerned with diffraction effects and we must therefore use wave optical methods to combine the various effects.

The problem of combining spherical aberration and diffraction coherently has been solved by Black and Linfoot[1] and forms a very good starting point for the analysis. Using a wave optical description of spherical aberration they show that it is possible to partially compensate the aberration effects using a small amount of defocus. This is analogous to the geometrical description but does not give the same numerical results.

If we consider the case of a perfect lens with no spherical aberration then the electron intensity in the probe can be described by the Airy function, or by its Fourier transform--the Optical Transfer Function or O.T.F.--which gives the capability of transmitting spatial frequencies from object to image. This function decreases monotonically from a value of 1 at zero spatial frequency to a value of zero at a frequency of $2\alpha / \lambda$ where α is the semi-angle of convergence of the probe at the focus.

If we now introduce a small amount of spherical aberration the transfer function begins to decrease and can even become negative in some regions. The most drastic changes occur in the frequency ranges around $r \sim 1.6\alpha / \lambda$ and $r \sim 0.6\alpha / \lambda$. Now if we introduce some defocus it is possible to partially restore the function. This corresponds to attempting to balance an r^4 effect with an r^2 compensation.

An effective way of looking at this effect is to plot contours of the fractional decrease of the transfer function in the neighborhood of these two frequencies[3]. This is most readily done in terms of two dimensionless parameters.

$$A = -\alpha^2\left(\frac{\Delta f}{2\lambda}\right) \tag{10}$$

$$B = -\alpha^4\left(\frac{C_s}{4\lambda}\right) \tag{11}$$

These contours are shown in Fig. 1. Inspection of this figure shows that a reasonable working point would be $A = -1$, $B = 1$ although other points nearby would be equally satisfactory. This is the choice made by Black and Linfoot[1].

This means that, if the lens has a spherical aberration constant C_s then there is an optimum convergence angle:

$$\alpha = [4\lambda / C_s]^{1/4} \tag{12}$$

and in this case the diffraction spot is changed only slightly from the case $C_s = 0$ using the same convergence angle. The central peak intensity is a little smaller and the surrounding rings have correspondingly greater intensity. One can still use the Rayleigh criterion, however, so that the resolution becomes:

$$\delta_d = 0.61\lambda / \alpha = 0.43C_s^{1/4}\lambda^{3/4} = 0.15C_s\alpha^3 \tag{13}$$

and the optimum focal plane is halfway between the paraxial and extreme foci. Note that the resolution is considerably better than would have been calculated geometrically ($0.25C_s\alpha^3$).

Now we can also use Figure 1 to include the effects of chromatic aberration. Suppose that the parameters are fixed for some particular operating voltage V. Then for some other voltage $V + \Delta V$ the operating point will not be at $A = -1$, $B = 1$, but instead will be displaced by some distance $\Delta A, \Delta B$. From the expressions for A and B one can easily see that the largest effect is that of changing the focal length. To a very good approximation $\Delta B = 0$ and

$$\Delta A = -\left(\frac{\alpha^2}{2\lambda}\right)\delta f. \tag{14}$$

Looking at Fig. 1 we might estimate that if we set $|\Delta A| < 0.2$ we would not seriously impair the transfer function. This then leads to:

$$\frac{|\Delta V|}{V} \leq \frac{2\delta_d^2}{f\lambda} \tag{15}$$

The final element we must take into account is the source size. Since this effect again adds incoherently we certainly require

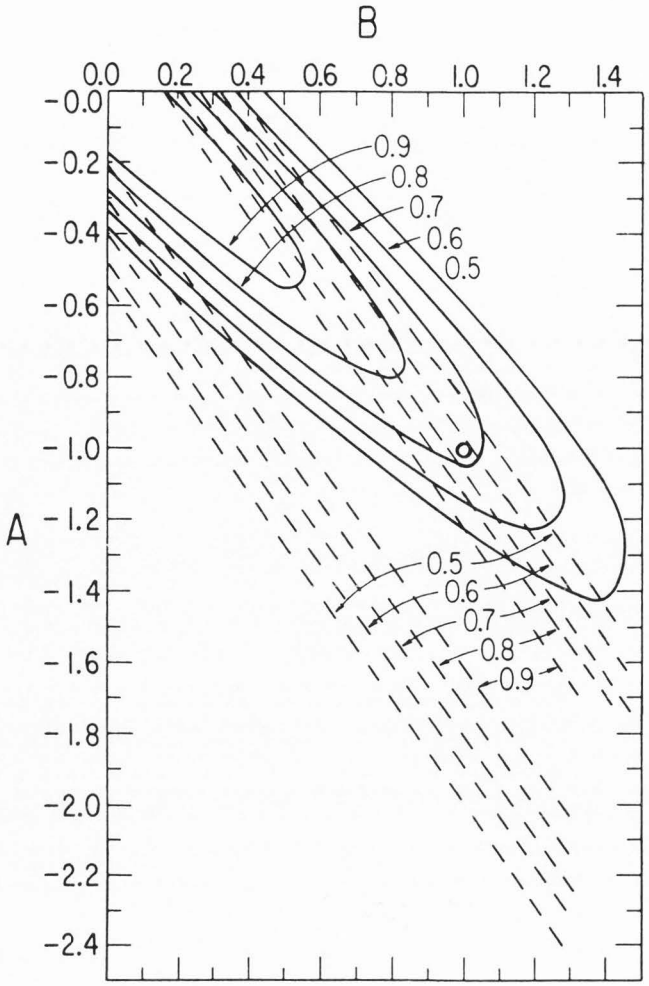

Fig. 1 The parameters A and B are dimensionless constants which represent the amount of defocus and spherical aberration respectively (see text). The contours represent the fractional deviation of the O.T.F. from the ideal for two spatial frequencies, one close to the Rayleigh limit (dotted) and one at a resolution about 3 times lower (solid). Resolution improves as B increases.

The optimum operating point is in the region A = -1, B = 1. The effect of chromatic aberration is to cause a spread in the value of A. It can be seen that one can tolerate a range of values $0.8 \leq A \leq 1.2$ but anything larger than this would seriously impair the O.T.F.

$$\left(\frac{\delta_{ss}}{\delta_d}\right) << 1 \tag{16}$$

and we can guess that a reasonable limit might be $(\delta_{ss} / \delta_d) \leq 0.2$. This would lead to an approximate resolution of:

$$\delta = \delta_d \left(1 + \left(\frac{\delta_{ss}}{\delta_d}\right)^2\right)^{1/2} \sim \delta_d \times 1.04 \tag{17}$$

To summarize, if we have an electron optical system whose spherical aberration constant is C_s and whose final probe-forming lens has a focal length f then we should place an aperture in that lens which defines a convergence angle of the beam at the final focus which has a value

$$\delta_d = [4\lambda / C_s]^{1/4} \tag{18}$$

and then the resolving power will be given by

$$\delta_d = 0.43 C_s^{1/4} \lambda^{3/4} \tag{19}$$

provided that the energy spread of electrons is such that

$$\frac{\Delta V}{V} \leq \frac{2\delta_d^2}{f\lambda} \tag{20}$$

and the source size is such that

$$\left(\frac{\delta_{ss}}{\delta_d}\right) \leq 0.2 \tag{21}$$

or alternatively that the probe current is such that

$$I_p \leq .04 K I_T. \tag{22}$$

The conditions given above are not easily met. For a normal electron source--a hot filament, there is little or no hope of achieving diffraction limited resolution unless inordinately long exposures are used (hours). Even the LaB_6 source cannot be used, the brightness is not great enough. Only the field emission source has a brightness adequate for the purpose. Even then one must choose the aperture size very carefully and an examination of these results will show that the permissible error is in the neighborhood of a few percent. In general this means that a physical aperture in the lens is unacceptable since its radius cannot be chosen with sufficient accuracy.

The condition on ΔV can easily be met by a field emission source at voltages above a few Kilovolts whereas a hot filament may require much higher voltages.

The Effect of Non-Local Interactions

The discussion above relates entirely to the matter of determining the size and intensity of the electron probe which determines the ultimate resolving power of instruments using such probes. In addition to this, however, we must also take into account the manner in which contrast is formed. Since we are only concerned here with the highest possible resolving power we will not take into account such things as multiple scattering or other thickness effects. However, there is one inescapable effect which we must take into account and that is the non-local nature of some scattering processes.

In order to provide image contrast we must take advantage of the interactions of the incident electron beam with the atoms and molecules of the specimen. In the case of the STEM the most commonly used interaction is the elastic scattering process. The backscattered electrons which are often used to provide contrast in the SEM also fall into this category providing the specimen is thin enough. This process is essentially a modified Rutherford scattering which is determined by the Coulomb field of the atomic nucleus. Since this field is shielded by the electron cloud around the atom it has a finite extension which we can call the atomic radius. This radius is considerably smaller than any electron probe that has so far been formed and therefore has no impact on the resolving power (although this may not be true in the near future).

All other contrast mechanisms can be considered to be due to one form or another of the inelastic scattering process whereby energy (or momentum) is transferred from the incoming electron to the specimen. Such interactions can be quite non-local in nature and are such that an electron can transfer momentum at

distances which may be large compared to the probe size itself, thereby causing a significant loss of resolution. This effect is a real one and has been shown to correspond to a resolution of ~7Å using 35 keV electrons on a Carbon film[4].

Unfortunately for our purpose here, the theoretical basis for this effect has not yet appeared so that we must resort to estimates.

Some theoretical progress has been reported by Rose[6] who calculated the shape of images of single atoms and estimated the effect due to a collection of non-interacting atoms. For our purposes here these results are not applicable and we resort to a more empirical estimate.

The characteristic angle of inelastic scattering can be written as[5]

$$\theta_E = \frac{\Delta E}{\beta^2(E_0 + m_0c^2)} \tag{23}$$

where ΔE is the energy loss (typically ~ 20 eV per event) , E_0 is the incident kinetic energy, m_0 is the rest mass of the electron and β_c is the velocity. In the non-relativistic approximation this becomes

$$\theta_E \cong \frac{\Delta V}{2V} \tag{24}$$

We can associate a characteristic distance with this angle. A precise method would be to determine the angular distribution of the scattering process and take the Fourier transform to relate this distribution to a distance. As an estimate, however, we can use the equivalent of equation (3) to write the characteristic distance δ_E as:

$$\delta_E \sim \frac{\lambda}{\theta_E} \tag{25}$$

so that we can write:

$$\delta_E = k\frac{V^{1/2}}{\Delta V} \tag{26}$$

where k is a constant to be determined experimentally. The dependence on V and ΔV is of some importance. The experimental results described above [4] correspond to the case where $V \sim$ 35kV, $\Delta V \sim$ 25eV, $\delta_E \sim 7$Å and we can immediately see that if we use electrons which have lost substantial amounts of energy (say in the X-ray region) then we can consider the events to be local, but if we use the low-lying losses (say <50eV) then the loss of resolution may be substantial. We can also see that if we use high energy electrons the situation becomes even worse.

In the case of the SEM secondary electrons are known to be generated in the low-lying energy loss processes so that a value of 25eV energy loss to produce one secondary electron would be a good average value. In that case we could expect that no matter how small we make the electron probe we could not achieve better than 10Å resolution with a 100 kV microscope and that one should use as low a voltage as possible if we are to obtain the best resolution.

Scanning and Display

The problem of acquiring data by scanning and then displaying the data--also by scanning--is a non-trivial one. In the past we have made a careful analysis of this area[2] and the conclusions, which are soundly based in Information Theory, are quite at odds with commercial practice, particularly in the matter of the display.

A display tube has an O.T.F. just like the microscope itself and this function accurately describes its capabilities and the information which it is capable of transmitting. The number of scan lines should be determined by this function and it rarely exceeds 1000 lines. As an example, with a true 2000 line capability one can display a printed page of text at full resolution. There are indeed some oscilloscopes which can do this but they cost more than any scanning microscope!

The reason why 2000 line (or more) systems are sold is that many users object to the visible line structure in SEM images so the manufacturers oblige by overscanning to remove or reduce that structure. *This is the wrong thing to do.* Information can be lost or even transmuted in this process. The correct way to avoid this is to display with the most visible line structure, the narrowest possible lines, and then use the properties of the eye itself to remove the line structure by holding the image far enough away (as one does automatically when viewing T.V.).

Conclusion

Clearly this analysis points the way to a totally different SEM than is commonly used. We have shown that no source other than field emission will suffice for the highest resolution, manufacturers claims notwithstanding, and even then great care must be used in designing the instrument, for example the aperture should *not* be placed in the objective lens. Contrary to the common belief going to higher voltages will not improve the SEM although it may enable one to use poor specimen preparations. Providing more scan lines may provide cosmetic appeal, but like cosmetics it may only serve to hide blemishes and falsify information.

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Discussion with Reviewers

T. Mulvey: The choice of the parameters A = -1 and B = 1, attributed by the author to Black and Linfoot seems very arbitrary. In particular the choice B = 1, leading to a convergence angle $\propto = [4\lambda / C_s]^{1/4}$, is equivalent to allowing a path difference between the paraxial and marginal rays of one wavelength. For an "ideal" instrument, according to Lord Rayleigh, only one

quarter wavelength can be tolerated. The corresponding resolution $\delta_d = 0.6\, C_s^{1/4}\lambda^{3/4}$, a worse value than $\delta_d = 0.43 C_s^{1/4}\lambda^{3/4}$ but the contrast will be higher. Similar considerations apply to the calculation of the permitted value of dV/V. The expression $dV/V = 2\delta_d^2 / f\lambda$ given in the paper appears, at first sight, to be unduly approximate in two respects. It assumes that the objective lens is weak so that the chromatic aberration coefficient $C_c \cong f$. In practice C_s will be perhaps $0.7f$. Secondly a path difference much greater than one quarter wavelength is implied. If these factors are taken into consideration, the voltage stability requirement will be appreciably more severe. Could the author please comment?
Author: The assignment A = -1, B = 1 is not arbitrary (see the Figure) because the range of acceptable values is so small. Since Lord Rayleigh did not consider spherical aberration, his "quarter wavelength" is not appropriate and, indeed, this was the very reason for the Black and Linfoot paper. The correct value for the resolution is indeed $0.43 C_s^{1/4}\lambda^{3/4}$ and has been verified experimentally by us. The use of $C_c \sim 0.7f$ does not materially change any of the arguments but I accept its validity.

J.J. Hren: Where should the aperture be placed?
T. Mulvey The author stresses the difficulty in arranging for an aperture of appropriate diameter to be placed in the final probe forming lens. From an instrumental point of view, every effort should be made to place the aperture in the final lens since this eliminates many unwanted electrons from the image that arise from defects further up the column. In addition it provides the most accurate method of defining the angle. Could it be that the difficulties mentioned by the author arise from his choice of too large an angle in the first place? If the Rayleigh criterion of allowing only one quarter of a wavelength path difference is followed, it will be found that a small error in the aperture angle, especially if this is slightly larger than the optimum Rayleigh angle will have a negligible effect on the size and shape of the electron probe. Could the author please comment?
Author: It is *not* a good idea to put the aperture in the final lens for the reasons given in the text. The best possible location is in the first anode of the electron gun. Any electrons scattered by this aperture will be quite out of focus in the final probe so that the "pedestal" of the radial distribution will be very small. Experimentally this has been verified here and has been the location of our aperture for many years.

As pointed out above, the Rayleigh criterion is not valid and one must use the results of Black and Linfoot or Crewe and Salzman to get the best results.

T. Mulvey: The author asserts that there is no agreed method of defining the resolution of the SEM. It may be that there is no simple test that will satisfy all concerned but has the author any positive suggestions to put forward concerning tests that would be acceptable to SEM manufacturers and users?
Author: I stated in the beginning of the article that the probe distribution can be measured in transmission. This should be the criterion used in judging SEMs.

J.J. Hren: What range of voltage is recommended?
Author: 3-8 kV.

J.J. Hren: What is practical vacuum without exhorbitant cost?
Author: 10^{-10} Torr for the tip and 10^{-8} Torr for the specimen. Cost can be reduced by careful engineering and should not be a problem.

J.J. Hren: Are T-F sources sufficient or a reasonable compromise to thermionic emission?
Author: T-F sources have too large an energy spread to be of value in attaining high resolution at low accelerating voltages but for some sources there is little published data so I cannot give a conclusive answer.

J.J. Hren: Should we use a CRT to record high resolution image data or would a computer be better utilized for this purpose?
Author: I do not understand the question since even a computer uses a CRT to provide a visual output. In any case a high resolution monitor is to be preferred and they are readily available at 1024x1024 pixels.

J.J. Hren: What specimen limitations are consistent with high resolution?
Author: One would need to use a thin (5Å) coating of high Z material (say Au).