Improving the coherence of a low-energy electron beam by modulation

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In a standard low-energy electron generator the beam is formed by particles traveling close to the axis of symmetry. However some electron trajectories are unstable and strongly dependent on the initial conditions. Numerical ray tracing shows that ultimate beam coherence is limited by these trajectories that pass far from the symmetry axis. This contribution can be partly eliminated by modulating the initial conditions and selecting the modulated response. This is exemplified with a low-energy electron beam used for electron diffraction, where the beam current modulation produces a modulated diffraction pattern that displays noteworthy improvement (sevenfold) in wave vector resolution. © 2003 American Institute of Physics. [DOI: 10.1063/1.1627954]

I. INTRODUCTION

Low energy electron beams are mainly used for surface diffraction. In the diffraction process, the diffracted pattern is a result of the accumulation of diffracted intensity from single electrons. Nevertheless each electron contributes very locally to image formation through wave packet reduction. So any change in the electron wave vector direction will result in a shift of the point where the wave packet reduction occurs. The diffraction image is built up statistically from a large number of such electrons, and as a consequence the incident electron trajectories must be perfectly aligned to avoid any blurring of the image. The quality of the electron trajectory alignment is related to beam coherence. It marks the limit above which the experiment cannot resolve details in wave vector space.

In this article we investigate the beam’s spatial coherence which is commonly related to the size of the source. We will show that at low current the beam spatial coherence of a standard electron beam can be significantly improved using a simple modulation process. Let us first analyze how a standard electrostatic low energy electron generator works. It is built by stacking two elements. The first one is an electron source formed by an oxide surface emitting electrons with a reasonable energy distribution (0.08 eV), and two electrodes that select particles in a small range of initial positions (40 µm in diameter), the Wehnelt and the extracting electrode (Fig. 1). The second element is a filter generally built around an Einzel lens, presented in Fig. 2.

Here we will show by numerical simulation that for such an arrangement the ultimate beam spatial coherence (hereafter referred to as “beam coherence”) is mainly limited by trans-Gaussian trajectories introduced by the Einzel lens (by trans-Gaussian we mean trajectories that pass far from the symmetry axis). This is related to the fact that the center electrode of this lens is also an aperture diaphragm that lies in a strong field gradient. It will be shown that the rejection of these unstable trajectories by a modulation process improves beam coherence. This increase in wave vector resolution will be exemplified with the modulated low-energy electron diffraction applied to the mica muscovite surface, which displays resolution of the order of δk = 2πl ≈ 0.09 nm⁻¹, which corresponds to transfer width l in real space of about 70 nm, compared with the 10 nm value observed for standard electron diffraction devices.

II. MODEL

In the literature, two classes of models have been developed in order to investigate beams of charged particles and the best conditions to achieve a highly coherent electron beam. The first one is based on charged particle optics and related aberration theory while the second one is ray tracing, based on calculation of the charged particle trajectories from the force due to the electrical field. Here we limit our investigation to cylindrical symmetry. In this case charged particle optics theory can be efficiently used within the paraxial approximation, which gives an excellent description of the trajectories close to the symmetry axis (Gaussian trajectories), but is unable to provide any correct description of trajectories far from it. Therefore, ray tracing was preferred in the present study because the loss in beam coherence is related to such particle trajectories that pass close to the electrodes and far from the symmetry axis, and are usually not taken into account in paraxial aberration theory. The beam properties were analyzed by “flying” the charged particles from the cathode to the gun exit.

In a standard charged particle beam, great care is taken in order to eliminate spurious trajectories. This is the role of diaphragms that select the trajectories located near the symmetry axis. They are also used to limit the aperture in order to reduce aberrations. Moreover such aperture limiters are placed in zero field regions to avoid submitting the charged particles to the strong field gradient that develops in the vicinity of a thin diaphragm. This is what is observed in Fig. 1, which displays the source part of our low-energy electron generator. The double extracting electrode (electrode E) acts as an aperture limiter and selects the center part of the beam. 

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only, thanks to the second diaphragm (E2) located in a low-field region. The electron generator design enables good separation of the electron source from the Einzel lens filter. Thus the modulation process can be analyzed simply by studying the trajectory evolution in the source region. To do that the trans-Gaussian trajectories are reversed, i.e., the particle charge is set to positive and the potentials are reversed, to analyze the complex modulation process. This is done using the (trans-Gaussian) image of the exit aperture through the Einzel lens as the particle "source."

A. Simulation of the electron trajectories

Simulation of the electron trajectories was performed using ray tracing software for charged particles, SIMION software. A finite difference method is used to solve the Laplace equation and to calculate the electrical field on a grid. The electron trajectories are then estimated using the Runge–Kutta method. A real beam is represented by a group of particles with a distribution of initial conditions. For each particle we measure on the target the impact position as well as the slope of the trajectories at impact. The beam coherence is then calculated from the variance of the slope weighted by the emission probability for such particles. The impact position is used to calculate the beam profile. Details of the simulation for regular trajectories are presented elsewhere. Here we focus on unstable (trans-Gaussian) trajectories. The three input parameters are the initial position, the initial energy and the initial charged particle direction. We observe that a good description of the initial conditions can be approximated by a fixed energy—here we chose 0.08 eV—and by the distribution of only two parameters: the initial position and the initial angle. Simulation is performed for a series of settings of Einzel lens potentials, A2 and focus (Fig. 2).

As stated in an earlier article, the optimum settings are obtained along a valley in parameter space, with the beam coherence order of magnitude around $5 \times 10^{-3}$. Nevertheless a series of peaks indicates that for special settings of the focus and A2 electrodes, the variance exceeds 1%, which is the standard performance expected for such an Einzel lens-based low-energy electron generator. The results presented here are unchanged if we halve the grid size used for simulation, so we are confident that the unstable trajectories presented here are not related to the size of the potential grid. If we investigate the origin of these peaks, we observe that these high variance values are systematically related to trans-Gaussian trajectories that are responsible for beam coherence degradation. These trajectories have low density but they display a large slope at impact, so they contribute heavily to the slope variance of the beam.

Our numerical simulation was performed for a series of discrete values of initial conditions, so it is difficult to give a complete quantitative evaluation of all the contributions from anomalous trajectories. We will not provide a full description of all the families of trans-Gaussian trajectories but will focus on a single one. This particular set of unstable trajectories, which results from the narrow range of initial conditions, is presented in Fig. 3. It will be used to evaluate the contribution of this type of family to beam variance and to show how it is rejected by a modulation process.

B. Filtering process

The Einzel lens acts as a filter that rejects trajectories that are not perfectly aligned with the symmetry axis. In the present investigation the center F electrode plays the key role. On the one hand, as exemplified in Fig. 2, its repulsive potential reduces the electron axial velocity, so that a particle with large transverse velocity deviates greatly from the symmetry axis and is rejected by the F diaphragm. This filter selects electrons in a narrow range of initial conditions where it is easier to form a coherent beam with the second part of the Einzel lens (see Fig. 2). On the other hand, the F diaphragm—which is placed in a strong field region—intercepts the beam. As a consequence, the electrons traveling close to the F electrode display anomalous trajectories.
Some of them not rejected by the exit diaphragm contribute negatively to the beam. This greatly spoils beam coherence. It must be noted that the very same process is also observed at the exit of the Einzel lens and may also result from geometrical imperfections of the diaphragm.

On the one hand, the more repulsive \( F \) is, the better the beam coherence, although at a cost of a decrease in regular (Gaussian) beam current. On the other hand, the beam current originating from trans-Gaussian trajectories like the one presented in Fig. 3 is somehow not filtered out by the repulsive electrode. Hence, the ultimate beam coherence is mainly limited by these trajectories.

In a previous article\(^3\) we have shown that these unwanted trajectories exhibit a common feature: they are all unstable with respect to small variation of the initial conditions. We therefore propose they be rejected using a filtering process that takes advantage of this property.

Oscillating the Wehnelt voltage effectively modulates the initial conditions, thus stable trajectories will produce a simple linear response while a set of unstable trajectories will display a strong nonlinear response, with only a weak contribution at fundamental frequency. So if we apply sinusoidal modulation to the beam intensity and if we correlatively extract the modulated part of the beam, we will be able to reject most of the contributions from unstable trajectories because they do not contribute to the intensity oscillation of the diffraction image at fundamental frequency. As we will see, this results in a beam whose modulated part displays significantly improved coherence compared with a standard beam.

**C. Analysis of the modulation process**

The modulation process was analyzed from a set of weighted trajectories that describe the whole beam. A simulated beam is formed by 400 particles, each corresponding to an initial condition on the cathode. Such a beam was investigated for 20 values of Wehnelt voltage which describe Wehnelt modulation. Within the framework of a simple model,\(^7\) the density of initial trajectories can be expressed by two parameters that describe the initial conditions at the cathode: the radial position \( R \) and the elevation angle \( \theta \). These two govern the weighting factor that characterizes a single trajectory. Because of the cylindrical symmetry the density of trajectories is proportional to \( R \) and we chose to use a simple model where the angular probability of emission is proportional to \( \cos \theta \). The beam intensity modulation is calculated by ray tracing from the weighted set of trajectories that reach the target, and is calculated as a function of the Wehnelt voltage.

For regular (Gaussian) trajectories, the cathode area where the particles that form the beam come from is a disk, which symmetrically shrinks around the symmetry axis as the Wehnelt voltage becomes more repulsive. This produces almost linear modulation of the beam intensity. Conversely, the initial conditions on the cathode for trans-Gaussian trajectories arise in a region located far from the symmetry axis. They come from a narrow ring with a large radius, thereby satisfying a strict relationship between the radial position and initial angle. As the Wehnelt voltage is varied, we find that the width and size of the ring move in opposite directions. For the whole trans-Gaussian beam, this results in nonlinear modulation and only a weak linear contribution at fundamental frequency.

Ray tracing was performed for a series of sets of trans-Gaussian trajectories. The simulation indicates that the modulation factor is reduced from 30% for regular trajectories to less than 5% for trans-Gaussian ones. Because we cannot analyze all trans-Gaussian trajectories, it is difficult to give a complete evaluation of their contribution to beam coherence. Nevertheless the simulation performed of a single family like the one of Fig. 3 clearly suggests that trans-Gaussian trajectories are only weakly associated with the modulation process. So their contribution to the modulated part of the diffraction pattern is essentially rejected, yielding significant improvement in effective beam coherence.

**III. EXPERIMENTAL RESULTS**

The experimental setup is built around standard reverse-view low-energy electron diffraction (LEED). It has been previously described.\(^3,8,9\) A sinusoidal voltage—typically 2 V peak to peak—is added to the Wehnelt repulsive voltage in order to produce 10% oscillation of the beam current intensity.

Then the image of the LEED diffraction pattern exhibits periodic brightness oscillation that is related to the beam current intensity modulation. The time dependence of the LEED pattern brightness is determined in phase with the beam modulation.

As explained in a previous article,\(^10\) our oscillating LEED method consists of recording the time-dependent pattern image using a video camera that is perfectly locked in phase with the beam current modulation. Details of the synchronization electronics may be found elsewhere.\(^8\)

The oscillating pattern is acquired as a series of digitized images that are stored as buffers in the random access memory (RAM) of a personal computer, thanks to a real-time acquisition process. A whole number \( N \) of images must be acquired per excitation period. Each image grabbed is numbered using a real-time electronic device to insure no discontinuity of the data stream during acquisition due to occasional loss of data.

After acquisition is completed, the \( N \) image buffers are numerically processed. Each buffer corresponds to a precise acquisition time along the excitation period, \( T \). The latter is simply computed as \( T = \frac{N}{25} \) (25 images per second). The frequency can range from about 0.04 to 5 Hz.

Two images are computed, pixel per pixel, from the \( N \) buffers.\(^11\) The first image is made from the average values of brightness intensities along a full period. It is called the “mean” image.\(^10\) It is nothing more than a diffraction pattern in conventional (dc) mode. The second image is obtained from the least-square fits of the brightness intensities to a sine wave at the frequency of the beam current modulation. Each calculated pixel of this “amplitude” image represents the magnitude of its oscillating component at the excitation frequency.
perimposed onto the large background of the Bragg peak.

The image width corresponds to 50% of the Brillouin zone diffraction pattern that centers on a single diffraction peak. The modulation frequency in the range of 0.05–5 Hz.

As expected the amplitude image is exclusively related to the modulated part of the beam, so it is a result of an effective beam with a strongly reduced contribution from trans-Gaussian trajectories. As a consequence, it displays the good coherence properties of trans-Gaussian trajectories by using the rejection process described in Sec. II C.

To test the dynamic filtering process we have applied the method to a standard surface. We have studied the electron diffraction of air-cleaved mica muscovite. This is one of the few surfaces that directly displays a good diffraction pattern in ultrahigh vacuum without requiring any surface preparation.

The experiments were performed with 145 eV low-energy electrons in order to avoid the surface charge effects that appear at lower energies. Moreover the beam current density was kept low enough to avoid temperature oscillation of the surface.\(^\text{12}\) The results were found to be independent of the modulation frequency in the range of 0.05–5 Hz.

In Fig. 4 we present an expanded view of part of the diffraction pattern that centers on a single diffraction peak. The image width corresponds to 50% of the Brillouin zone (i.e., \(0.5K_f = \pi/a\) with \(a = 0.52\) nm). Figures 4(a) and 4(b) display normal diffraction and modulated diffraction, respectively. The fine structures revealed in Fig. 4(b) correspond to nanostructures of the mica muscovite surface.\(^\text{10}\) They are superimposed onto the large background of the Bragg peak.

This background was filtered out by Fourier transform and rejection of the long wave components. The result is presented in Fig. 4(c), which displays structures with obvious high resolution in reciprocal space. The lower limit for resolution of wave vector \(K\) was calculated from the full width at half maximum (FWHM) of the finest structures as well as from the high-frequency component of the Fourier transform. We found 0.7% of \(K_f\), which corresponds to a transfer width of about 70 nm. This is seven times the typical value of an ordinary LEED device.

IV. CONCLUSION

With numerical simulations of particle trajectories using the ray tracing method, we have shown that at low current the coherence of a standard low energy electron beam can be improved by almost one order of magnitude in the case of a standard LEED device. This improvement arises from modulation of the beam intensity as well as from correlated analysis of the diffraction pattern oscillating part using real-time video acquisition coupled with video signal digital processing. It is worth noting that the latter can be efficiently performed using a personal computer. The whole process acts as dynamical filtering that efficiently rejects the unstable trajectories that are responsible for most of the loss in beam coherence. We have applied our experimental method to a standard mica muscovite surface, and it has enabled the observation of surface nanostructures that indicate wave vector resolution corresponding to instrumental transfer width greater than 70 nm, compared with the typical 10 nm value of standard devices.

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