

Experimental reconstruction of source 4D phase space without prior knowledge of transfer matrix

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We experimentally demonstrate a method for reconstructing the transverse 4D phase space of an electron beam at the time of emission from downstream diagnostics of the 4D phase space. This method does not rely on detailed knowledge of the beamline transport, besides assuming that linearity and symplecticity are satisfied. We apply this method to measure the transverse position and momentum phase space of electrons emitted from a spatially structured alkali-antimonide cathode. This method can uncover local correlations between emission location and momentum spread. We formulate this method analytically and investigate resolution limits.

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I. INTRODUCTION

Understanding the physics of photoemission is critical to many applications of particle beams. Cathode photoemission performance, often characterized by the mean transverse energy (MTE) and quantum efficiency (QE), determines (in part) the maximum achievable brightness of a beam in a linear accelerator for which Liouville's theorem applies to the 6D phase space distribution. Brightness is a key metric for various applications, such as ultrafast electron microscopy [1,2], x-ray free-electron lasers [3,4], and colliders [5,6]. Brightness can be defined in several ways; nearly all definitions of brightness include a factor that depends on the transverse 4D phase space distribution. Our work focuses on a new method to measure the source 4D transverse phase space distribution.

There has been much work done, both theoretically [7–11] and experimentally [12–15], to study the QE and MTE of cathodes of various materials and surface preparations in accelerator contexts, in high surface field and charge/current regimes. However, experimental work has yet to bridge the gap with the theory in exploring the

photoemission process at a microscopic level beyond ensemble quantities such as QE and MTE. Specifically, the full distribution of source momentum, as well as local correlations with surface deformities (physical and chemical), is not frequently measured in accelerators, which can hamper the prediction of beam dynamics and comparison to photoemission theories. As such, there is a need for an accessible experimental diagnostic that can measure the beam in an accelerator and reconstruct its source 4D phase space.

The MTE of a cathode is typically measured through several techniques [16], such as scans of electromagnetic optics (solenoid, quadrupole, accelerating field/voltage) [16–18], or aperture/pepperpot measurements [19]. These measurements are either performed in actual accelerators or in smaller characterization chambers. Often, these methods do not directly measure the source momentum distribution, but instead measure the normalized beam emittance, $\epsilon_n = \sqrt{\langle x^2 \rangle \langle p_x^2 \rangle - \langle xp_x \rangle^2} / mc$, where x and p_x are the transverse position and momentum, respectively, m is the particle mass, and c is the speed of light. The MTE is then given by $\text{MTE} = mc^2 (\epsilon_n / \sigma_x)^2$, where σ_x is the rms transverse size of the beam in real space at the cathode. To do this, scans of optics (like solenoid scans) typically require accurate fieldmaps that describe the beamline elements throughout the beam transport. However, unintentional defects in the optics, such as higher-order multipole components in magnet fields, can introduce errors to the transport, and subsequently the measured

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emittance/MTE. In addition, it can be nontrivial to measure the rms transverse size of the beam, σ_x , at the cathode, e.g., in cases where the QE or drive laser intensity varies rapidly in space, or in cases with significant multiphoton photoemission [20,21].

Some advanced probes, such as photoemission electron microscopy (PEEM) [22,23] and angle-resolved photoemission spectroscopy (ARPES) [24], do measure the full momentum distribution of the photoemitted electrons. However, most PEEMs require a complex set of lens calibration procedures, which can be expensive or time-consuming to set up. The hemispherical analyzers used in ARPES also typically require eV-scale electron kinetic energies, which, for a photocathode driven by visible or near/mid-ultraviolet light, requires postacceleration, which invariably adds lensing effects that must be accounted for [24]. Despite these challenges, PEEM and ARPES are well-established methods and provide the highest resolution images of photoemission momentum. Yet, these excellent probes are not likely to be available in the accelerator itself and do not trivially (i.e., without tomographic techniques) resolve local-position-momentum correlations at the source. Methods like direct single-shot momentum space imaging [25] take a step toward making these capabilities more accessible to accelerators, but like PEEM and ARPES, do not trivially resolve local-position-momentum correlations at the source.

In this paper, we demonstrate a method where downstream 4D phase space measurements, achieved via aperture scans, can be used to reconstruct the source transverse phase space without prior knowledge of the transfer matrix. We deduce the transfer matrix by measuring the experimentally accessible matrix elements (for us, these are the position-position and position-momentum elements), and then exploiting the symplectic condition to infer the values of the unknown transfer matrix elements (in our case the momentum-position and momentum-momentum elements). Here, the momentum-position and momentum-momentum transfer matrix elements are experimentally inaccessible since we do not have a means to deterministically vary the momentum of the beam at emission. Once the transfer matrix is known, the source phase space can be determined via application of the inverse transfer matrix to the measured downstream phase space.

We first discuss the theory behind this source reconstruction method in Sec. II, our experimental setup in Sec. III, and then discuss the practical implementation of this method and error considerations in Secs. IV and V.

II. THEORY

A linear transfer matrix, $\mathbf{M}$, is often a good approximation for relating the source position and momentum of a particle to its final position and momentum downstream near the design trajectory of a beamline,

$$\begin{pmatrix} x \\ p_x \\ y \\ p_y \end{pmatrix}_f = \mathbf{M} \begin{pmatrix} x \\ p_x \\ y \\ p_y \end{pmatrix}_i$$

$$\mathbf{M} = \begin{pmatrix} m_{11} & m_{12} & m_{13} & m_{14} \\ m_{21} & m_{22} & m_{23} & m_{24} \\ m_{31} & m_{32} & m_{33} & m_{34} \\ m_{41} & m_{42} & m_{43} & m_{44} \end{pmatrix}, \quad (1)$$

where x, y are transverse coordinates and p_x, p_y are transverse (physical) momenta. In this work, we restrict consideration to 4 dimensions, but many of our results can be generalized to 6D provided a means to measure some of the longitudinal transfer matrix elements.

According to Hamiltonian mechanics, the transfer matrix must satisfy the symplectic condition, which is expressed in an unconventional form here,

$$\mathbf{M}^{-1} = -\Omega \mathbf{M}^T \Omega$$

$$= \begin{pmatrix} m_{22} & -m_{12} & m_{42} & -m_{32} \\ -m_{21} & m_{11} & -m_{41} & m_{31} \\ m_{24} & -m_{14} & m_{44} & -m_{34} \\ -m_{23} & m_{13} & -m_{43} & m_{33} \end{pmatrix}$$

$$\Omega = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}. \quad (2)$$

Note that the symplectic condition constrains the inverse significantly: it is a simple rearrangement and sign modification of the original transfer matrix in Eq. (1). This, as we will show, allows us to calculate the full source momentum distribution without full knowledge of the transfer matrix.

In principle, we can measure components of the transfer matrix by linearly fitting the final position and momentum of a particle measured at a beamline diagnostic to its source position and momentum. In practice, for a beam of finite size, its centroid in 4D phase space transforms like a single particle. To determine transfer matrix elements from a particle source, we often only have control over the source position centroid. In the case of a photocathode, this can be done by moving the laser driving photoemission a known displacement on the cathode surface.

For each spatial displacement of the emission site, the *phase space displacement* of the centroid (a 4D vector) of the beam at the diagnostic can be measured by a phase space diagnostic. For example, as shown in Fig. 1, we

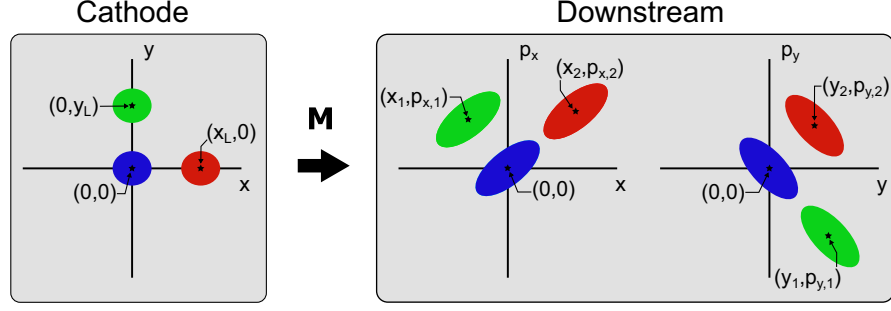


FIG. 1. A cartoon demonstrating the measurement of the partial transfer matrix. At the cathode (left), the beam is moved on the emission surface to positions $(x_L, 0)$ and $(0, y_L)$. At a downstream diagnostic (right), after evolving with the transfer matrix $\mathbf{M}$, the 4D phase space of the beam is measured and labeled by its centroids (indicated by stars). Each phase space is measured with the beam emitted at the correspondingly colored cathode position.

measure phase space centroids of $(x_1, p_{x,1}, y_1, p_{y,1})$ and $(x_2, p_{x,2}, y_2, p_{y,2})$ for a laser displacement of $(y_L, 0)$ and $(x_L, 0)$, respectively.

Altogether, this allows us to determine the first and third columns of the transfer matrix, which will be referred to as the partial transfer matrix,

$$\begin{pmatrix} m_{11} & m_{13} \\ m_{21} & m_{23} \\ m_{31} & m_{33} \\ m_{41} & m_{43} \end{pmatrix} = \begin{pmatrix} x_2/x_L & x_1/y_L \\ p_{x,2}/x_L & p_{x,1}/y_L \\ y_2/x_L & y_1/y_L \\ p_{y,2}/x_L & p_{y,1}/y_L \end{pmatrix}. \quad (3)$$

In practice, the partial transfer matrix will be determined by linearly fitting the measured phase space centroids to

$$\begin{pmatrix} x \\ p_x \\ y \\ p_y \end{pmatrix}_i = \mathbf{M}^{-1} \begin{pmatrix} x \\ p_x \\ y \\ p_y \end{pmatrix}_f = \begin{pmatrix} m_{22} & -m_{12} & m_{42} & -m_{32} \\ -m_{21} & m_{11} & -m_{41} & m_{31} \\ m_{24} & -m_{14} & m_{44} & -m_{34} \\ -m_{23} & m_{13} & -m_{43} & m_{33} \end{pmatrix} \begin{pmatrix} x \\ p_x \\ y \\ p_y \end{pmatrix}_f.$$

It follows that the source transverse momentum $p_{x,i}$ and $p_{y,i}$ are then related to the measured 4D phase space by the measured partial transfer matrix given by Eq. (3),

$$\begin{pmatrix} p_x \\ p_y \end{pmatrix}_i = \begin{pmatrix} -m_{21} & m_{11} & -m_{41} & m_{31} \\ -m_{23} & m_{13} & -m_{43} & m_{33} \end{pmatrix} \begin{pmatrix} x \\ p_x \\ y \\ p_y \end{pmatrix}_f = \begin{pmatrix} \frac{-p_{x,2}}{x_L} & \frac{x_2}{x_L} & \frac{-p_{y,2}}{x_L} & \frac{y_2}{x_L} \\ \frac{-p_{x,1}}{y_L} & \frac{x_1}{y_L} & \frac{-p_{y,1}}{y_L} & \frac{y_1}{y_L} \end{pmatrix} \begin{pmatrix} x \\ p_x \\ y \\ p_y \end{pmatrix}_f. \quad (4)$$

Given a measured 4D phase space, this directly yields the source momentum phase space of the beam, from which the MTE can be calculated as

$$\text{MTE} = \frac{1}{m} \sqrt{\langle p_x p_x \rangle_i \langle p_y p_y \rangle_i}. \quad (5)$$

the measured laser displacements. Note that this requires us to assume that the source momentum centroid does not vary with emission location. Our formalism does allow the momentum *width* (e.g, local MTE) to vary across the emitter surface. Also note that all matrix elements of the form m_{nl} where l is a momentum index (i.e., m_{nl} acts on the source momentum $p_{x,i}, p_{y,i}$), and $n \in [1, 4]$ remain unknown, as we typically do not have a means to change the source momentum centroid systematically.

Even without the full transfer matrix, we can still calculate the source transverse momentum $p_{x,i}$ and $p_{y,i}$ by applying the inverse transfer matrix given by the symplectic condition in Eq. (2) to a point in the measured 4D phase space,

So far we have reconstructed the source transverse momentum distribution. With a few additional assumptions, we can also solve for the full 4×4 transfer matrix and hence reconstruct the source 4D phase space. We first generate a system of nonlinear equations from expanding a slightly different form of the symplectic condition in

Eq. (2), $\mathbf{M}\mathbf{M}^T = \mathbf{\Omega}$. This yields 5 independent nonlinear equations (after accounting for redundancy in the original 16).

Yet, this is not enough equations to solve for the remaining 8 unknown transfer matrix elements. Just as we measured the downstream centroids of the 4D phase space to obtain information about the transfer matrix, we can also measure higher-order statistical moments of the beam. The next order statistical moment is the beam covariance matrix, which evolves in the beamline with the transfer matrix as

$$\mathbf{M}^{-1}\Sigma_f(\mathbf{M}^{-1})^T = \Sigma_i, \quad (6)$$

where Σ_f and Σ_i are the measured final and the source beam covariance matrices, respectively. As usual, the elements of the beam covariance matrices are defined as $\Sigma_{ij} = \langle v_i v_j \rangle$, for $v = \{x, p_x, y, p_y\}$.

Since we choose to use a cathode that is disordered and polycrystalline, as is typical, we assume that the position and momentum are independent, or in other words, the source position-momentum correlation is zero. This yields another 4 independent nonlinear equations, $\langle xp_x \rangle_i = \langle xp_y \rangle_i = \langle yp_x \rangle_i = \langle yp_y \rangle_i = 0$, which is related to the measured beam covariances and transfer matrix by Eq. (6). Note that this average is taken over the whole beam, and nonzero correlation is permitted locally.

As a result, this provides a total of 9 independent nonlinear equations. There are 8 unknown transfer matrix elements, fewer than the number of equations, making this an overdetermined system of equations. We can then apply the Gauss-Newton method to numerically find a best-fit solution, which yields the full transfer matrix. Once the full transfer matrix is acquired, it can be inverted and applied to a measured 4D phase space to reconstruct the entire 4D phase space at emission. In the Supplemental Material [26], we present the full system of equations used to solve for the transfer matrix, and simulation benchmarking of errors potentially introduced by the experiment to the 4D transfer matrix, the reconstructed source beam size, and MTE. Our procedure, via the symplectic condition, enforces unity determinant of the transfer matrix and preserves 4D emittance; since we are using physical momenta, this remains true in transfer matrices with acceleration.

III. EXPERIMENTAL DEMONSTRATION METHODS

We measured the 4D phase space of a beam using the PHOTOCATHODE Epitaxy and Beam Experiments (PHOEBE) test beamline at Cornell University [27]. Photoemission is driven at the cathode by a continuous-wave diode laser, and the position of the laser on the cathode is controlled by mirrors mounted on motorized linear translation stages. A beamsplitter splits the laser

right before it enters the gun chamber, and the reflected laser is viewed by a CMOS camera acting as a virtual cathode, which measures the laser position.

For the purposes of demonstrating this method, we used a micropatterned alkali-antimonide cathode—see Supplemental Material [26] for more details. The cathode consisted of a Si/SiO₂ substrate with a layer of copper deposited on top with a periodic lattice of fiducial markers of varying geometries, such that the underlying Si/SiO₂ is exposed. A thin film of Na-K-Sb was then grown on top of the substrate using molecular beam epitaxy. In our growth conditions, the QE of the Na-K-Sb film grown on the copper is larger than Si/SiO₂; therefore periodically modulating the QE across the cathode when photoemission is driven at 405 nm.

Electrons emitted by the cathode are accelerated by a DC gun biased at 15 kV. The beam is focused by a solenoid onto a circular aperture with a diameter of 30 μm at which the 4D phase space of the beam is measured, as shown in Fig. 2(a). After the aperture, the transmitted beam traveled through a approximately 0.5 m drift section until it reached the detector. The detector consisted of a microchannel plate, which multiplied electrons and accelerated them onto a YAG scintillator screen imaged by a sCMOS camera.

Approximating the aperture as a point source, the transverse spatial distribution imaged by the detector trivially yields the transverse momentum distribution of the transmitted beam by dividing the detector position by the drift length and multiplying by the longitudinal momentum, which is inferred from the DC gun voltage bias. This transverse momentum distribution was measured continuously as two corrector magnets, one for each transverse axis, scan the beam across the aperture in a 2D grid. Each corrector magnet consists of two air-core dipole magnets wired in series and is calibrated such that the magnet current measured at every step of the 2D grid corresponds to a known point in the $x - y$ position phase space. As such, for each point in the $x - y$ position phase space, there is an associated transverse momentum distribution. After subtracting the momentum kick added by the corrector magnet from the measured transverse momentum, the 4D phase space can be composed, an example of which is shown in Fig. 2(b). For analysis, we will visualize the 4D phase space in 2D projections onto the transverse coordinate axes, like in Fig. 2(c).

To measure the partial transfer matrix, we use a small laser spot size such that the beam is ideally emitted from the uniform regions of the cathode, excluding the patterned fiducial markers. The laser is moved around the cathode, within a 200 μm by 200 μm region, with the 4D phase space of the beam measured at 8 positions. The 4D phase spaces measured at each laser position are similar to that shown in Figs. 2(b)–2(c). The clean phase spaces allow us to fit the 2D phase space projections [e.g. Fig. 2(c)] to a 2D superGaussian, which then supplies the beam covariances

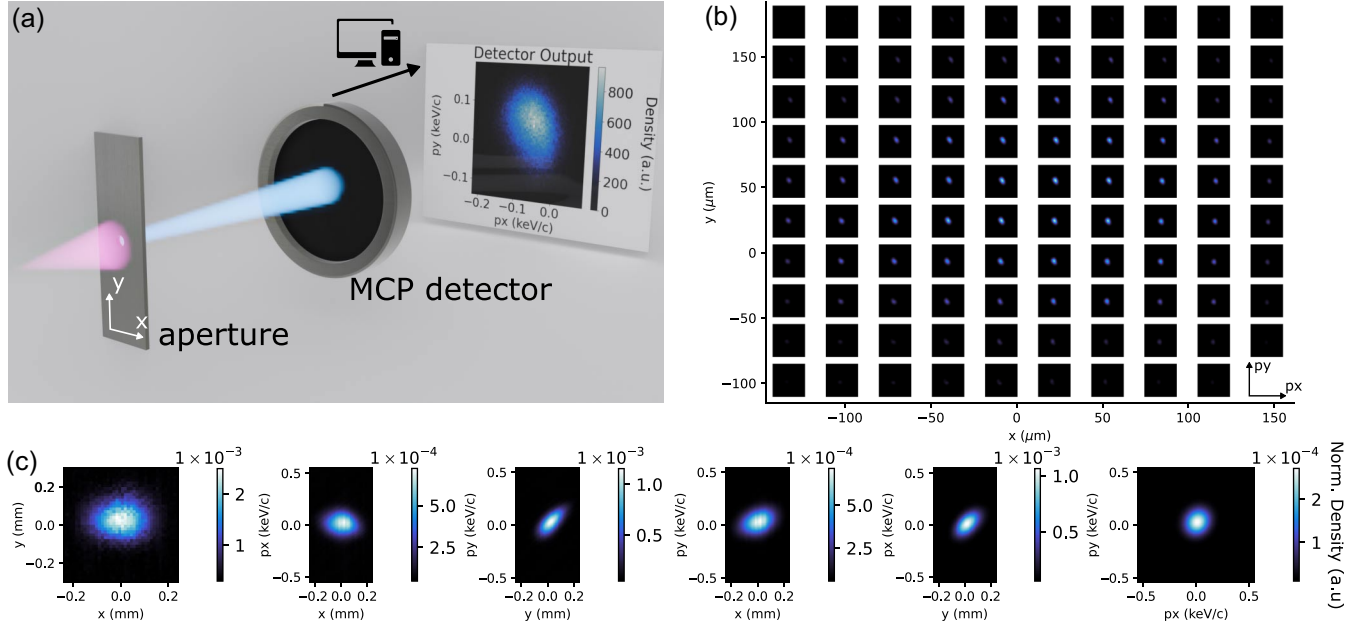


FIG. 2. (a) Diagram of the aperture scan measurement. Beam (pink) is scanned over the aperture, and the transverse spatial distribution of the transmitted beam (blue) is imaged by the detector, which is converted into a transverse momentum distribution. (b) Example of a measured 4D phase space, where a subset of the data is shown. Each image is a (p_x, p_y) distribution measured when the beam is at the (x, y) position on the aperture. (c) The 4D phase space in b) projected into 2D planes along the (x, p_x, y, p_y) axes.

required to enforce zero source position-momentum correlation when solving for the full 4D transfer matrix. We then switch to a larger laser spot that covers the patterned fiducial markers, measure the 4D phase space of the resulting beam, and reconstruct the source 4D phase space using the solved transfer matrix.

IV. EXPERIMENTAL RESULTS

Driving the photoemission with a large laser spot that covers multiple patterned markers on the cathode, we measure a 4D phase space using the aperture scan, shown

in Fig. 3(a). During the aperture scan, we only scan over a part of the entire beam in the $x - y$ position phase space to increase the 2D spatial resolution. Both the hard edges of the scan range and the modulation of QE on the cathode surface lead to sharp edges and intricate intensity modulations not present in the example phase space shown in Fig. 2(c). Following the process laid out in Sec. II, we reconstruct the 4D transfer matrix and the source 4D phase space of the beam at the cathode, shown in Fig. 3(b). An example of a transfer matrix we measured and the uncertainties of the elements is shown in Supplemental Material [26].

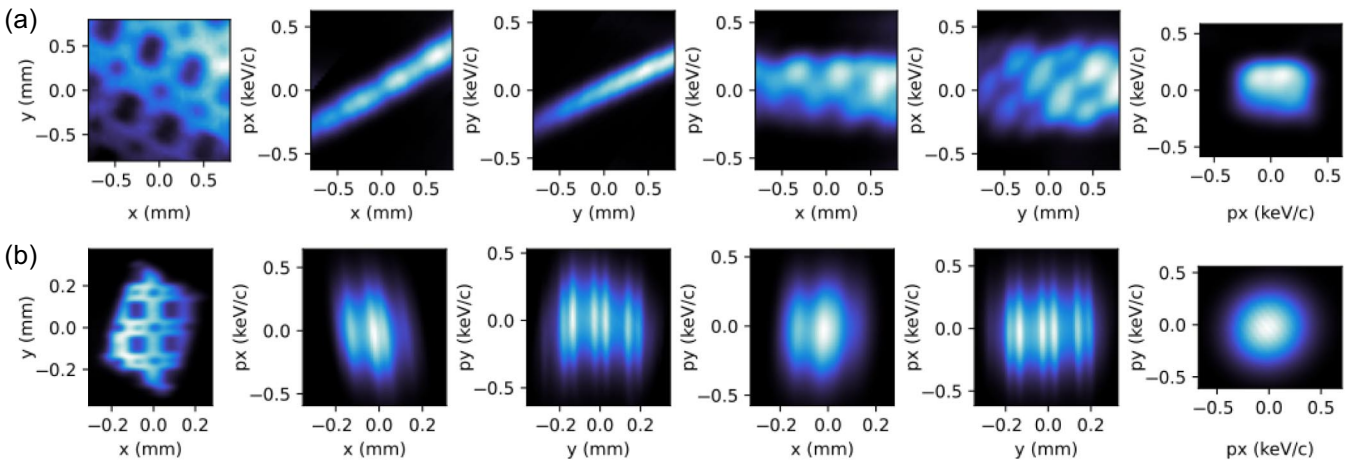


FIG. 3. (a) Measured 4D phase space of the beam at the aperture. Only a $1200 \mu\text{m}$ by $1200 \mu\text{m}$ part of the beam was measured. (b) Reconstructed source 4D phase space of the beam at the cathode.

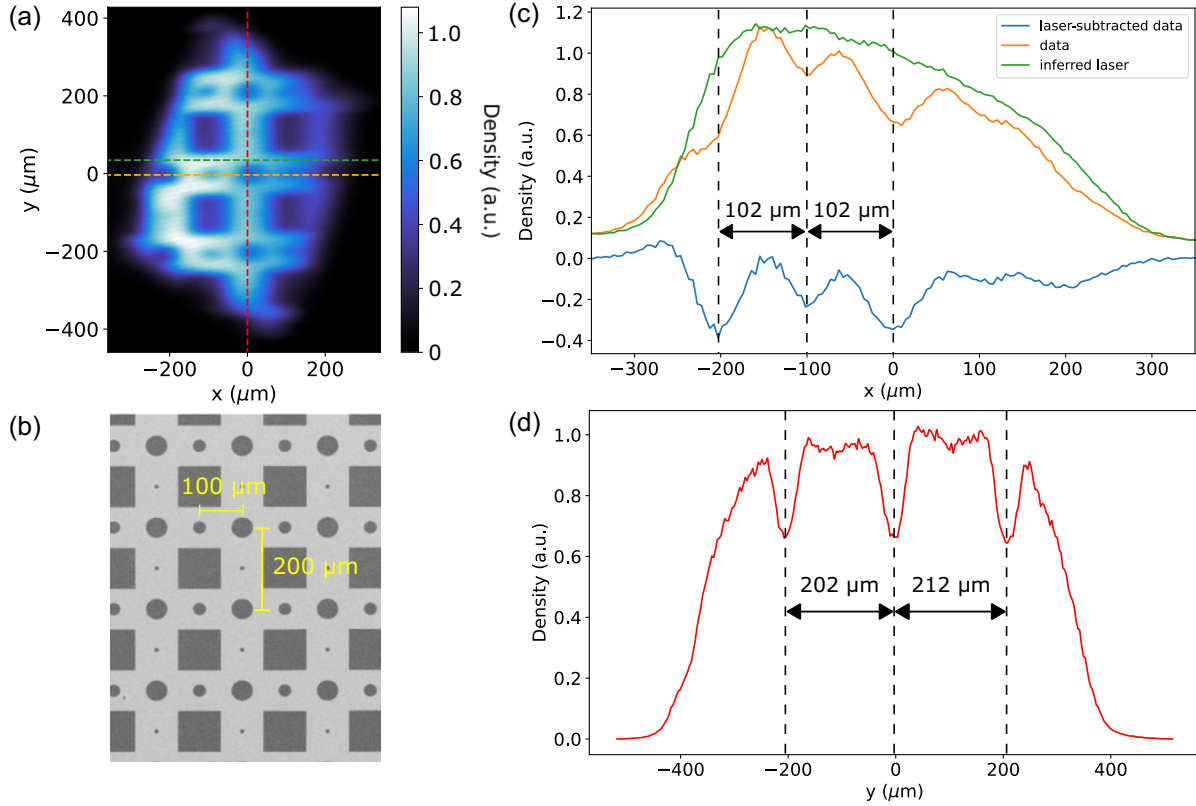


FIG. 4. (a) Detailed image of the reconstructed source $x - y$ position phase space. Linecut profiles are indicated by the dashed lines and correspondingly colored with the displayed profiles in (c) and (d). (b) Scanning electron microscope image of the substrate. Dark regions correspond to SiO₂, and copper for light regions. (c) Horizontal linecut profiles, taken on (orange) and off (green) the features in (a). The off-feature linecut is treated as background and subtracted from the on-feature linecut, yielding the linecut in blue. (d) Vertical linecut profile. Black dashed lines in (c) and (d) indicate the position of features corresponding to known QE modulations induced by the substrate pattern.

Upon first inspection of the reconstructed phase space in Fig. 3(b), we note that the position-momentum phase spaces ($x - p_x$, $y - p_y$, $x - p_y$, $y - p_x$) display little correlation between the position and momentum, on average over all the electrons, which is expected from a randomly disordered cathode. Since we do not use the measured 4D phase space [Fig. 3(a)] in solving for the transfer matrix, this is not trivially a result of constraining the source position-momentum correlation to be zero.

The $p_x - p_y$ momentum phase space also displays little average correlation and is highly symmetric, which is expected for a polycrystalline cathode where the band structure is not well-defined and has a randomly disordered surface that allows electrons to uniformly scatter into all energetically allowed transverse momentum [9,11]. The fact that this simple momentum distribution arises from such a complex phase space, without enforcing it as a constraint on the transfer matrix, is evidence that the reconstruction does indeed produce physically sensible results.

We analyze the reconstructed $x - y$ position phase space, shown in Fig. 4(a), by investigating linecut profiles of the density taken across features induced by the

substrate micropattern, shown in Fig. 4(b). Looking at the horizontal linecut profile in Fig. 4(c), there is a noticeable background slope in the data, which can be attributed to variation in the laser intensity. To account for this, we take a linecut profile nearby, which does not intersect the substrate micropattern features, and subtract it from the data. The features appear as troughs in the density, and we measure the center-to-center distance. The average center-to-center distance comes out to $102 \pm 4 \mu\text{m}$, which matches the spacing between the corresponding substrate fiducial markers, measured by a scanning electron microscope (SEM) in Fig. 4(b) to be 100 μm . The uncertainties of the average center-to-center distances here are propagated from the resolution of the aperture scan measurement. Similarly, we measure the center-to-center distance between features in a vertical linecut profile in Fig. 4(d), and the average center-to-center distance comes out to $207 \pm 5 \mu\text{m}$. This is slightly larger than the 200 μm spacing measured by an SEM, but still within 2σ . While acknowledging that some deviations may occur due to the cathode growth and QE modulations not perfectly corresponding with the substrate micropattern, we nevertheless observe relatively good agreement

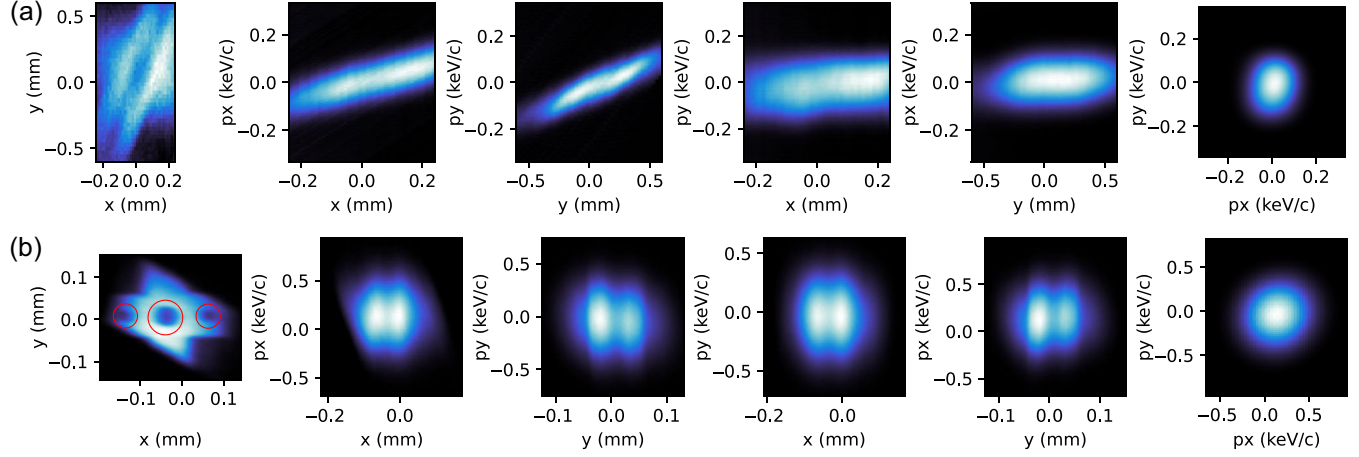


FIG. 5. (a) 2D projections of a 4D phase space of the beam measured at beamline optics settings where the intensity modulations in the $x - y$ phase space are significantly distorted. (b) Source 4D phase space reconstructed from (a). In the source spatial distribution, the dark circular features within the red circles correspond with fiducial markers on the cathode.

between the position of features in the reconstructed $x - y$ position phase space and the position of the corresponding fiducial markers measured by SEM.

As noted earlier, we only measured part of the beam in Fig. 3(a), so reconstructions of the source 4D phase space could be frustrated since we may not be measuring all of the electrons being emitted from the reconstructed region on the cathode. To understand this effect, we performed General Particle Tracer simulations, tracking the beam emitted from a point on the cathode with the measured MTE to the aperture. From these simulations, we found that the beam forms a roughly $45 \mu\text{m}$ rms spot at the aperture. Given that we scan the beam within a $1200 \mu\text{m}$ by $1200 \mu\text{m}$ region, we can safely say that we measure all of the electrons emitted from the region of the cathode that was reconstructed in the $x - y$ position phase space of Fig. 3(b) except for near the edges of that phase space.

We also attempt to reconstruct the source 4D phase space of the beam from a 4D phase space, shown in Fig. 5(a), measured by performing the aperture scan at a different solenoid focusing strength. The intensity modulation in the $x - y$ position phase space here [Fig. 5(a)] is now significantly distorted compared with its counterpart in the 4D phase space that we analyzed earlier [Fig. 3(a)]. In the reconstructed source $x - y$ position phase space, shown in Fig. 5(b), the average center-to-center distance between the circular features is $94 \pm 6 \mu\text{m}$. This agrees with the distance between the corresponding fiducial markers on the cathode [Fig. 4(b)], measured by SEM imaging to be $100 \mu\text{m}$. The accurate reconstruction of the source spatial distribution from a distorted 4D phase space signifies that our calculated transfer matrix successfully incorporates the momentum of the measured beam to “unscramble” the distorted $x - y$ phase space that was measured at the aperture.

The other primary goal of reconstructing source 4D phase space is to accurately measure the MTE of the cathode. To check that the MTE calculated from the reconstructed source momentum distribution is correct, we compare it to the MTE measured by an emittance measurement via the aperture scan. We measured 4D phase spaces while varying the source beam sizes at the cathode, σ_x , and reconstructed the source 4D phase spaces for each source beam size. Fitting each reconstructed source $p_x - p_y$ momentum phase space to a 2D supergaussian for $\langle p_x p_x \rangle_i$, $\langle p_y p_y \rangle_i$, and $\langle p_x p_y \rangle_i$, we calculate the MTE as given by Eq. (5) to be $73 \pm 2 \text{ meV}$. The uncertainty of the MTE here is propagated from the uncertainty of the measured partial transfer matrix through a Monte Carlo simulation. To check this MTE value, we calculated the 4D emittance [26], ϵ , of each measured 4D phase space and linearly fitted it as a function of σ_x , $\epsilon = \sigma_x \sqrt{\text{MTE}/m_e c^2}$, where m_e is the electron mass. This is shown in Fig. 6, yielding a MTE of $69 \pm 2 \text{ meV}$. This fitted MTE value agrees with the MTE calculated from the reconstructed $p_x - p_y$ momentum phase spaces, validating the source $p_x - p_y$ momentum phase space reconstruction. The MTE we expect for a NaKSb cathode can be calculated given the photo-excitation energy, $h\nu \approx 3 \text{ eV}$, and the work function, $\phi \approx 2 \text{ eV}$ [28,29], as $\text{MTE} = (h\nu - \phi)/3 \approx 330 \text{ meV}$ [7]. In comparison, the MTE we measure is quite small, but this is not necessarily unexpected given that the cathode’s QE has degraded by a few orders of magnitude since it was grown, and we are likely emitting near the photoemission threshold.

The agreement between the position of features measured in the reconstructed source position phase space and the known position of fiducial markers in the substrate micropattern suggests that we have correctly reconstructed the source position phase space of the beam. Together with the confirmation of the MTE and the low

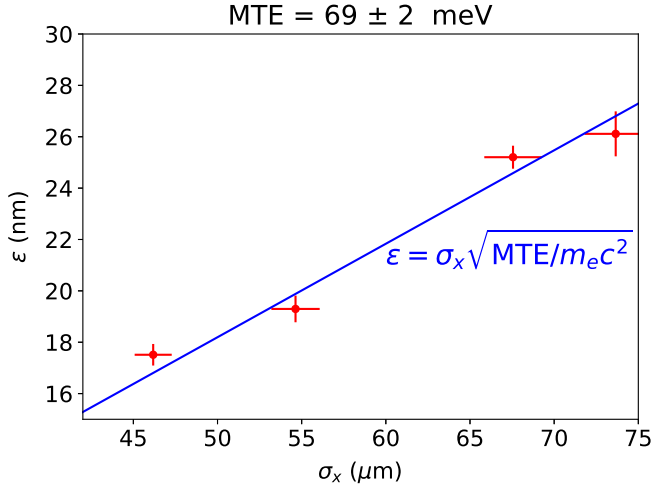


FIG. 6. 4D emittance, ϵ , measured as a function of beam size at the cathode, σ_x , and linearly fitted to yield an MTE of 69 ± 2 meV. The fit requires $\epsilon \rightarrow 0$ as $\sigma_x \rightarrow 0$.

position-momentum correlations aligning with our expectations of the cathode's electronic and physical structure, we have likely reconstructed the entire source 4D phase space with good fidelity.

The reconstructed source 4D phase space still includes measurement errors and artifacts, such as background noise, point spread function blurring of the measured phase space, and others. We now discuss these measurement errors

and artifacts in detail and how they are accounted for in our prior analysis.

V. UNCERTAINTY CONSIDERATIONS

A. Camera background noise

While measuring the 4D phase space, there is an intrinsic background noise added by the detector itself. To account for this, we perform an aperture scan without a beam, achieved by blocking the driving laser and turning off the DC gun power supply, which yields the background noise in the measured 4D phase spaces. Having solved for the full transfer matrix in previous measurements, we can invert it and apply it to the measured 4D background noise, yielding the background noise in the source 4D phase space. This background noise can then be subtracted from the reconstructed source 4D phase space of a beam, the resulting difference being shown earlier in Fig. 3(b).

Here, we focus on the reconstructed $p_x - p_y$ momentum phase space, shown in Fig. 7(a), but the full source 4D phase space and its background noise can be found in the Supplemental Material [26]. Projecting the reconstructed source $p_x - p_y$ background noise onto either p_x and p_y , as in Figs. 7(c) and 7(d), we can see that the background noise appears Gaussian-like. Doing the same 1D projection for the reconstructed $p_x - p_y$ momentum phase space of the beam we measured previously, fully shown here

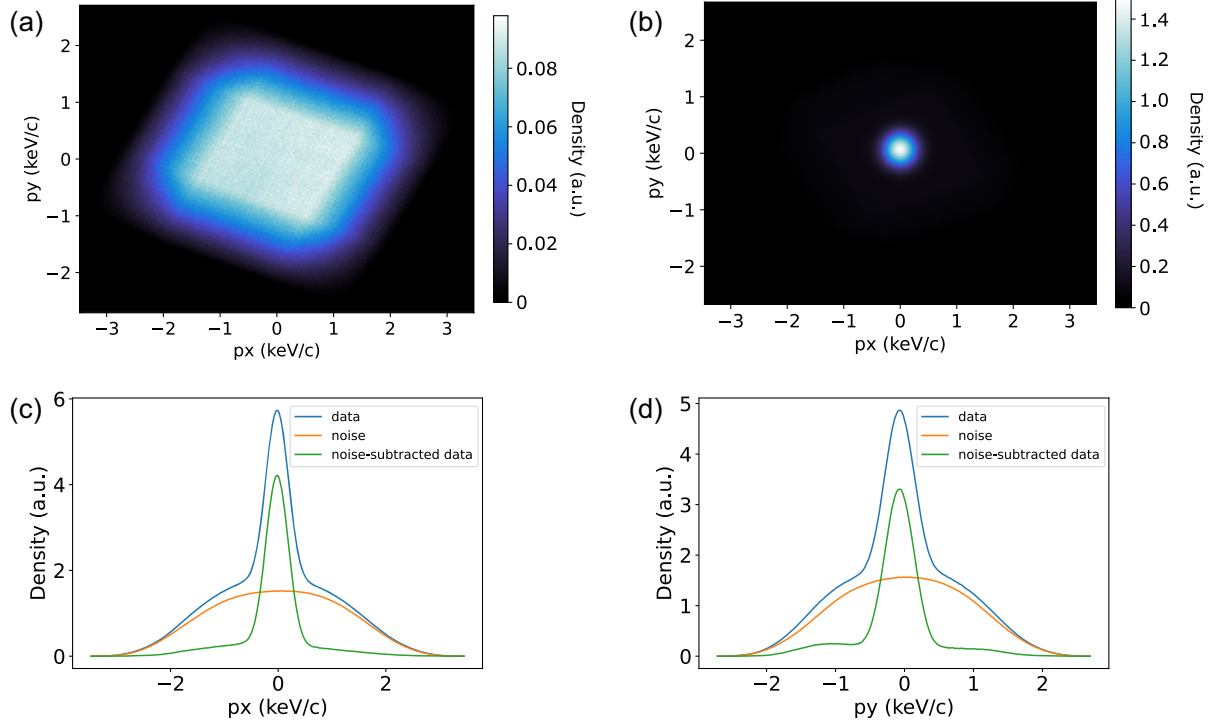


FIG. 7. (a) Isolated background noise in reconstructed $p_x - p_y$ momentum space due to camera background noise. (b) Measured source $p_x - p_y$ momentum space of a beam. (c) and (d) show, respectively, projections of the background noise (green) and the measured source $p_x - p_y$ momentum space (blue) onto the p_x and p_y axes, as well as the background-subtracted distribution (orange).

in Fig. 7(b), we see that the background noise matches the tail of the data distribution. Subtracting the background noise from the data then produces a much cleaner distribution that can be easily fitted with a supergaussian and yields a more accurate MTE.

There is some residual background leftover after the background noise subtraction, which can be attributed to other sources of noise, such as the presence of stray beam leaking out past the aperture sidewalls and hitting the detector. Evidence of stray beam can be seen in the phase space fit residuals, shown in Fig. S5b in Supplemental Material [26].

B. Effect of finite aperture size and detector point spread function

When measuring the 4D phase space of the beam with the aperture scan, the finite size of the aperture will blur the measured $x - y$ position phase space. To understand this, we can imagine the case where the beam is a point source. Scanning the beam across the aperture then produces an $x - y$ position phase space of uniform density that matches the shape of the aperture, a circle with diameter A . In the case of a beam of nonzero size at the aperture, the measured $x - y$ position phase space is then a convolution of the aperture with the actual $x - y$ position phase space, where, for simplicity, we represent the aperture as a Gaussian with an rms spread of $\sigma_A = A/\sqrt{12}$. As a result, the finite aperture size blurs the $x - y$ position phase space.

The effect of the detector point spread function (PSF) is similar, where a point source object is imaged by the detector as a Gaussian with an rms spread of σ_D . Like the $x - y$ position phase space, the detector PSF is convolved

with the actual $p_x - p_y$ momentum phase space, thus blurring it as well. Since it is so similar, we will also use the term PSF to refer to both aperture and detector blurring.

Knowing the detector PSF, we can deconvolve the detector images of the beam measured during the aperture scan to obtain the true 4D phase space. However, direct deconvolution can produce inaccurate results in the case where the signal-to-noise ratio is low. Instead, if we are only interested in statistical quantities like MTE, we need only to account for the aperture and detector PSFs in the measured beam covariance matrix and propagate it to the beam covariance at the source.

Assuming the $x - y$ and $p_x - p_y$ phase spaces are 2D Gaussians, the convolution of the phase space with the aperture and detector PSFs results in the following relationship between the actual beam covariance matrix Σ_f and the measured beam covariance matrix Σ'_f ,

$$\Sigma'_f = \Sigma_f - \begin{pmatrix} \sigma_A^2 & & & \\ & \sigma_D^2 & & \\ & & \sigma_A^2 & \\ & & & \sigma_D^2 \end{pmatrix}.$$

We can then propagate the PSF-corrected beam covariances to the cathode by applying the inverted transfer matrix to Σ'_f , like in Eq. (6), yielding the source beam covariance matrix corrected for the aperture and detector PSF. For measuring MTE, we are particularly interested in the corrected source momentum covariances, $\langle p_x p_x \rangle'_i$, $\langle p_y p_y \rangle'_i$, and $\langle p_x p_y \rangle'_i$,

$$\begin{aligned} \langle p_x p_x \rangle'_i &= \langle p_x p_x \rangle_i - m_{11}^2 \sigma_D^2 - m_{21}^2 \sigma_A^2 - m_{31}^2 \sigma_D^2 - m_{41}^2 \sigma_A^2 \\ \langle p_y p_y \rangle'_i &= \langle p_y p_y \rangle_i - m_{13}^2 \sigma_D^2 - m_{23}^2 \sigma_A^2 - m_{33}^2 \sigma_D^2 - m_{43}^2 \sigma_A^2 \\ \langle p_x p_y \rangle'_i &= \langle p_x p_y \rangle_i - m_{11} m_{13} \sigma_D^2 - m_{21} m_{23} \sigma_A^2 - m_{31} m_{33} \sigma_D^2 - m_{41} m_{43} \sigma_A^2. \end{aligned}$$

Here, $\langle p_x p_x \rangle_i$, $\langle p_y p_y \rangle_i$, and $\langle p_x p_y \rangle_i$ are calculated from fitting the reconstructed source momentum phase space. With our measured source momentum phase space, this results in a roughly 15% decrease in the MTE when using an aperture with a diameter of 30 μm and a detector with a PSF spread of $\sigma_D = 100 \mu\text{m}$, which yields the aforementioned MTE of $73 \pm 2 \text{ meV}$ in Sec. IV.

C. Other sources of error

Experimental drift in the beam phase space over time may cause subsequent measurements of the beamline transfer matrix and source phase space to be inaccurate. This drift may originate from small changes in the laser optics positions due to vibrations or temperature shifts, time-varying laser intensities, and the cathode's QE and

MTE changing over time. To address changes in the laser position and intensity, we monitored them using the virtual cathode camera over the course of an aperture scan measurement. We did not observe any significant drift in the laser position. However, there are noticeable variations in the laser intensity. Assuming linear photoemission, we account for this by normalizing the images of the beam taken during the aperture scan by the laser intensity measured simultaneously. As for cathode's QE and MTE, we did not observe significant changes in either over the typical timescale of a measurement, which is roughly 15 min for an aperture scan. We performed multiple aperture scans of the same phase space over 12 h and saw no significant drift in the beam emittance calculated from the measured phase spaces. These measurements also

experimentally determined the statistical uncertainty of the phase space centroids and the uncertainty of phase space covariance matrix elements. The uncertainties of the partial transfer matrix were then obtained from the error-weighted linear fit of the phase space centroids to the laser displacements, as given by Eq. (3). Finally, the uncertainties of the reconstructed 4D transfer matrix were propagated from the partial transfer matrix uncertainties and the beam covariance uncertainties through a Monte Carlo simulation of the Gauss-Newton method. An example of the 4D transfer matrix and the uncertainties is shown in Supplemental Material [26].

Another source of error is beam energy spread, introducing dispersion into the position and momentum measured by the aperture scan. The full effect of dispersion is discussed in Supplemental Material [26], where we perform General Particle Tracer simulation benchmarking of the full 4D reconstruction method while allowing for beam energy jitter. In particular, we also estimate the dispersion added by our corrector magnets used to scan the beam across the aperture. Within the observed beamline conditions, we determine that the uncertainty added to the position and momentum from dispersion is negligible compared with the other uncertainties, such as the finite aperture size and angular resolution limits.

VI. CONCLUSIONS

In this paper, we present a method for determining the 4D transfer matrix of a beamline by using a simple aperture scan diagnostic to measure the dependence of the 4D phase space on the source emission position. This method is experimentally applied to find the transfer matrix of the PHOEBE test beamline and reconstruct the source 4D phase space of a beam emitted from a micro-patterned cathode. Analyzing the reconstructed source 4D phase spaces, we fit the $p_x - p_y$ momentum phase space to directly determine the MTE and found that it agreed with aperture scan measurements of MTE. We also confirmed that the source $x - y$ position phase space is reconstructed successfully across varying beamline optics settings by observing that the spacing between features in the reconstructed $x - y$ position phase space matches that of the corresponding fiducial markers patterned onto the cathode. Altogether, this is suggestive that we are able to solve for the beam transfer matrix and apply it to reconstruct the source 4D phase space with good fidelity.

A feature of this method is the ability to image source position-momentum correlation at microscopic scales. We could exploit this ability in future work by deterministically engineering physical features, like steps in height on the cathode surface, or chemical features, such as interfaces between deposited metals of different work functions, and studying the effects on the momentum of electrons emitted nearby. Studies like these, aiming to understand local-position-momentum correlations, could

open up the development of “designer photocathodes” with physical and chemical surface features engineered to shape the emission of electrons in a controllable fashion.

Finally, this source reconstruction method is accessible to existing accelerators, requiring only linear beam transport, a method of measuring 4D phase space (aperture scans, pepperpot, etc), and a means to deterministically control the source position (or momentum) of the beam. By requiring beam transport to be linear, accelerators must operate at beam currents where space charge is negligible and include only linear optics. In addition, there can be no coupling of the transverse coordinates to time or energy, as they are not measured by 4D phase space measurements. However, this method could be extended to include time and energy in the transfer matrix and source phase space if the 5D or 6D phase space of the beam is measured. Given that all these conditions are satisfied, our source reconstruction method can be applied to measure the beamline transfer matrix for arbitrary linear optics and the phase space of the beam at the source.

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J. M. is a co-founder of Cayuga Beam Systems.

DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

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