

Efficient STEM-EBIC Simulation Using an Adjoint Drift-Diffusion Model

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Abstract—Scanning transmission electron microscopy electron-beam-induced current (STEM-EBIC) imaging provides nanometer-scale maps of carrier collection in semiconductor devices, but quantitative drift-diffusion simulation normally requires one nonlinear solve per beam position. We formulate STEM-EBIC simulation as a discrete adjoint problem for the first-order beam-induced response of the fully coupled drift-diffusion system linearized about a selected DC operating point. For each selected bias, one beam-free DC solve and one transposed linear solve per collecting contact yield an adjoint solution, so each beam position is evaluated by an inner product with the corresponding beam-generation source. The adjoint implementation is verified against forward nonlinear beam-on Newton simulations, while a finite-injection sweep quantifies the validity range of the first-order response. The zero-bias adjoint profile is further compared with an experimental STEM-EBIC profile of a Si p-n junction lamella. Measured timings and scaling projections show orders-of-magnitude computational savings in the tested 2D case and indicate that the corresponding full-device 3D adjoint simulation is computationally feasible.

Index Terms—STEM-EBIC, adjoint method, drift-diffusion simulation, reciprocity, semiconductor device simulation.

I. INTRODUCTION

Electron-beam-induced current (EBIC) imaging is a long-established method for semiconductor and device characterization [1]. When performed in a scanning transmission electron microscope, STEM-EBIC enables nanometer-scale maps of carrier collection in semiconductor devices [2]. In a STEM-EBIC experiment, a focused electron beam generates electron-hole pairs that are separated by internal electric fields and collected at the contacts; scanning the beam position relative to the device produces a spatial map of the resulting current. Quantitative interpretation, however, generally requires self-consistent device simulation because the EBIC signal depends on generation, carrier transport, and recombination throughout the device volume. The conventional approach solves the full nonlinear drift-diffusion (DD) system separately for every beam position, requiring N_{beam} Newton solves at each bias. This cost is prohibitive for the pixel counts typical of STEM-EBIC maps, especially in three dimensions.

Adjoint and reciprocity methods offer an alternative to repeated source-by-source simulation. Donolato related the collected current to an auxiliary minority-carrier problem [3], but this formulation relies on the minority-carrier approximation and does not directly describe the fully coupled

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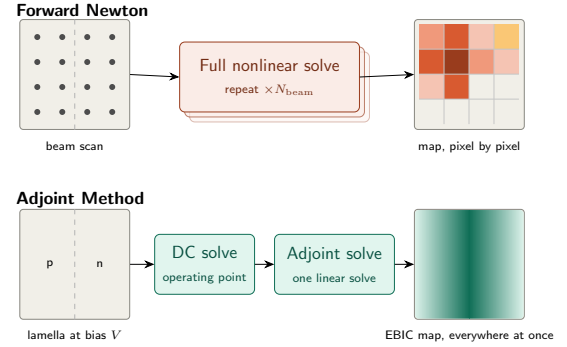


Fig. 1. Forward Newton (top) vs. the adjoint method (bottom). The direct approach performs one full nonlinear drift-diffusion solve per beam position, filling the EBIC map pixel-by-pixel at cost $\propto N_{\text{beam}}$. The adjoint method performs one nonlinear DC solve at the chosen bias, followed by a single linear solve per collecting contact, and recovers the EBIC map over the prescribed scan grid by source-adjoint inner products.

DD response around a biased operating point. More general transposed-system ideas originate from circuit sensitivity and noise analysis [4] and were later applied to multidimensional physics-based DD noise analysis [5]. These approaches suggest that the response to many localized generation sources can be evaluated from a single adjoint solution.

In this work, we formulate the linearized beam-induced STEM-EBIC response directly from the discretized, fully coupled DD system. Instead of solving the nonlinear DD equations separately for every beam position, the proposed method computes the beam-free DC operating point and then uses one adjoint solve per collecting contact to evaluate the EBIC response at all beam positions. This keeps the per-pixel evaluation inexpensive while preserving the fully coupled DD response at the selected bias. We verify the adjoint implementation against forward nonlinear beam-on Newton simulations and compare the zero-bias adjoint profile with an experimental STEM-EBIC profile. Runtime tests in one, two, and three dimensions show that eliminating the per-pixel nonlinear solve gives large practical speedups and makes bias-dependent 3D STEM-EBIC simulation feasible.

II. ADJOINT FORMULATION

At a fixed terminal bias, a STEM-EBIC scan changes the center of a finite electron-beam generation profile, while the device geometry, contacts, operating point, and measured

terminal-current functional remain fixed. The problem therefore has the many-sources/one-observable structure for which an adjoint formulation is especially effective. We formulate this response directly from the fully coupled drift–diffusion system linearized about the beam-free DC operating point.

After spatial discretization, the drift–diffusion equations and contact boundary conditions are written as a nonlinear residual system

$$\mathbf{F}(\mathbf{u}; \{V_k\}, \mathbf{s}) = \mathbf{0},$$

where $\mathbf{u}$ contains the electrostatic potential and carrier-density unknowns, $\{V_k\}$ denotes the applied terminal-bias vector, and $\mathbf{s}$ denotes an externally imposed generation source. For a chosen DC bias and in the absence of electron-beam excitation, the beam-free operating point is obtained from

$$\mathbf{F}(\mathbf{u}_0; \{V_k^0\}, \mathbf{0}) = \mathbf{0},$$

with

$$\mathbf{u}_0 = \begin{bmatrix} \psi_0 \\ \mathbf{n}_0 \\ \mathbf{p}_0 \end{bmatrix}, \quad (1)$$

where ψ_0 , $\mathbf{n}_0$, and $\mathbf{p}_0$ are the discretized electrostatic potential, electron density, and hole density, respectively.

An electron beam centered at position $\mathbf{r}_b$ introduces a localized electron–hole-pair generation profile $G_b(\mathbf{r}; \mathbf{r}_b)$. After discretization, this profile gives a sparse source vector $\mathbf{s}_b(\mathbf{r}_b)$, which enters the electron and hole continuity-equation rows at the mesh vertices affected by the beam. Here $\mathbf{s}_b$ is defined as the signed source contribution after moving the beam-generation term to the right-hand side of the linearized system. If the beam-induced perturbation is small relative to the DC operating point, the perturbed state can be written as

$$\mathbf{u} = \mathbf{u}_0 + \delta\mathbf{u}, \quad \delta\mathbf{u} = \begin{bmatrix} \delta\psi \\ \delta\mathbf{n} \\ \delta\mathbf{p} \end{bmatrix}. \quad (2)$$

Linearizing the drift–diffusion residual about $\mathbf{u}_0$ gives

$$\mathbf{J}_0 \delta\mathbf{u} = \mathbf{s}_b(\mathbf{r}_b), \quad \mathbf{J}_0 = \left. \frac{\partial \mathbf{F}}{\partial \mathbf{u}} \right|_{\mathbf{u}_0}. \quad (3)$$

Here, $\mathbf{J}_0$ is the full coupled drift–diffusion Jacobian at the selected bias point. The linearization therefore retains electrostatic coupling, carrier transport, recombination, and the derivatives of the contact boundary conditions included in the nonlinear DD residual. This is the standard first-order linearization used in physics-based DD noise analysis [5], with the electron-beam generation treated as the perturbing source. The approximation is valid as long as the beam-induced perturbation remains within the linear response of the chosen DC operating point.

For a collecting contact ℓ , the EBIC signal is the beam-induced change in terminal current. To first order,

$$\Delta I_\ell^{(1)}(\mathbf{r}_b) = \mathbf{c}_\ell^T \delta\mathbf{u}, \quad \mathbf{c}_\ell = \left. \frac{\partial I_\ell}{\partial \mathbf{u}} \right|_{\mathbf{u}_0}, \quad (4)$$

where I_ℓ is the terminal-current functional evaluated at contact ℓ . The adjoint field $\boldsymbol{\lambda}_\ell$ is defined by the transposed linear system

$$\mathbf{J}_0^T \boldsymbol{\lambda}_\ell = \mathbf{c}_\ell. \quad (5)$$

Substituting $\delta\mathbf{u} = \mathbf{J}_0^{-1} \mathbf{s}_b(\mathbf{r}_b)$ into Eq. (4) and using Eq. (5) gives

$$I_{\text{EBIC},\ell}^{(1)}(\mathbf{r}_b) \equiv \Delta I_\ell^{(1)}(\mathbf{r}_b) = \boldsymbol{\lambda}_\ell^T \mathbf{s}_b(\mathbf{r}_b). \quad (6)$$

The superscript (1) emphasizes that this is the first-order EBIC response about the beam-free DC operating point. For a given bias and collecting contact, $\mathbf{J}_0$, $\mathbf{c}_\ell$, and $\boldsymbol{\lambda}_\ell$ do not change during the scan; only the source vector $\mathbf{s}_b(\mathbf{r}_b)$ depends on the beam position. Thus, one nonlinear DC solve and one adjoint linear solve per collecting contact replace the sequence of nonlinear beam-on solves required by a direct scan. The remaining map evaluation consists only of source assembly and evaluation of the inner product between the adjoint solution and the source vector.

This structure is particularly well matched to STEM-EBIC: the beam source has finite spatial support and is sparse after discretization, the measured quantity is a scalar terminal current, and a typical scan contains many beam positions at the same device bias. If the LU factors of $\mathbf{J}_0$ from the converged DC Newton solve are retained, the transposed adjoint system can reuse the same factors and does not require an additional matrix factorization.

III. RESULTS

A. Simulation setup and bias-dependent EBIC maps

All simulations in this work were performed with an in-house drift–diffusion solver based on the finite-volume method. The governing system consists of Poisson’s equation and the electron and hole continuity equations. Electron and hole fluxes at the control-volume faces are discretized using the Scharfetter–Gummel scheme [6], and the resulting coupled nonlinear system is solved by a Newton–Raphson method. The mobilities are assumed constant. Carrier recombination is described by Shockley–Read–Hall (SRH)-type models [7], [8]; in the present simulations, the bulk-recombination model assumes midgap traps and uses doping-dependent carrier lifetimes given by the Scharfetter lifetime relation [9].

The electron-beam excitation is represented by a localized pair-generation profile $G_b(\mathbf{r}; \mathbf{r}_b)$. The profile is distributed over the prescribed beam cross section and extends along the transmitted beam path through the lamella thickness. The total generation rate is set by the experimental beam current and the stopping power of 200 keV electrons in silicon [10], [11].

As a representative test case, we consider a two-dimensional cross section of a Si p–n junction lamella with $N_D = N_A = 1 \times 10^{17} \text{ cm}^{-3}$ and a thickness of 300 nm, based on the FIB-prepared STEM-EBIC device structure of Schneider et al. [12]. The p- and n-terminals are treated as ideal ohmic contacts. The applied voltage V denotes the p-terminal bias relative to the grounded n-terminal. For the bias sweep $V = -2, -1, 0, +1, +2 \text{ V}$, the operating point and adjoint solution

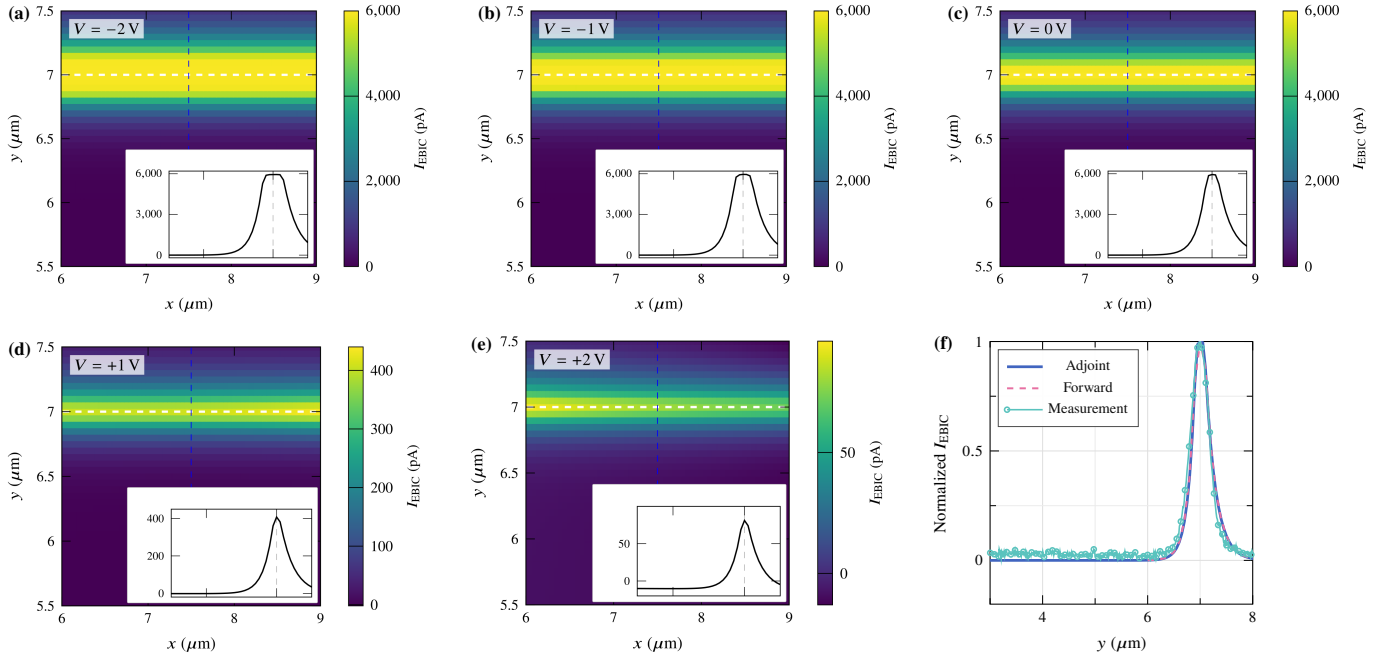


Fig. 2. Bias-dependent EBIC maps simulated by the adjoint method. Panels (a)–(e) show $V = -2, -1, 0, +1, +2$ V, respectively, applied at the p-terminal with the n-terminal grounded, zoomed to the junction region ($x \in [6, 9]$ μm , $y \in [5.5, 7.5]$ μm). The blue dashed line marks the vertical line cut at $x = 7.5$ μm ; the insets show the EBIC profiles obtained by scanning the beam along this line cut, and the white dashed line indicates the p–n junction. Panel (f) compares the zero-bias adjoint, forward Newton, and experimental profiles [12] along the same line cut.

are recomputed once at each bias, after which the EBIC map is obtained by source–adjoint inner products.

Fig. 2 shows a pronounced bias-dependent reshaping of the EBIC distribution around the p–n junction, with forward bias suppressing the collected current and reverse or zero bias retaining a high-collection region near the junction. Compared with a single zero-bias profile, such bias-dependent maps can provide additional sensitivity to junction electrostatics, including doping variations and the built-in potential [13]. At $V = 0$, the adjoint and forward Newton profiles agree to within a pA-

level absolute-current difference, and the normalized adjoint profile in Fig. 2(f) also follows the experimental measurement along the same vertical line cut, showing that the simulated collection profile is consistent with the measured STEM-EBIC signal.

B. Finite-injection validity

The adjoint relation in Eq. (6) is exact for the linearized drift–diffusion problem. To quantify the range over which this first-order response remains valid for a finite beam source, we use the same Si p–n junction lamella and bias points as in Sec. III-A and compare the adjoint prediction with full nonlinear beam-on simulations while scaling the nominal generation rate by $\alpha = G/G_{\text{nom}}$. For each $\alpha > 0$, the nonlinear EBIC increment divided by α is compared with the adjoint first-order prediction. We define the normalized first-order error as

$$\varepsilon_{1\text{st}}(\alpha, V) = \frac{\max_{\mathbf{r}_b} \left| \alpha^{-1} \Delta I_{\text{NL}}(\mathbf{r}_b; \alpha, V) - I_{\text{adj}}^{(1)}(\mathbf{r}_b; V) \right|}{\max_{\mathbf{r}_b} \left| I_{\text{adj}}^{(1)}(\mathbf{r}_b; V) \right|}. \quad (7)$$

Here ΔI_{NL} denotes the nonlinear beam-on terminal-current increment relative to the beam-free DC solution, and $I_{\text{adj}}^{(1)}$ denotes the first-order adjoint EBIC response. Because the mismatch is maximized over all beam positions, $\varepsilon_{1\text{st}}$ gives a conservative worst-position measure of finite-injection effects at each bias.

Fig. 3 shows the deviation between the scaled nonlinear beam-on response and the first-order adjoint response as the

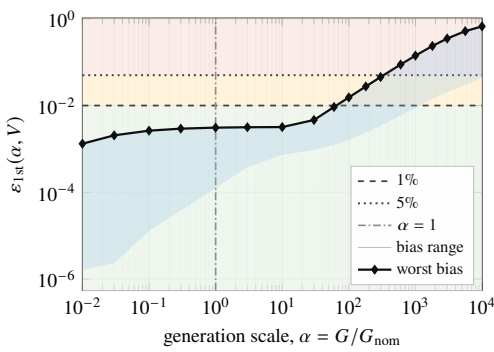


Fig. 3. Finite-injection validity of the linearized adjoint EBIC response. The normalized first-order error $\varepsilon_{1\text{st}}$ compares the scaled nonlinear beam-on current increment $\alpha^{-1} \Delta I_{\text{NL}}$ with the first-order adjoint prediction $I_{\text{adj}}^{(1)}$ as the generation amplitude is varied. The shaded band spans the tested bias range $V = -2, -1, 0, +1, +2$ V, and the solid curve gives the worst-bias envelope. The vertical dashed line marks the nominal generation level $\alpha = 1$; the horizontal dashed lines mark 1% and 5% error.

generation amplitude is varied. At the nominal beam strength, $\alpha = 1$, the error remains well below the percent level for all tested biases, indicating that the nominal STEM-EBIC source lies within the linear-response regime of the selected DC operating point. As α is increased, finite-injection effects gradually become visible and exceed the percent level only at substantially larger generation levels.

C. Runtime scaling

We next evaluate the computational scaling using representative wall-clock setup and per-position timings from the 1D, 2D, and 3D implementations. The absolute timings are hardware- and implementation-dependent; here they are used to parameterize the scaling model and to compare the direct and adjoint workflows under the same timing methodology. File I/O and device initialization are excluded from the reported timing estimates. The timing model is

$$T_{\text{fwd}}(N) = Nt_{\text{NL}}, \quad T_{\text{adj}}(N) = T_{\text{setup}} + Nt_{\text{pix}}, \quad (8)$$

where t_{NL} is the mean time for one direct nonlinear solve at a single beam position, T_{setup} is the one-time cost of obtaining the beam-free operating point and adjoint solution at the selected bias, and t_{pix} is the mean time for source assembly and adjoint inner-product evaluation. The solid curves in Fig. 4 show the projected cost of repeating the direct nonlinear Newton solve over N_{beam} positions, whereas the dashed curves show the adjoint timing model using the measured setup and per-position evaluation costs. The corresponding asymptotic speedups are obtained from the large- N limit

$$\lim_{N \rightarrow \infty} \frac{T_{\text{fwd}}(N)}{T_{\text{adj}}(N)} = \frac{t_{\text{NL}}}{t_{\text{pix}}},$$

giving 2×10^6 , 4×10^7 , and 5×10^8 for the tested 1D, 2D, and 3D cases, respectively. For finite maps, the realized speedups are smaller than these large- N limits because the adjoint runtime still includes the one-time setup cost. For the present 2D map ($N_{\text{beam}} = 48\,051$), the runtime is reduced from an estimated 8.8 days for the direct scan to 16 s with

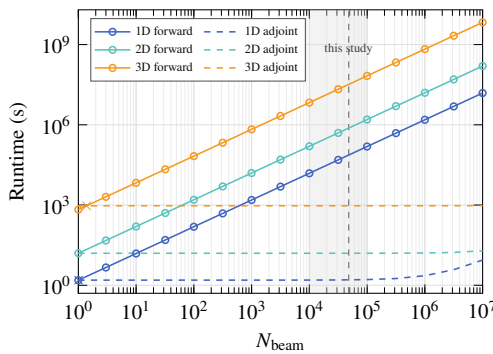


Fig. 4. Wall-clock runtime versus N_{beam} for forward Newton (solid) and adjoint (dashed) evaluation in 1D, 2D, and 3D. The shaded band marks the pixel-count range of typical STEM-EBIC maps; the vertical dashed line marks this work ($N_{\text{beam}} = 48\,051$). Over the STEM-EBIC pixel-count range shown, the adjoint runtime is dominated by the one-time setup cost because the per-pixel cost is negligible compared with a nonlinear beam-on solve.

the adjoint method. For the tested full-device 3D case, the same timing model projects approximately 376 days for the forward scan, whereas the adjoint method requires 16 min. These results show that the adjoint formulation shifts the dominant cost from repeated nonlinear beam-on solves to the one-time setup, enabling large bias-dependent STEM-EBIC maps to be computed efficiently.

IV. CONCLUSION

We presented a linearized adjoint drift-diffusion formulation for the first-order beam-induced STEM-EBIC response and applied it to a Si p-n junction lamella. At each selected DC bias, the method replaces N_{beam} nonlinear beam-on solves with one beam-free DC operating-point solve, one transposed linear solve per collecting contact, and N_{beam} source-adjoint inner products.

Direct nonlinear beam-on calculations verify the adjoint implementation, and the normalized zero-bias comparison with experiment shows that the simulated collection profile captures the measured STEM-EBIC line shape. The finite-injection sweep further shows that the nominal beam source remains in the first-order regime over the tested bias range.

The timing analysis shows that removing the per-pixel nonlinear solve shifts the dominant cost to the one-time setup, enabling efficient computation of quantitative, bias-dependent STEM-EBIC maps at experimentally relevant pixel counts.

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