Supporting Information

Optimizing and Understanding amorphous SiN Thin Film Deposition for GaN-High-Electron-Mobility Transistors Using Machine Learning and Causal Discovery

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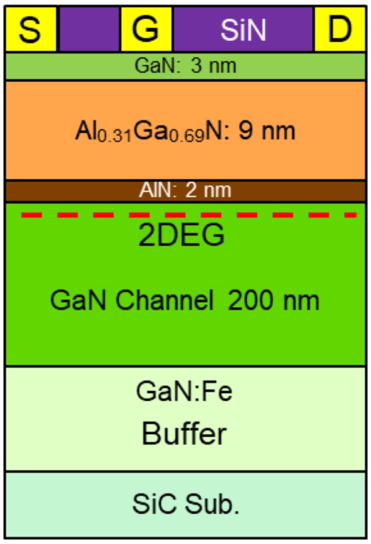

Figure S1. Cross section of the AlGaN/GaN high electron-mobility transistor (HEMT) structure used in this study.

Table S1. Predicted characteristic values and independent variables for 160 individuals selected via genetic algorithm (GA) evaluation. The model used for prediction was constructed from the initial seven datasets. The individual No. 56 (marked in green) represents condition (i), and the individual No. 4 (marked in blue) denotes condition (ii).

Individual number	V_{SiH4} (SCCM)	P_{RF} (W)	T_{anneal} (°C)	t_{anneal} (min.)	V_{BD} ($\mathrm{V\cdot nm^{-1}}$)	ΔV (V)	R_{sh} ($\Omega\cdot\mathrm{sq.}^{-1}$)
1	2.3	30	700	0	0.8	0.2	352
2	0.8	60	676	24	2.6	4.2	618
3	1.4	58	700	0	1.6	2.1	418
4	1.6	37	699	11	1.3	2.4	405
5	1.4	60	700	4	1.8	2.3	445
6	1.4	59	698	5	1.8	2.4	450
7	2.2	30	700	2	0.8	0.3	351
8	1.3	58	675	18	2.2	3.3	529
9	1.4	60	698	6	1.8	2.4	458
10	0.8	61	676	25	2.6	4.2	607
11	1.1	59	700	30	2.4	3.9	543
12	1.3	58	698	3	1.7	2.3	435
13	1.3	60	687	19	2.2	3.4	539
14	1.3	58	700	14	2.1	3.0	517
15	1.6	35	693	11	1.3	2.2	395
16	0.8	61	683	28	2.5	4.2	590
17	1.1	61	692	35	2.3	4.0	525
18	1.4	60	699	2	1.7	2.2	431
19	1.1	58	700	31	2.3	4.0	537
20	1.3	58	686	14	2.2	3.1	524
21	2.1	30	698	4	0.9	0.5	353
22	1.6	34	700	13	1.3	2.4	399
23	1.8	30	700	11	1.1	1.7	380
24	1.9	30	698	6	1.0	1.0	361
25	2.1	30	699	1	0.8	0.4	350
26	1.7	31	697	9	1.1	1.8	378
27	1.4	59	698	8	1.9	2.5	469
28	1.9	30	699	7	1.0	1.1	364
29	1.4	59	698	1	1.6	2.2	421
30	1.6	34	680	13	1.3	2.5	400
31	0.9	58	680	31	2.5	4.2	564
32	2.0	30	699	6	0.9	0.8	359
33	1.4	58	698	1	1.6	2.2	424
34	1.4	60	698	12	2.0	2.8	498
35	2.1	30	699	3	0.9	0.4	352
36	1.4	61	698	19	2.2	3.3	526
37	1.3	61	698	20	2.3	3.4	546
38	1.7	36	700	13	1.3	2.3	402
39	1.2	58	699	31	2.3	3.9	527
40	1.7	34	680	13	1.2	2.0	394
41	1.4	60	700	11	2.0	2.8	489
42	1.3	60	698	18	2.3	3.3	544
43	2.1	30	699	6	0.9	0.6	356
44	1.4	60	698	20	2.2	3.4	531
45	1.7	32	700	10	1.1	1.8	380
46	0.8	60	683	27	2.5	4.2	593
47	0.9	60	684	28	2.5	4.2	587
48	1.1	60	684	29	2.4	4.0	549
49	1.4	59	700	2	1.6	2.2	427
50	2.1	30	699	4	0.9	0.5	353
51	1.4	60	700	11	2.0	2.7	491
52	2.0	30	699	4	0.9	0.7	355
53	1.6	35	700	11	1.2	2.2	394
54	0.8	61	678	24	2.6	4.2	617
55	1.4	59	700	9	1.9	2.6	481
56	1.4	59	698	2	1.7	2.2	430
57	1.3	59	696	14	2.1	3.0	520
58	1.4	58	686	9	1.9	2.6	478
59	1.3	60	699	18	2.2	3.3	537
60	1.6	31	697	12	1.2	2.2	389
61	1.4	60	698	12	2.0	2.8	499
62	1.3	58	700	14	2.1	3.0	515
63	1.9	30	697	10	1.0	1.3	372
64	1.4	60	697	7	1.9	2.5	467
65	0.9	61	687	33	2.4	4.2	548
66	1.4	60	698	11	2.0	2.8	496
67	1.0	61	679	30	2.5	4.1	562
68	1.4	60	698	12	2.0	2.8	501
69	1.6	34	700	12	1.3	2.3	395
70	1.4	60	700	3	1.7	2.3	439
71	1.2	59	700	28	2.4	3.9	550
72	1.4	59	698	4	1.7	2.3	443
73	1.4	61	698	3	1.7	2.3	438
74	1.8	30	700	10	1.1	1.6	378
75	2.1	30	698	6	0.9	0.6	357
76	1.3	59	696	14	2.1	3.0	520
77	1.1	60	700	30	2.4	4.0	545
78	1.9	30	678	9	1.0	1.2	370
79	1.7	32	699	11	1.2	1.9	384
80	1.4	60	682	8	1.9	2.6	475
81	1.1	61	694	27	2.4	3.9	564
82	1.7	33	699	11	1.2	2.0	388
83	1.0	62	680	31	2.4	4.1	558
84	2.2	30	700	0	0.8	0.2	351
85	1.4	58	699	2	1.7	2.2	428
86	1.4	60	697	8	1.9	2.5	471
87	1.4	60	698	20	2.2	3.4	531
88	1.0	62	698	35	2.3	4.1	530
89	1.4	61	700	7	1.8	2.4	461
90	1.0	62	698	31	2.4	4.1	557
91	1.4	60	696	6	1.8	2.4	455
92	1.2	63	700	29	2.3	3.9	537
93	1.9	30	676	7	1.0	1.2	366
94	1.4	59	698	1	1.6	2.2	423
95	1.4	60	700	8	1.9	2.6	474
96	1.9	30	700	7	1.0	1.1	365
97	1.4	58	698	10	2.0	2.7	487
98	1.7	30	700	7	1.1	1.7	372
99	0.9	62	681	29	2.5	4.1	575
100	2.1	30	699	3	0.9	0.4	351
101	1.4	58	697	6	1.8	2.4	453
102	1.9	30	700	6	1.0	1.0	362
103	1.3	60	698	13	2.1	2.9	511
104	2.0	30	700	4	0.9	0.8	357
105	1.7	32	699	7	1.1	1.7	375
106	1.4	60	700	4	1.7	2.3	441
107	1.4	60	698	3	1.7	2.3	438
108	0.9	60	674	29	2.5	4.2	576
109	1.0	61	698	30	2.5	4.1	561
110	1.3	61	699	18	2.2	3.3	538
111	1.3	60	683	13	2.1	2.9	512
112	1.7	32	697	9	1.1	1.9	380
113	1.4	60	700	5	1.8	2.4	452
114	2.0	30	698	3	0.9	0.8	355
115	1.6	32	698	12	1.2	2.2	390
116	1.3	60	692	16	2.2	3.1	526
117	0.9	59	681	29	2.5	4.1	576
118	1.4	57	692	13	2.0	2.9	502
119	1.9	30	698	5	1.0	0.9	359
120	1.3	60	694	15	2.2	3.1	524
121	0.9	60	679	29	2.5	4.2	578
122	1.1	60	700	28	2.4	3.9	556
123	1.4	59	699	11	2.0	2.7	493
124	1.0	62	680	29	2.5	4.1	573
125	1.7	32	700	12	1.2	1.9	387
126	1.7	32	697	9	1.1	1.9	380
127	1.2	59	699	25	2.4	3.8	562
128	1.4	58	689	10	1.9	2.7	481
129	1.3	60	687	26	2.3	3.7	536
130	1.3	59	691	15	2.2	3.1	526
131	1.4	59	698	7	1.9	2.5	462
132	0.8	61	694	27	2.5	4.2	598
133	1.9	30	699	11	1.1	1.3	375
134	1.8	31	698	9	1.1	1.4	374
135	1.9	30	699	11	1.1	1.3	375
136	2.1	30	698	6	0.9	0.6	357
137	1.6	37	699	11	1.3	2.4	405
138	1.8	30	699	8	1.0	1.4	369
139	1.4	57	699	10	2.0	2.7	486
140	1.4	58	698	10	2.0	2.7	483
141	1.3	58	689	15	2.2	3.1	528
142	1.3	58	698	13	2.1	2.9	508
143	1.6	32	698	12	1.2	2.2	391
144	1.7	31	699	12	1.2	1.9	384
145	1.3	60	698	4	1.7	2.3	442
146	2.0	30	698	6	1.0	0.9	360
147	1.7	33	698	11	1.2	2.0	387
148	1.7	34	699	11	1.2	2.1	389
149	1.4	59	698	9	1.9	2.6	477
150	1.6	34	700	12	1.3	2.3	397
151	1.7	32	698	12	1.2	2.0	388
152	1.3	58	688	15	2.2	3.1	529
153	0.8	62	679	29	2.5	4.2	580
154	1.3	58	700	12	2.1	2.9	507
155	1.7	34	699	9	1.2	2.0	385
156	0.8	61	676	26	2.6	4.2	603
157	1.4	60	698	12	2.0	2.8	494
158	1.2	59	676	30	2.3	4.0	537
159	1.4	60	698	13	2.1	2.9	503
160	1.9	30	699	7	1.0	1.1	365

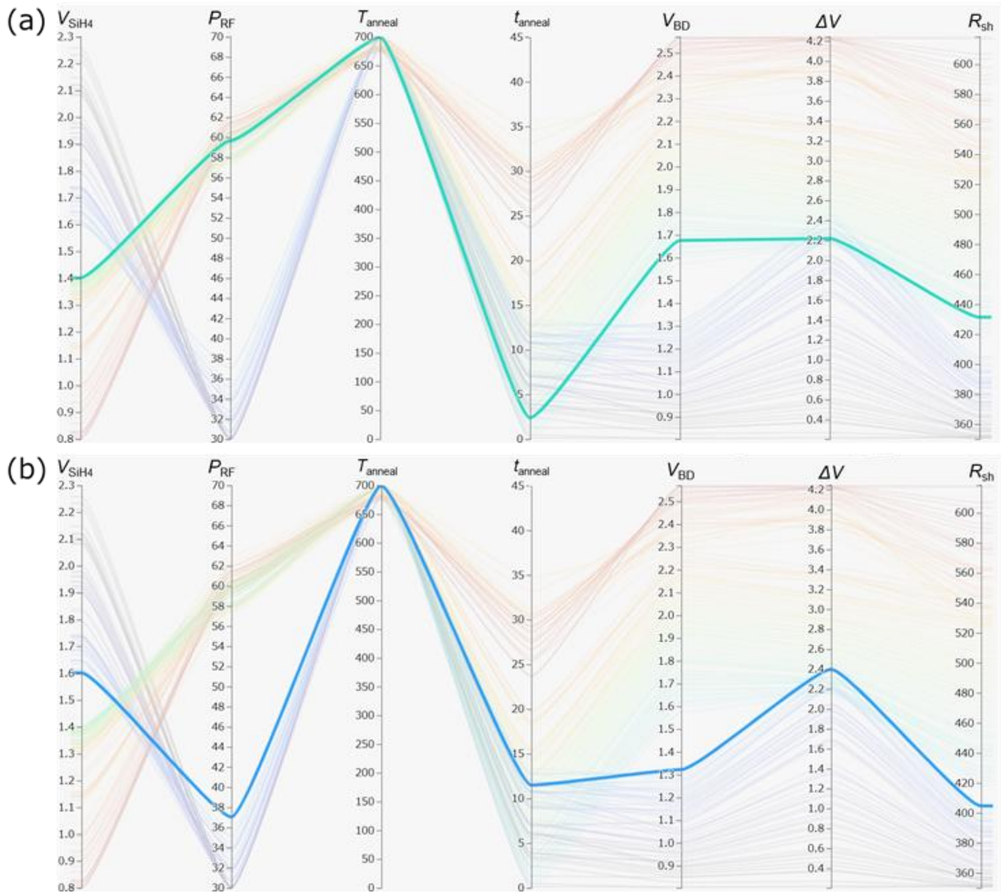

Figure S2. Predicted characteristics for recommended conditions: (a) Condition (i): V_{SiH4}: 1.4 SCCM, P_{RF}: 60 W, T_{anneal}: 700 °C, and t_{anneal}: 2 min. Predicted characteristics: V_{BD}: 1.7 V·nm^{-1}, ΔV: 2.2 V, and R_{sh}: 430 Ω·sq^{-1} (Individual No. 56). (b) Condition (ii): V_{SiH4}: 1.6 SCCM, P_{RF}: 37 W, T_{anneal}:_700 °C, and t_{anneal}: 2 min. Predicted characteristics: V_{BD}: 1.3 V·nm^{-1}, ΔV: 2.4 V, and R_{sh}: 404 Ω·sq^{-1} (Individual No. 4). Condition (iii): *Note: Not shown in figure*. Intermediate values of independent variables from conditions (i) and (ii): V_{SiH4}: 1.5 SCCM, P_{RF}: 49 W, T_{anneal}: 700°C, and t_{anneal}: 7 min.

Table S2. Predicted characteristic values and independent variables for 160 individuals selected via GA evaluation. The model used for prediction was constructed from 10 data sets.

Individual number	V_{SiH4} (SCCM)	P_{RF} (W)	T_{anneal} (°C)	t_{anneal} (min.)	V_{BD} ($V \cdot nm^{-1}$)	ΔV (V)	R_{sh} ($\Omega \cdot sq.^{-1}$)
1	1.0	61	701	21	2.3	3.2	622
2	2.2	30	701	1	0.7	0.2	359
3	1.4	63	701	8	2.3	2.6	493
4	1.2	61	701	15	2.3	3.1	557
5	1.6	38	701	11	1.2	1.6	369
6	2.0	58	701	1	1.4	1.2	388
7	1.5	62	701	7	2.3	2.5	484
8	1.9	59	701	1	1.7	1.5	403
9	2.0	32	701	4	0.7	0.5	361
10	1.1	61	701	16	2.3	3.2	565
11	2.1	30	701	1	0.7	0.5	358
12	1.9	59	701	1	1.6	1.2	398
13	1.7	36	701	9	1.1	0.9	366
14	1.5	60	700	2	2.1	1.3	454
15	1.9	59	701	1	1.6	1.2	396
16	1.9	33	701	5	0.8	0.6	361
17	1.6	38	701	11	1.2	1.5	370
18	1.5	61	701	2	2.1	1.3	457
19	1.0	59	701	19	2.3	3.3	599
20	1.5	61	701	3	2.1	1.4	462
21	1.9	33	701	5	0.8	0.6	361
22	1.6	38	701	11	1.2	1.2	369
23	1.5	61	701	5	2.2	1.8	465
24	1.9	35	701	6	0.9	0.7	361
25	1.7	36	701	8	1.0	0.9	365
26	1.8	35	701	8	1.0	0.8	364
27	1.7	37	699	9	1.1	0.9	367
28	1.8	59	701	1	1.8	1.7	411
29	1.8	59	701	1	1.9	1.8	411
30	1.6	37	701	9	1.2	1.1	367
31	1.5	62	701	5	2.2	1.6	479
32	1.8	59	701	1	1.8	1.7	409
33	1.5	61	701	3	2.1	1.2	467
34	1.9	59	701	1	1.8	1.6	408
35	1.6	38	701	11	1.2	1.4	370
36	1.6	37	701	10	1.2	1.3	368
37	1.9	59	701	1	1.7	1.4	402
38	1.6	36	701	10	1.1	0.9	368
39	1.8	59	701	1	1.8	1.6	409
40	1.9	34	701	6	0.8	0.6	362
41	2.0	33	701	5	0.8	0.5	361
42	1.8	35	701	7	0.9	0.7	362
43	1.5	62	701	6	2.3	2.2	479
44	1.0	61	701	21	2.3	3.2	618
45	1.8	35	701	7	1.0	0.8	363
46	1.6	38	701	10	1.2	1.1	368
47	1.7	58	701	1	2.0	1.8	423
48	1.9	58	701	1	1.6	1.3	395
49	1.0	58	701	20	2.3	3.3	590
50	1.5	61	701	3	2.1	1.4	459
51	1.0	58	701	21	2.3	3.3	588
52	1.5	61	701	4	2.2	1.6	461
53	1.5	61	701	2	2.1	1.2	461
54	1.5	60	701	3	2.1	1.4	457
55	1.9	58	701	1	1.7	1.5	401
56	2.0	33	701	4	0.7	0.5	360
57	2.1	31	701	1	0.7	0.3	358
58	2.1	30	701	1	0.7	0.5	358
59	1.6	38	701	11	1.2	1.5	369
60	1.5	61	701	5	2.2	1.8	473
61	1.0	58	701	20	2.3	3.3	592
62	1.9	58	701	1	1.6	1.3	397
63	1.5	62	701	6	2.3	2.0	482
64	1.8	58	701	1	1.8	1.7	406
65	1.0	60	701	20	2.3	3.3	607
66	1.2	62	701	15	2.3	3.1	565
67	1.5	62	701	5	2.2	1.8	477
68	2.0	58	701	1	1.5	1.2	389
69	1.6	36	701	10	1.1	0.9	368
70	1.9	59	701	1	1.6	1.2	397
71	1.9	59	701	1	1.7	1.5	405
72	1.6	37	701	9	1.1	1.0	367
73	1.8	35	701	7	1.0	0.8	363
74	1.5	62	701	5	2.2	1.7	479
75	1.5	60	701	4	2.2	1.7	454
76	1.0	57	701	19	2.3	3.4	577
77	1.5	61	701	6	2.2	2.1	474
78	1.5	61	701	2	2.1	1.4	457
79	1.7	35	701	8	1.0	0.8	364
80	2.0	32	701	4	0.7	0.5	361
81	1.9	59	701	1	1.6	1.2	395
82	1.9	58	701	1	1.7	1.4	399
83	1.8	58	701	1	1.9	1.9	413
84	1.6	60	701	1	2.0	1.7	437
85	1.9	34	701	6	0.8	0.7	361
86	1.7	58	701	1	2.0	1.8	418
87	1.6	38	701	10	1.2	1.4	368
88	1.9	59	700	1	1.7	1.6	405
89	1.7	58	701	1	1.9	1.9	416
90	1.8	35	701	7	0.9	0.7	363
91	1.1	61	701	17	2.3	3.2	581
92	1.5	62	701	7	2.3	2.4	484
93	1.7	36	701	9	1.1	0.9	366
94	1.7	35	701	7	1.0	0.9	363
95	1.6	59	701	1	2.0	1.7	432
96	1.4	61	701	4	2.2	1.3	469
97	1.5	62	701	7	2.3	2.3	482
98	1.5	62	701	6	2.3	2.1	482
99	1.0	58	701	21	2.3	3.3	597
100	2.0	58	701	1	1.5	1.2	390
101	1.9	59	701	1	1.6	1.3	399
102	1.7	36	701	9	1.1	0.9	366
103	1.1	60	701	17	2.3	3.2	578
104	1.7	36	701	8	1.0	0.8	365
105	1.0	60	701	20	2.3	3.2	611
106	1.8	59	701	1	1.9	1.8	413
107	1.6	59	701	1	2.0	1.7	434
108	2.0	58	701	1	1.5	1.2	391
109	1.7	58	701	1	2.0	1.8	419
110	1.8	59	701	1	1.9	1.8	412
111	1.9	58	701	1	1.5	1.2	393
112	1.8	58	701	1	1.8	1.6	405
113	1.9	58	701	1	1.6	1.3	397
114	1.9	59	701	1	1.7	1.4	402
115	1.7	58	701	1	2.0	1.8	420
116	1.8	35	701	7	0.9	0.7	363
117	1.5	62	701	5	2.2	1.9	479
118	2.0	59	701	1	1.5	1.1	393
119	1.7	58	701	1	1.9	1.9	415
120	1.8	35	701	7	0.9	0.7	362
121	1.0	60	701	21	2.3	3.2	613
122	1.5	61	701	4	2.2	1.5	470
123	1.7	36	701	8	1.0	0.8	365
124	1.9	59	701	1	1.6	1.3	400
125	1.1	62	701	16	2.3	3.2	574
126	1.9	34	701	5	0.8	0.6	361
127	1.5	61	701	6	2.3	2.3	471
128	2.1	31	701	1	0.7	0.3	358
129	1.8	59	701	1	1.8	1.8	411
130	2.0	58	701	1	1.4	1.2	388
131	1.6	37	701	10	1.2	1.0	367
132	1.1	61	701	16	2.3	3.3	567
133	2.0	59	701	1	1.5	1.1	394
134	1.0	60	701	20	2.3	3.3	607
135	1.5	61	701	5	2.2	1.8	464
136	1.9	34	701	6	0.9	0.7	362
137	1.6	59	701	1	2.0	1.7	431
138	1.9	58	701	1	1.7	1.6	404
139	1.9	59	701	1	1.7	1.4	402
140	1.9	34	701	6	0.8	0.6	361
141	1.7	58	701	1	1.9	1.9	414
142	1.6	38	701	10	1.2	1.1	368
143	1.8	58	701	1	1.9	1.9	411
144	1.9	58	701	1	1.7	1.4	399
145	2.0	58	701	1	1.5	1.2	391
146	1.5	61	701	4	2.2	1.6	468
147	1.5	61	701	4	2.2	1.5	469
148	1.5	61	701	4	2.2	1.8	464
149	1.5	62	701	5	2.2	1.9	479
150	1.5	62	701	7	2.3	2.3	487
151	1.4	61	701	4	2.2	1.3	469
152	1.6	38	701	11	1.2	1.3	369
153	1.8	58	701	1	1.8	1.6	405
154	2.0	59	701	1	1.5	1.1	394
155	1.6	58	701	1	2.0	1.8	426
156	2.0	32	701	4	0.7	0.5	361
157	1.8	35	701	7	0.9	0.7	364
158	1.1	61	701	16	2.3	3.3	568
159	1.5	62	701	7	2.3	2.2	484
160	1.1	61	701	17	2.3	3.2	578

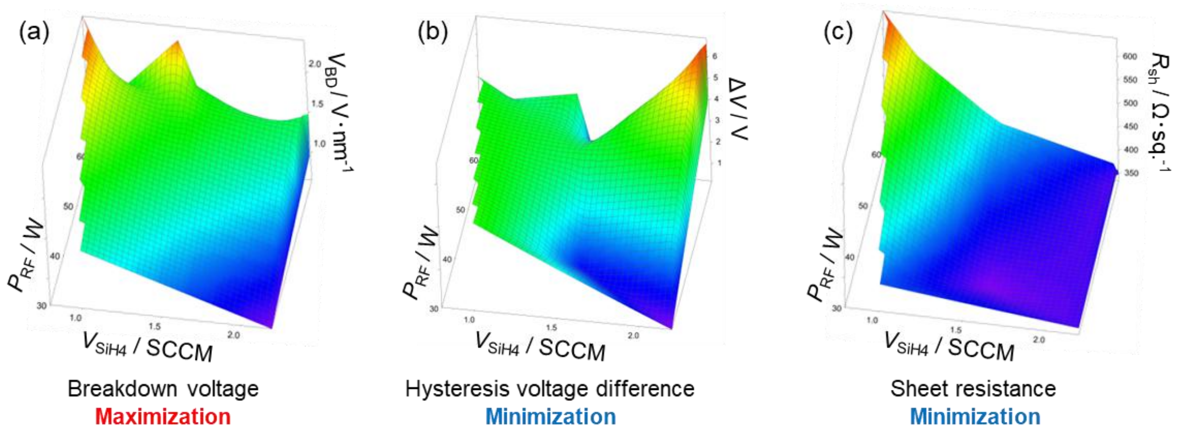

Figure S3. Heatmaps of each objective function. The axes represent the main independent parameters, V_{SiH4} and P_{RF}, using data from 700 °C annealing. The optimization directions are as follows: (a) maximize breakdown voltage, (b) minimize hysteresis voltage difference, (c) minimize sheet resistance.

Table S3. Data sets comprising intermediate variable information for 10 samples.

Sample No.	V_{SiH4} (SCCM)	P_{RF} (W)	T_{anneal} (°C)	t_{anneal} (min.)	n	Ns (cm^{-2})	μ_{2DEG} ($cm^2 \cdot V^{-1} \cdot s^{-1}$)	ρ ($g \cdot cm^{-3}$)	$I_{Si–N}$ (a. u.)	$v_{Si–N}$ (cm^{-1})	$I_{N–H}$ (a. u.)	$v_{N–H}$ (cm^{-1})	$\Delta\lambda_{N–H}$ (cm^{-1})	$I_{Si–H}$ (a. u.)	$v_{Si–H}$ (cm^{-1})	$\sigma_{in\text{-}plane}$ (MPa)	V_{BD} ($V \cdot nm^{-1}$)	ΔV (V)	R_{sh} ($\Omega \cdot sq.^{-1}$)
1	2.2	60	350	45	2.011	9.00E+12	2069	2.52	0.0689	833.1	0.0025	3349.8	138	0.0062	2173.4	-620	1.6	7.1	346
2	2.2	60	700	1	2.047	9.40E+12	1963	2.57	0.0712	837	0.0019	3357.5	125.25	0.0027	2177.2	-356	1	3.9	369
3	1.5	60	700	1	1.902	8.50E+12	1930	2.6	0.0733	844.7	0.0028	3338	138.302	0.0011	2179.2	-1451	1.7	0.6	428
4	1	60	700	1	1.805	7.10E+12	1566	2.6	0.055	873.6	0.0055	3336	167.845	0	2180	-2887	1.5	3.2	552
5	2.2	30	700	1	2.311	8.00E+12	2128	2.58	0.076	833.1	0.0018	3334.3	151.715	0.00364	2165.7	-2510	0.7	0.2	349
6	1	30	700	1	1.887	9.50E+12	2027	2.58	0.071	848.5	0.0033	3349.7	156.6	0.00075	2183	-3432	1.4	4.4	393
7	0.8	60	685	15	1.794	7.00E+12	1567	2.6	0.052	883.2	0.0052	3332	150.059	0	2180	-4967	2.4	4.1	641
8	1.4	60	700	2	1.885	8.00E+12	1762	2.6	0.0513	819	0.0128	3451	91.074	0	2180	767	2.2	3.7	450
9	1.6	37	700	11	2.087	9.00E+12	2055	2.55	0.058	815.7	0.0117	3448	91.584	0	2180	-219	1.2	1	334
10	1.5	49	700	7	1.941	8.39E+12	2036	2.59	0.054	817.7	0.0123	3448	91.68	0	2180	-2438	1.6	3.6	380

Table S4. Summary of causal strengths. Bold values represent causal influences included in the causal graph. Leftmost column shows source variables, and top row displays the target variables.

		Independent variable				Intermediary variable												Objective function		
		V_{SiH4}	T_{anneal}	P_{RF}	t_{anneal}	n	N_s	μ_{2DEG}	ρ	$I_{Si–H}$	$v_{Si–H}$	$I_{N–H}$	$v_{N–H}$	$\Delta\lambda_{N–H}$	$I_{Si–N}$	$v_{Si–N}$	$\sigma_{in\text{-}plane}$	V_{BD}	ΔV	R_{sh}
Independent variable	V_{SiH4}	0	0	0	0	**0.76**	**0.36**	**0.56**	**-0.93**	**0.54**	**0.79**	0	**1.73**	0	**1.46**	0	**0.31**	**-1.71**	0	**-0.76**
	T_{anneal}	0	0	0	0	**1.02**	**1.15**	0	**0.64**	**-0.6**	**-0.27**	0	**-0.86**	**-0.47**	**-1.5**	0	**-0.95**	**0.47**	**-0.28**	**0.52**
	P_{RF}	0	0	0	0	**-0.47**	**-0.62**	**-0.27**	**0.54**	**0**	**-0.34**	0	**-0.25**	0	**-0.5**	0	**0.58**	**0.56**	0	**0.35**
	t_{anneal}	0	0	0	0	**0.46**	**0.61**	**0.25**	**-0.48**	0	0	0	**0.75**	**-1.13**	**-0.57**	0	**-1.45**	**1.54**	**-0.74**	**0.42**
Intermediary variable	n	0	0	0	0	0	-1.03	0	-0.29	0	-0.59	0	0	-0.54	0	0	0	**0.71**	**-0.93**	0
	N_s	0	0	0	0	0	0	0	-0.27	0	0	0	0	-0.51	0	0	0	**0.73**	**1**	0
	μ_{2DEG}	0	0	0	0	0	0.66	0	0	0	0	0	0	0	0	0	0	**-0.75**	0	**-0.61**
	ρ	0	0	0	0	0	0	0	0	0	0	0	0	-0.72	0	0	0	**1.14**	0	0
	$I_{Si–H}$	0	0	0	0	0.74	0.78	-0.44	0.45	0	-0.99	0	-2.91	0.42	-1.71	-0.45	1.62	0	**1.31**	0
	$v_{Si–H}$	0	0	0	0	0	1.01	0	-0.61	0	0	0	0	0	0	0	0	**-0.68**	**-0.59**	**-0.38**
	$I_{N–H}$	0	0	0	0	1.44	-1.63	0	0	0	0	0	0	0	0	-0.69	2.16	**-0.5**	**-0.65**	0
	$v_{N–H}$	0	0	0	0	-0.82	0.64	0	-0.29	0	0.45	0.71	0	-0.34	-0.89	-0.68	3.97	0	0	0
	$\Delta\lambda_{N–H}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	$I_{Si–N}$	0	0	0	0	0.49	0	0.63	-0.31	0	-0.41	-0.34	0	0.33	0	-0.81	3.33	**-0.43**	**-2.06**	**-0.29**
	$v_{Si–N}$	0	0	0	0	0.42	-0.25	-0.6	-1.01	0	0.55	0	0	0.36	0	0	4	**-0.97**	**-0.56**	0
	$\sigma_{in\text{-}plane}$	0	0	0	0	0	0.5	-0.38	-0.33	0	0	0	0	0	0	0	0	0	**-0.4**	0
Objective function	V_{BD}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	ΔV	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	R_{sh}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

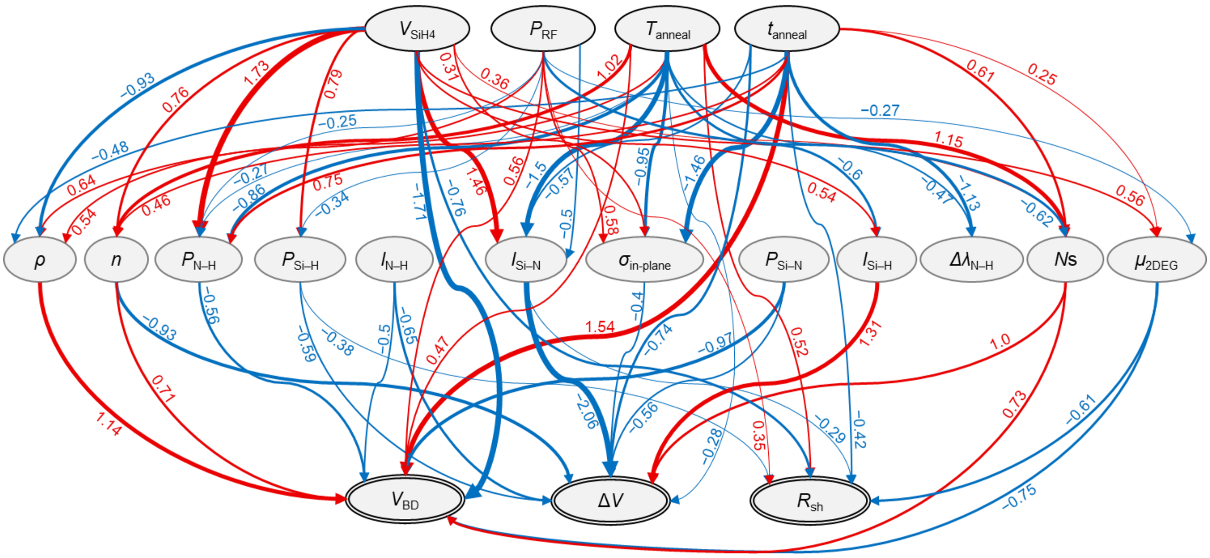

Figure S4. Causal graph derived from the 10 experimental data sets. Positive correlations are indicated in red, and negative correlations are represented in blue. Relationships between intermediate variables are not shown.