Materials Informatics at NASA GRC

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Material Informatics

It takes 20 years to go from material discovery to commercial use [1,2]

Materials Genome Initiative– is a federal initiative for discovering, manufacturing, and deploying advanced materials twice as fast and at a fraction of the cost compared to traditional methods. Announced by Obama in 2011. Thanks Obama!

Material Informatics – application of informatics (statistics, data science, machine learning, AI, etc.) to materials science and engineering to improve the understanding, development, and discovery of materials.

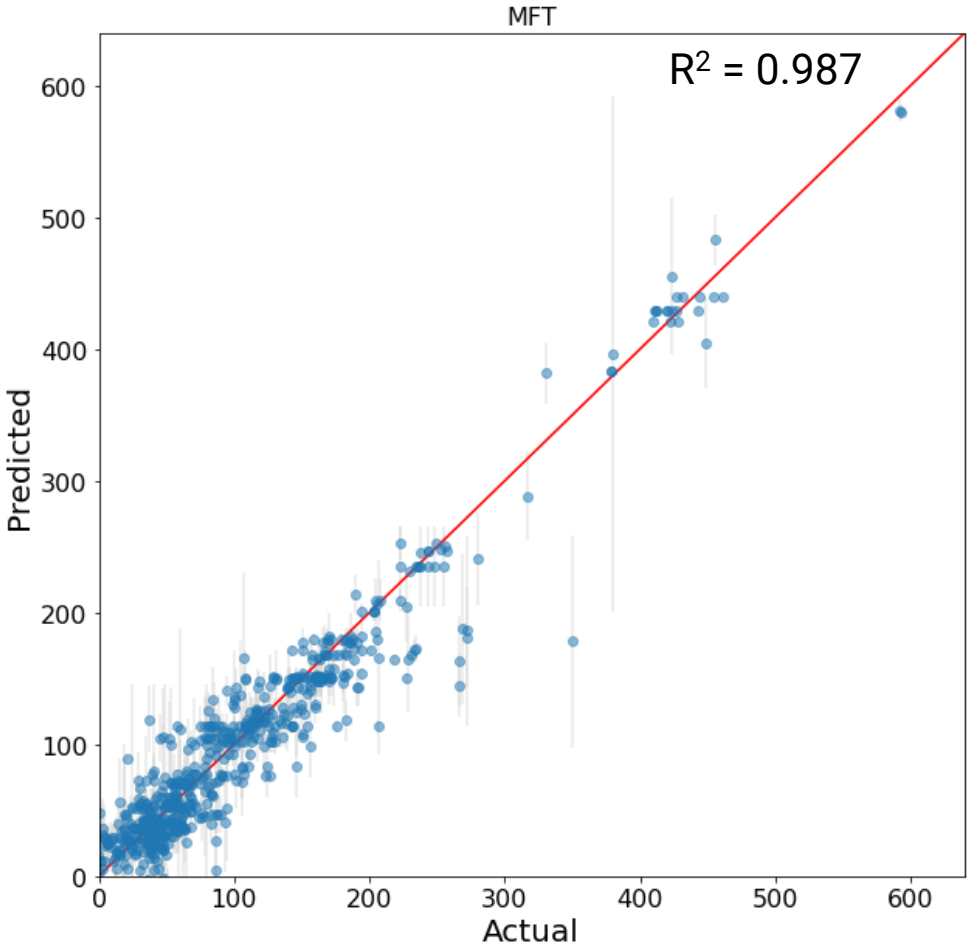
[1] Faster: Accelerating the transition from materials discovery to commercial deployment. Alexander H. King. https://www.osti.gov/pages/servlets/purl/1556925
[2] T.W. Eagar, Technology Review, 98, 43 (1995)

Predictive Models

Shape Memory Alloys

- Continuous features
  - Ni %
  - Ti %
  - Element 3 %
  - Element 4 %
  - Heat treat 1 time
  - Heat treat 1 temp
  - Heat treat 2 time
  - Heat treat 2 temp
  - Heat treat 3 time
  - Heat treat 3 temp
  - Lower Cycle Temperature
  - Higher Cycle Temperature
  - Austenite Start temp
  - Austenite finish temp
  - Martensite start temp
  - Martensite finish temp
- Categorical features
  - Element 3
  - Element 4
  - Test type
  - Processing method

Martensite Finish Temperature



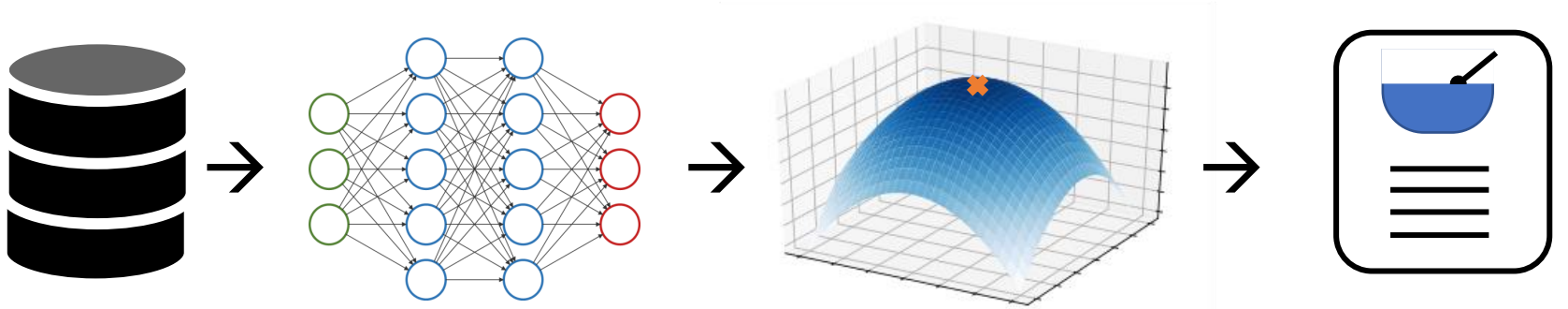
Inverse Design

Processing → Properties
Properties → Processing

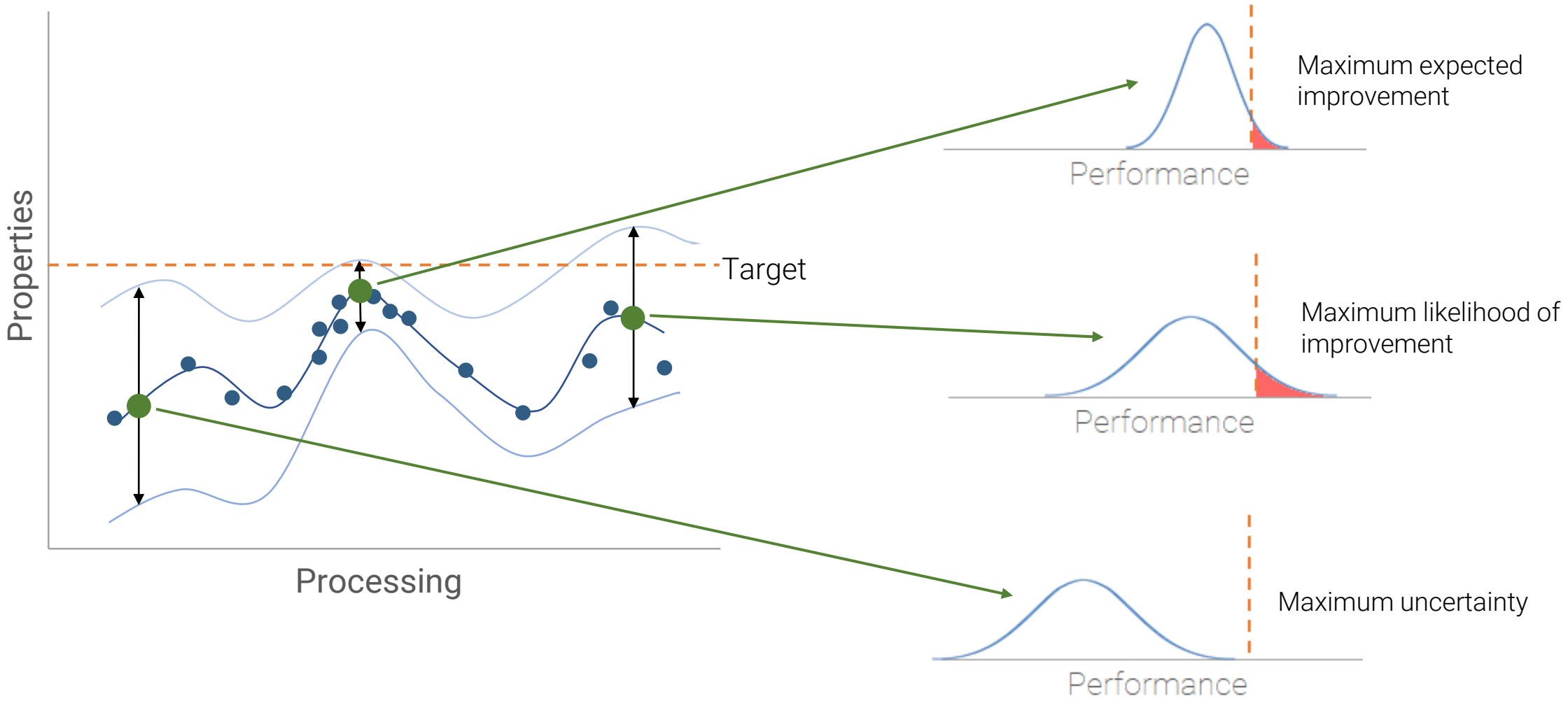
x y

$$y = F(x)$$

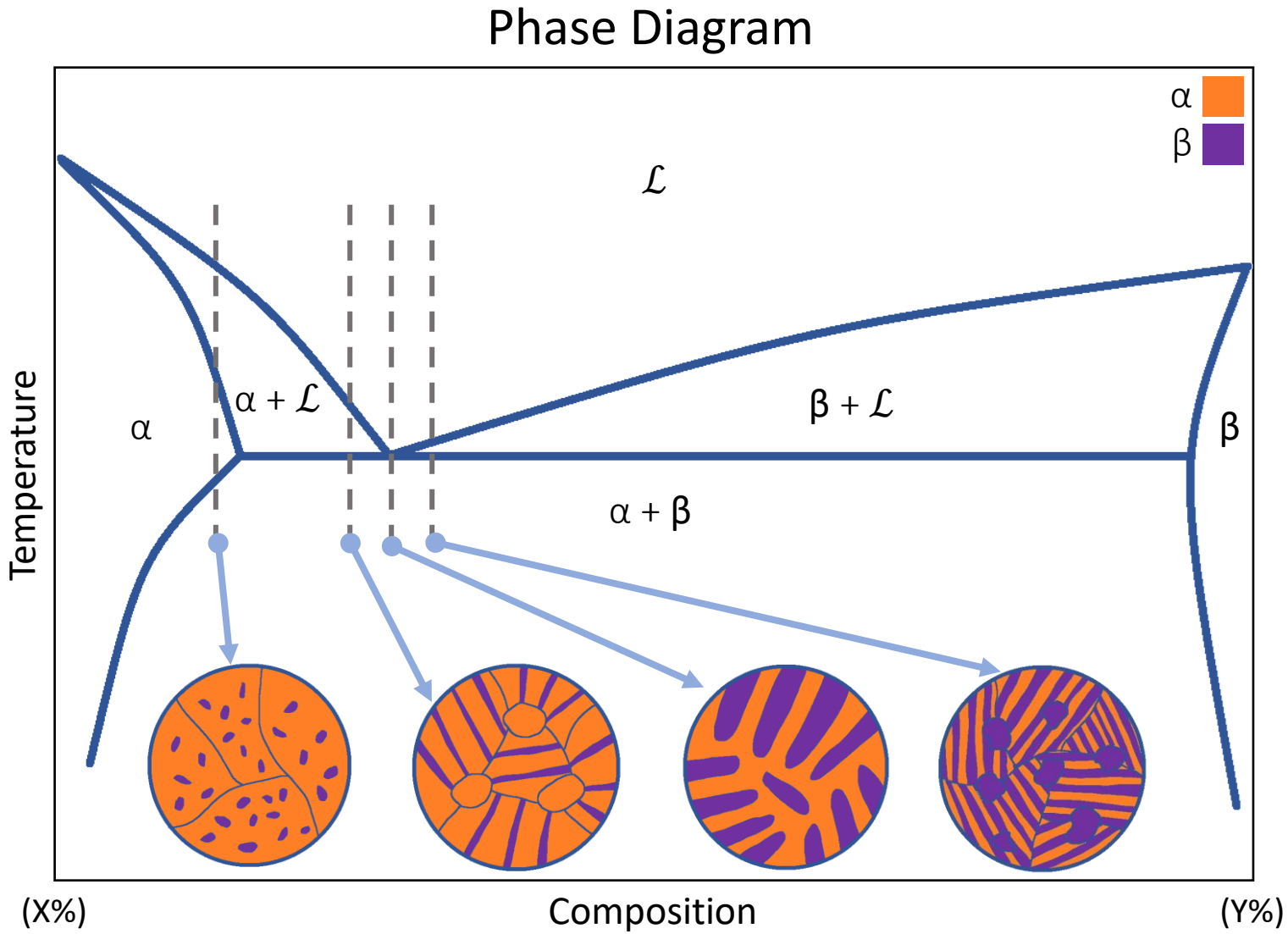
processing: $x^* = \text{argmax}(F(x))$



Sequential Learning



Microstructure

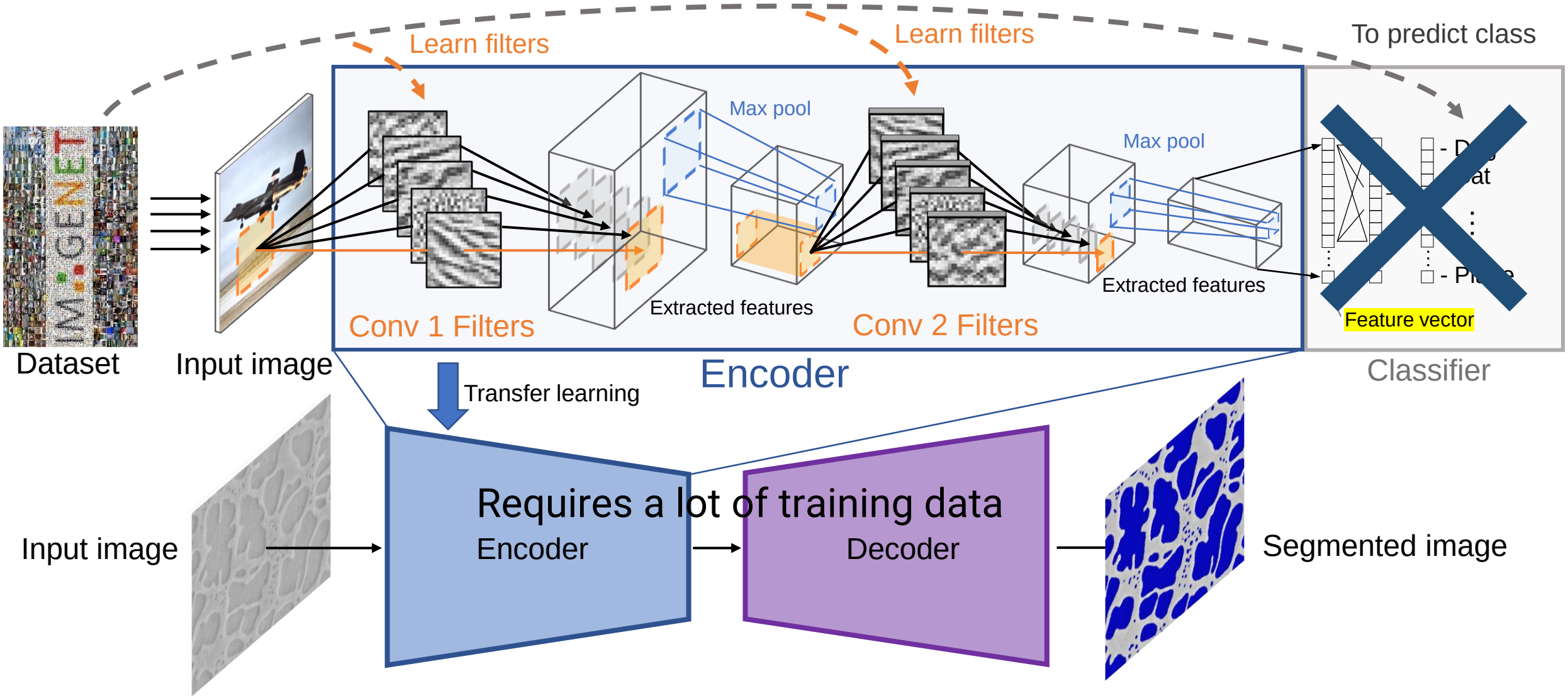


Microstructure

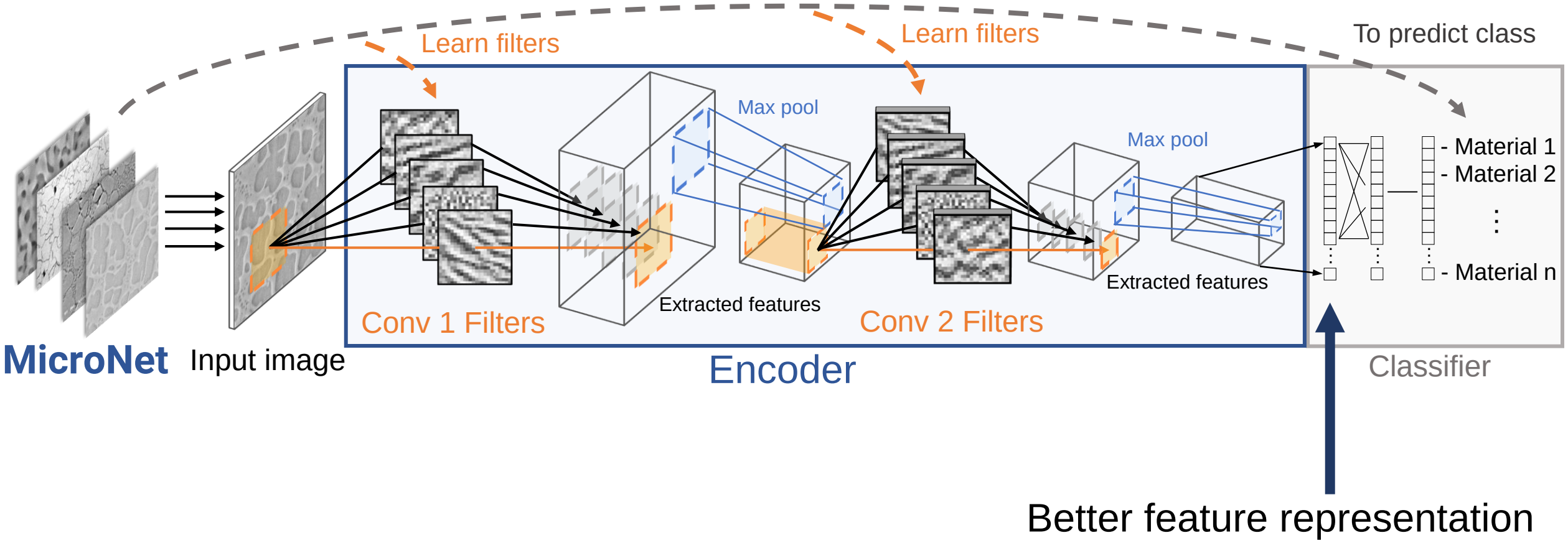
Processing → Structure → Properties
x z y

$$y = F(x,z)$$

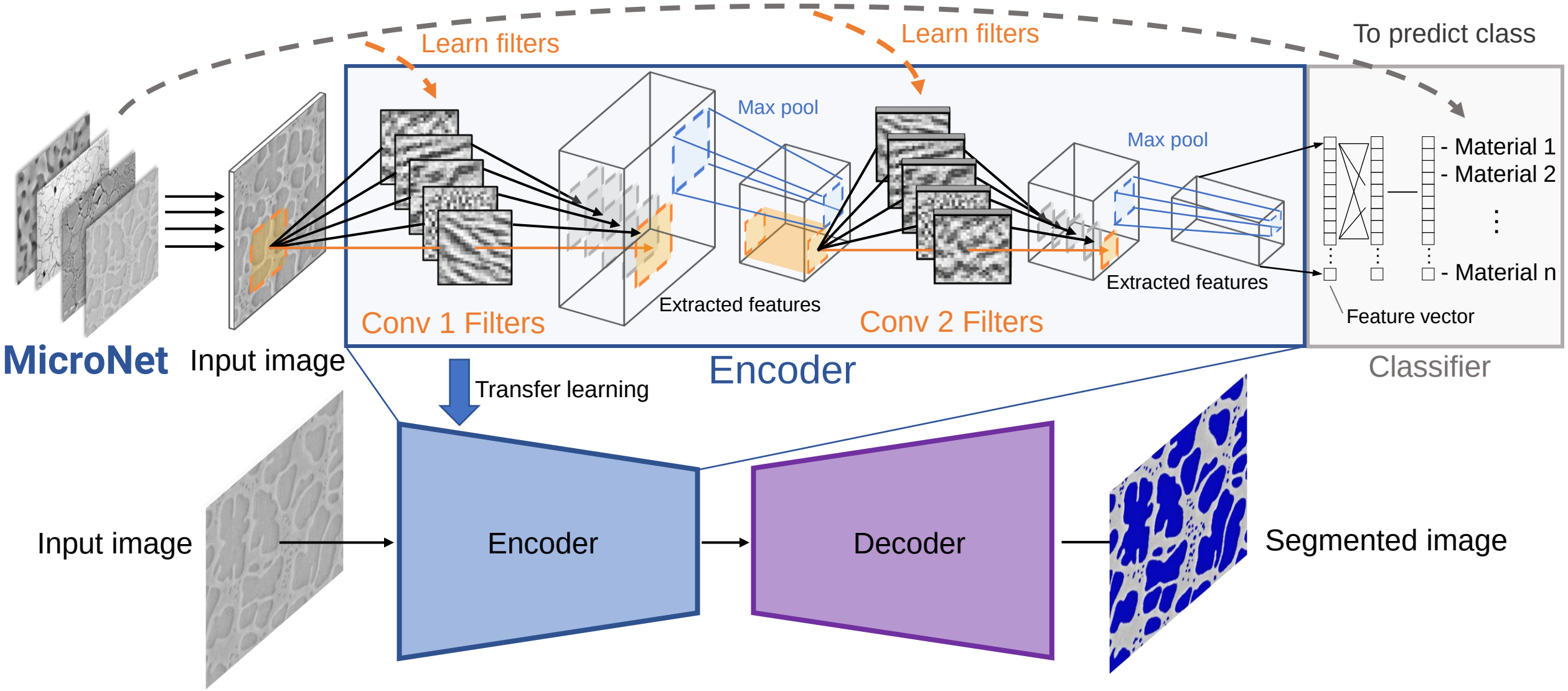
Computer Vision



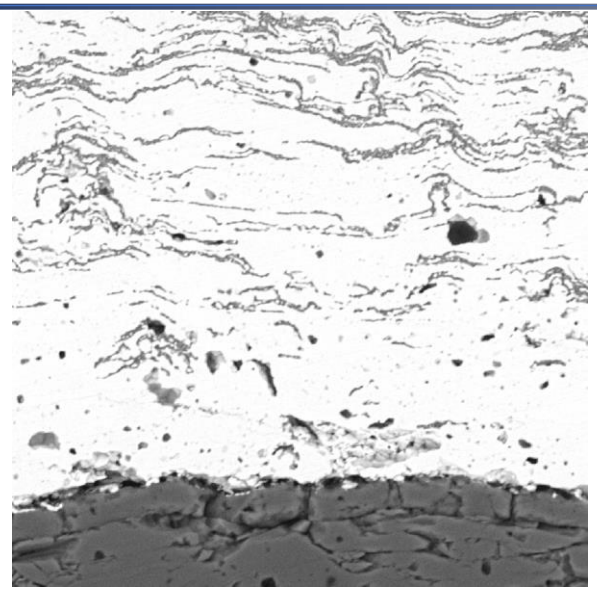
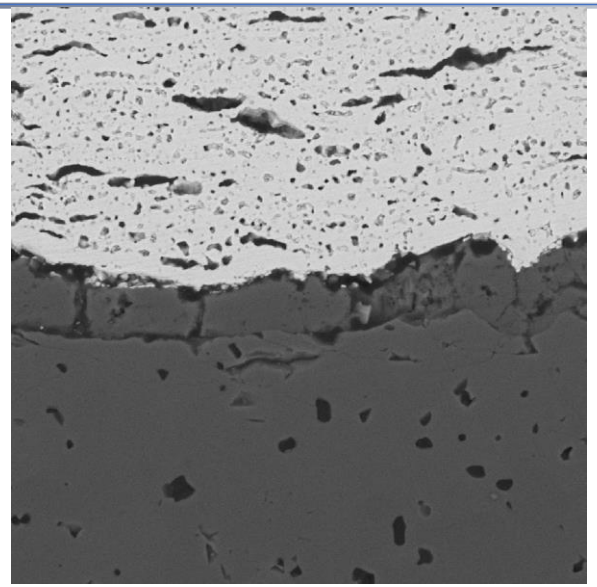
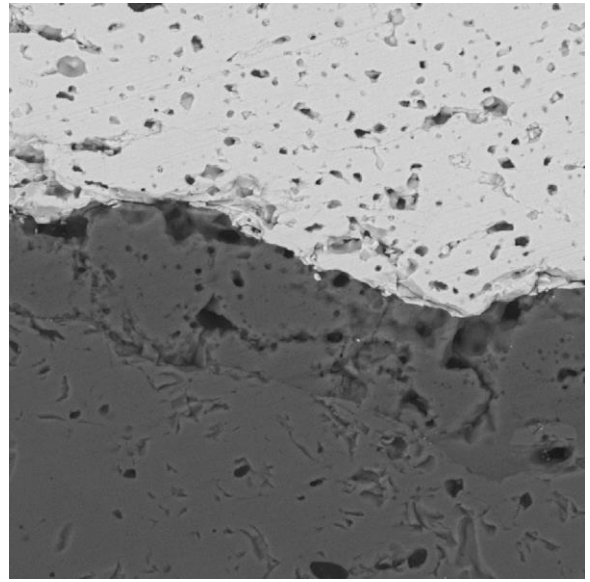
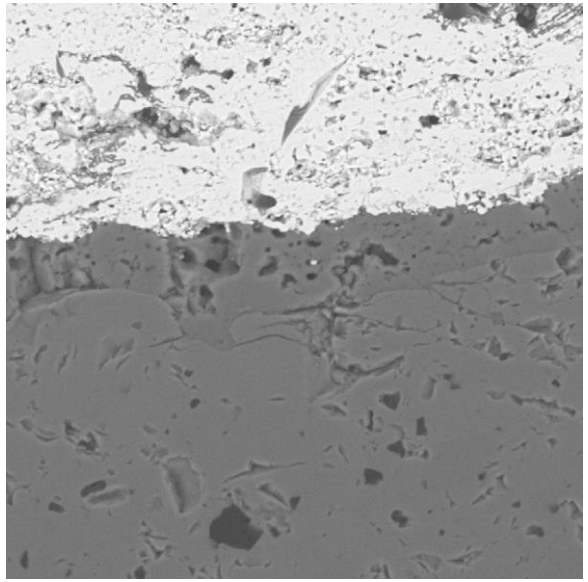
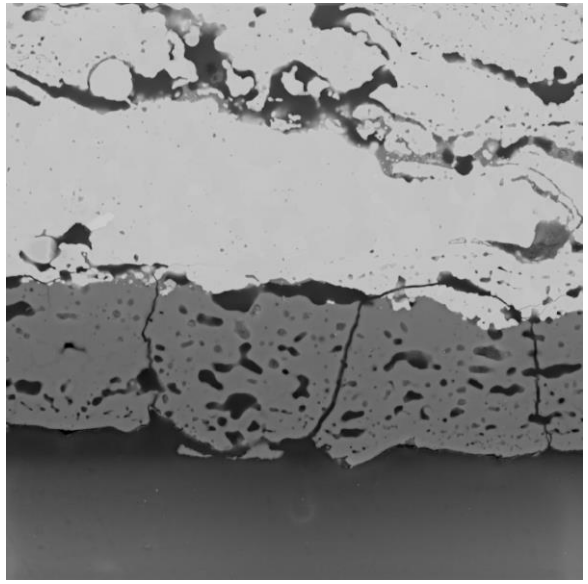
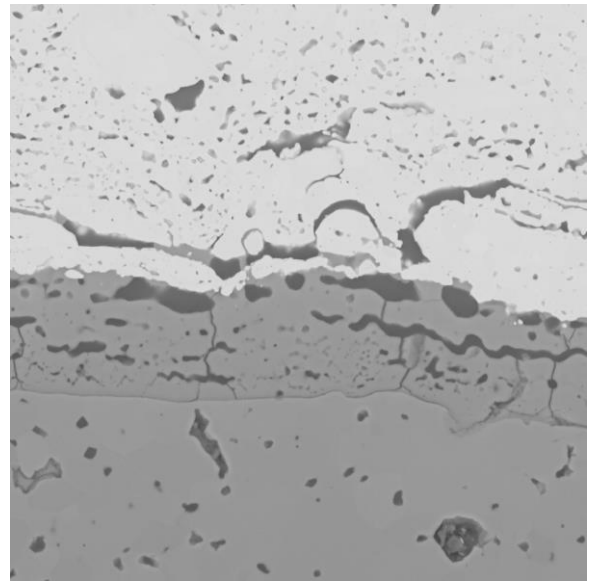
Computer Vision



Computer Vision



Automatic Microstructure Analysis

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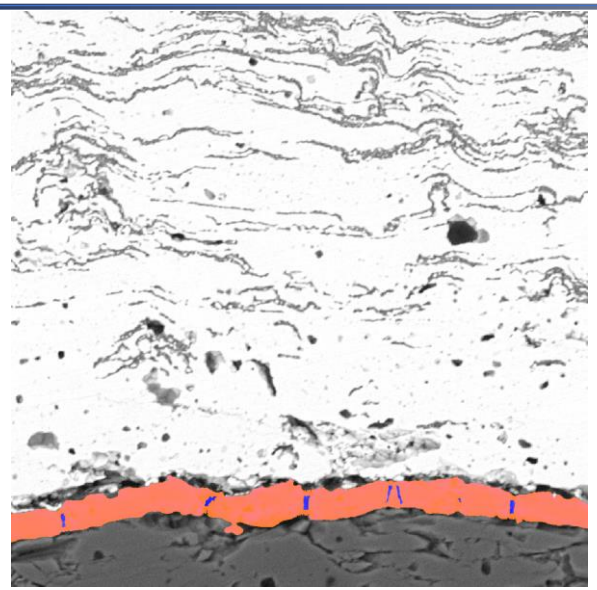
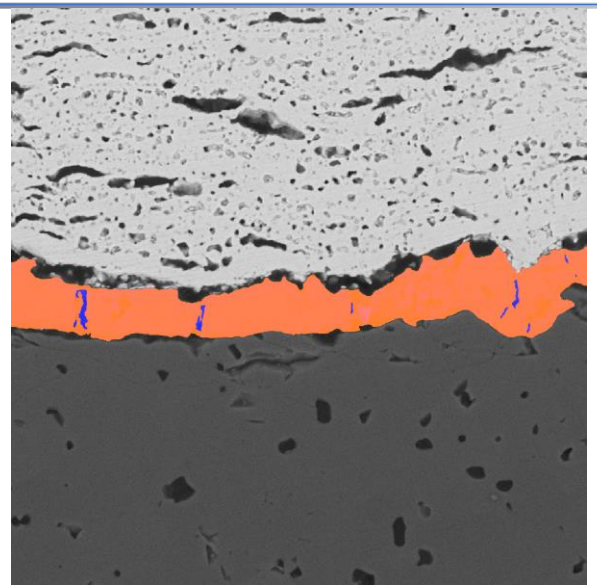
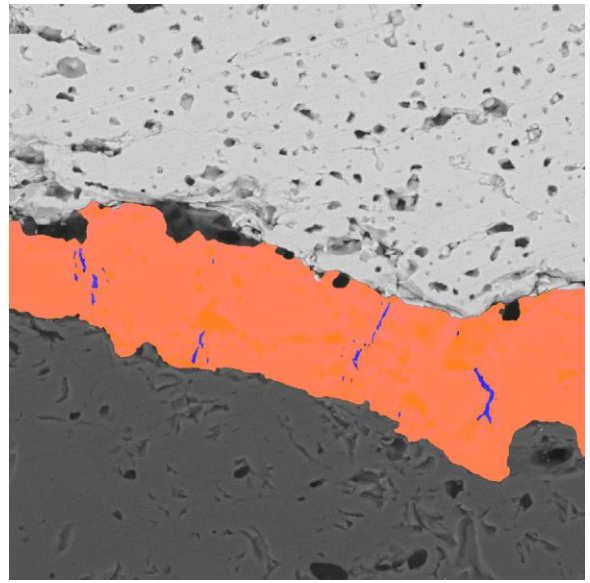
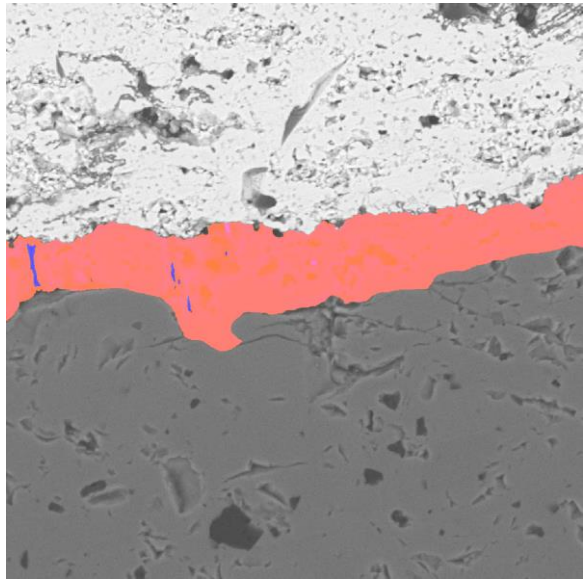
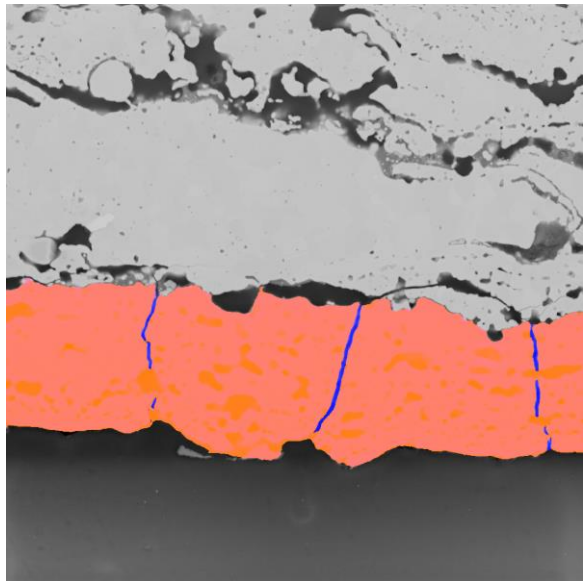
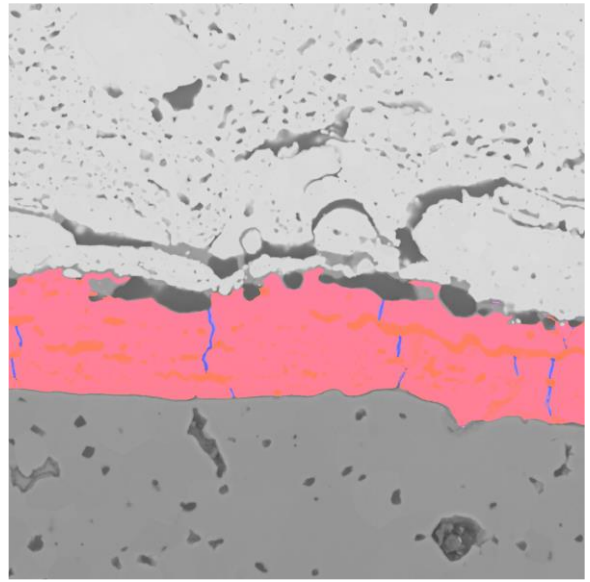

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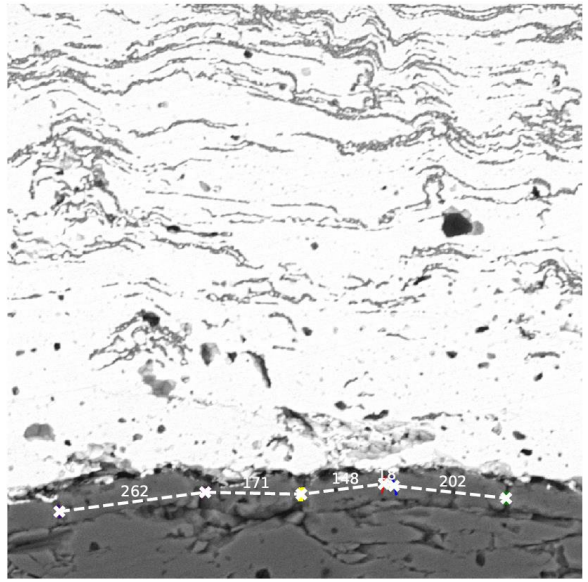

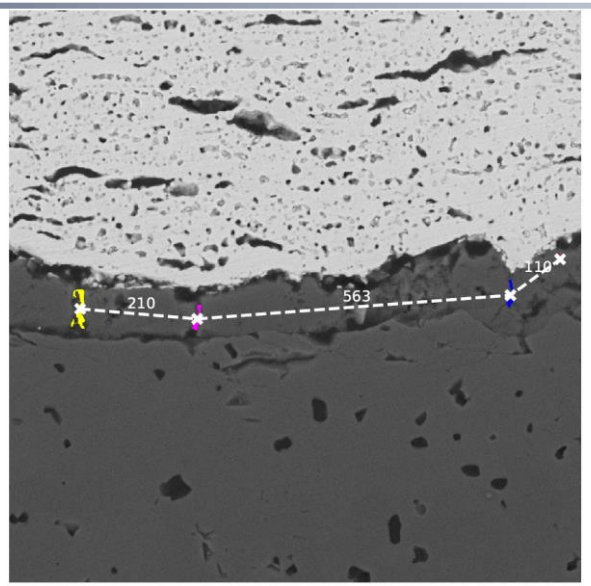

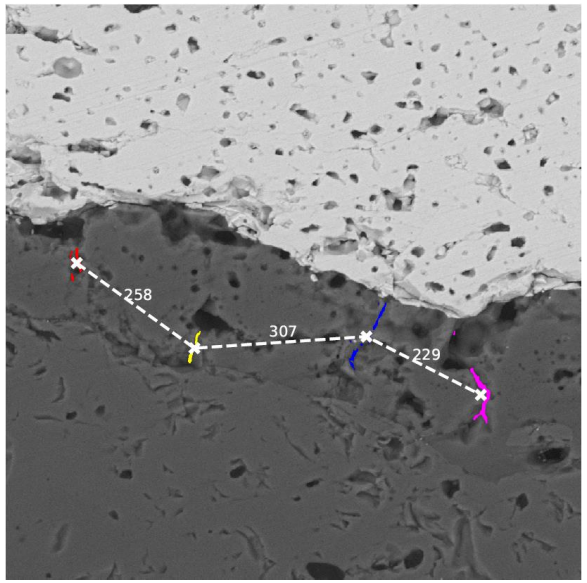

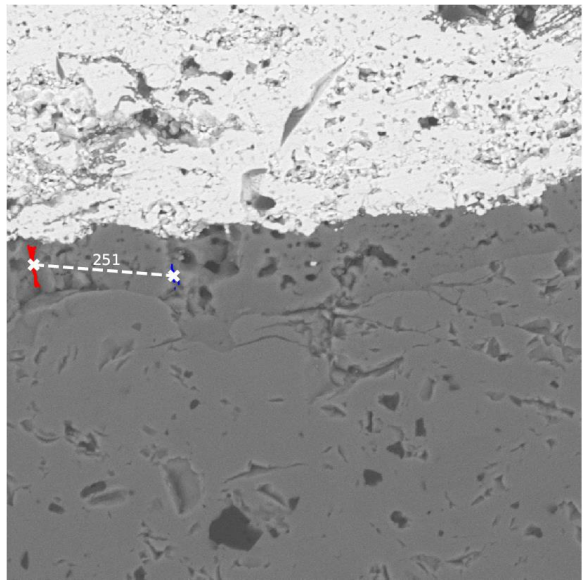

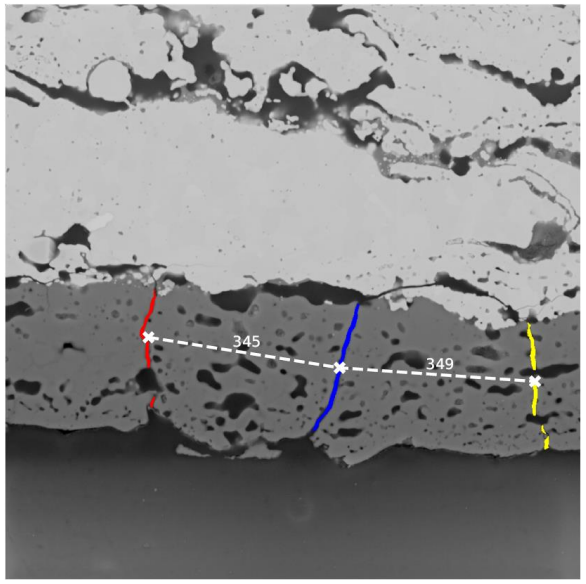

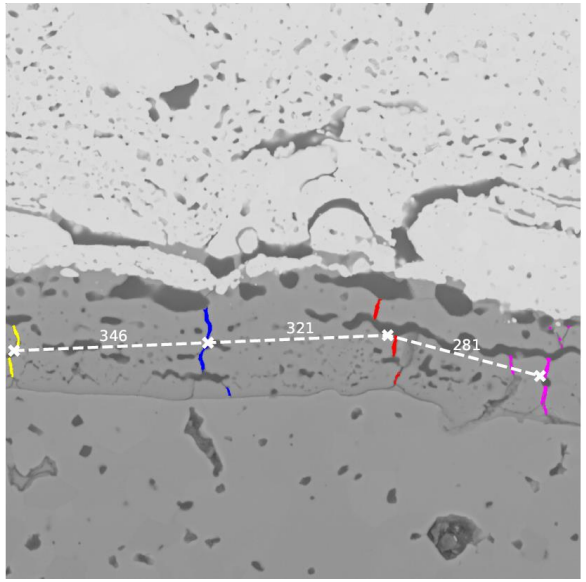

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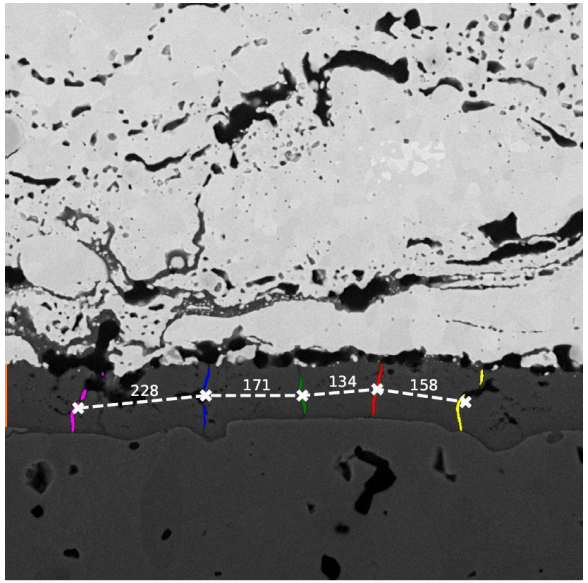
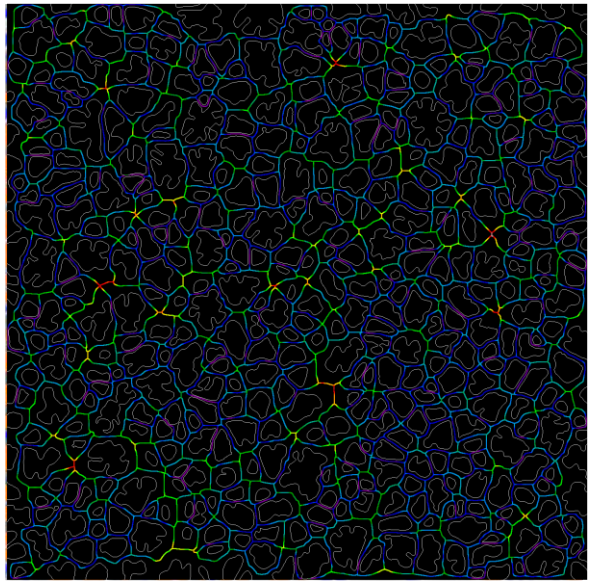
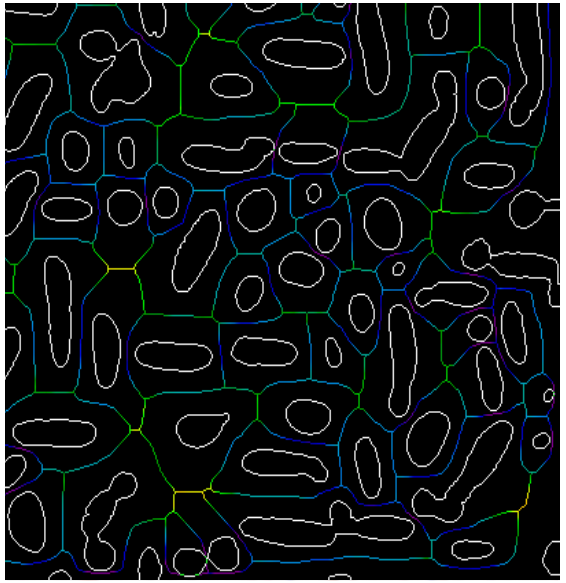
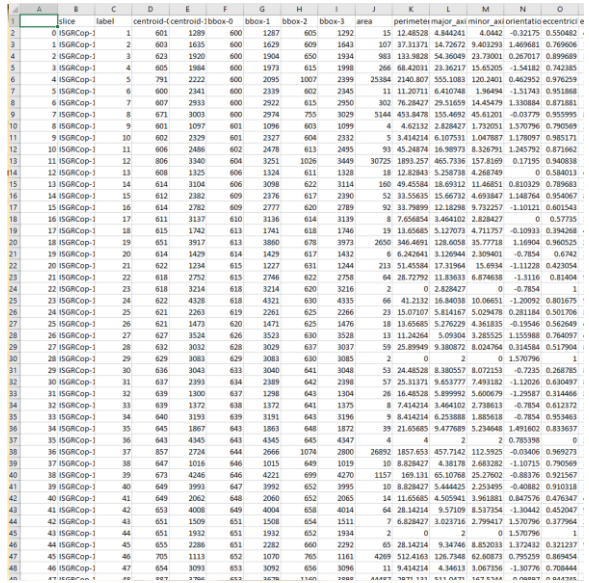
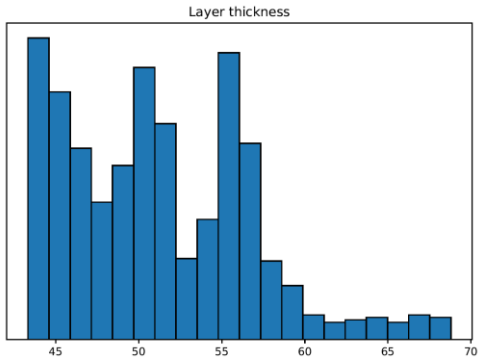


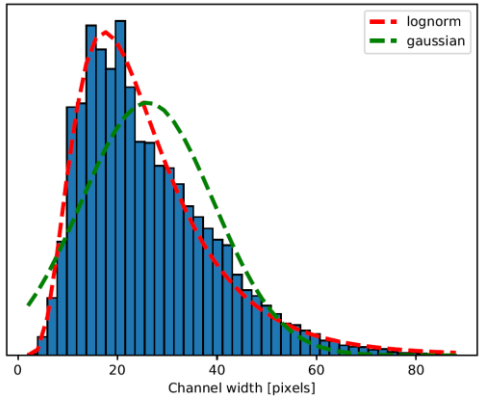


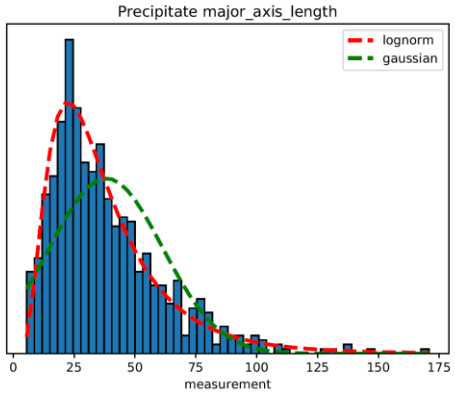


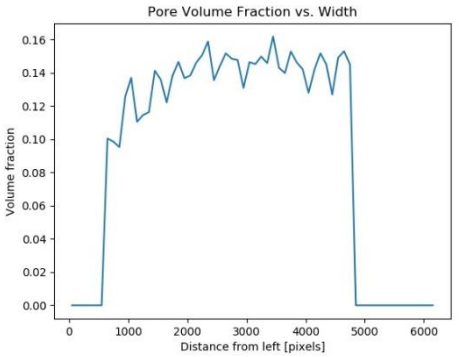


	slice	label	centroid-0	centroid-1	bbox-0	bbox-1	bbox-2	bbox-3	area	perimeter	major_axi	minor_axi	orientatio	eccentricit
0	ISGRCop-1	1	601	1289	600	1287	605	1292	15	12.48528	4.844241	4.0442	-0.32175	0.550482
1	ISGRCop-1	2	603	1635	600	1629	609	1643	107	37.31371	14.72672	9.401293	1.469681	0.769606
2	ISGRCop-1	3	623	1920	600	1904	650	1934	983	133.9828	54.36049	23.73001	0.267017	0.899689
3	ISGRCop-1	4	605	1984	600	1973	615	1998	266	68.42031	23.36217	15.65205	-1.54182	0.742385
4	ISGRCop-1	5	791	2222	600	2095	1007	2399	25384	2140.807	555.1083	120.2401	0.462952	0.976259
5	ISGRCop-1	6	600	2341	600	2339	602	2345	11	11.20711	6.410748	1.96494	-1.51743	0.951868
6	ISGRCop-1	7	607	2933	600	2922	615	2950	302	76.28427	29.31659	14.45479	1.330884	0.871881
7	ISGRCop-1	8	671	3003	600	2974	755	3029	5144	453.8478	155.4692	45.61201	-0.03779	0.955995
8	ISGRCop-1	9	601	1097	601	1096	603	1099	4	4.62132	2.828427	1.732051	1.570796	0.790569
9	ISGRCop-1	10	602	2329	601	2327	604	2332	5	3.414214	6.107531	1.047887	1.178097	0.985171
10	ISGRCop-1	11	606	2486	602	2478	613	2495	93	45.24874	16.98973	8.326791	1.245792	0.871662
11	ISGRCop-1	12	806	3340	604	3251	1026	3449	30725	1893.257	465.7336	157.8169	0.17195	0.940838
12	ISGRCop-1	13	608	1325	606	1324	611	1328	18	12.82843	5.258738	4.268749	-0	0.584013
13	ISGRCop-1	14	614	3104	606	3098	622	3114	160	49.45584	18.69312	11.44851	0.810329	0.789683
14	ISGRCop-1	15	612	2382	609	2376	617	2390	52	33.55635	15.66732	4.693847	1.148764	0.954067
15	ISGRCop-1	16	614	2782	609	2777	620	2789	92	33.79899	12.18298	9.732257	-1.10121	0.601543
16	ISGRCop-1	17	611	3137	610	3136	614	3139	8	7.656854	3.464102	2.828427	0	0.57735
17	ISGRCop-1	18	615	1742	613	1741	618	1746	19	13.65685	5.127073	4.711757	-0.10933	0.394268
18	ISGRCop-1	19	651	3917	613	3860	678	3973	2650	346.4691	128.6058	35.77718	1.16904	0.960525
19	ISGRCop-1	20	614	1429	614	1429	617	1432	6	6.242641	3.126944	2.309401	-0.7854	0.6742
20	ISGRCop-1	21	622	1234	615	1227	631	1244	213	51.45584	17.31964	15.6934	-1.11228	0.423054
21	ISGRCop-1	22	618	2752	615	2746	622	2758	64	28.72792	11.83633	6.874638	-1.3116	0.81404
22	ISGRCop-1	23	618	3214	618	3214	620	3216	2	0	2.828427	0	-0.7854	1
23	ISGRCop-1	24	622	4328	618	4321	630	4335	66	41.2132	16.84038	10.06651	-1.20092	0.801675
24	ISGRCop-1	25	621	2263	619	2261	625	2266	23	15.07107	5.814167	5.029478	0.281184	0.501706
25	ISGRCop-1	26	621	1473	620	1471	625	1476	18	13.65685	5.276229	4.361835	-0.19546	0.562649
26	ISGRCop-1	27	627	3524	626	3523	630	3528	13	11.24264	5.09304	3.285525	1.155988	0.764097
27	ISGRCop-1	28	632	3032	628	3029	637	3037	59	25.89949	9.380872	8.024764	0.314584	0.517904
28	ISGRCop-1	29	629	3083	629	3083	630	3085	2	0	2	0	1.570796	1
29	ISGRCop-1	30	636	3043	633	3040	641	3048	53	24.48528	8.380557	8.072153	-0.7235	0.268785
30	ISGRCop-1	31	637	2393	634	2389	642	2398	57	25.31371	9.651777	7.491182	-1.12026	0.630497
31	ISGRCop-1	32	639	1300	637	1298	643	1304	26	16.48528	5.899992	5.600679	-1.29587	0.314466
32	ISGRCop-1	33	639	1372	638	1372	641	1375	8	7.414214	3.464102	2.738613	-0.7854	0.612372
33	ISGRCop-1	34	640	3193	639	3191	643	3196	9	8.414214	6.253888	1.885618	-0.7854	0.953463
34	ISGRCop-1	35	645	1867	643	1863	648	1872	39	21.65685	9.477685	5.234648	1.491602	0.833637
35	ISGRCop-1	36	643	4345	643	4345	645	4347	4	4	2	2	0.785398	0
36	ISGRCop-1	37	857	2724	644	2666	1074	2800	26892	1857.653	457.7142	112.5925	-0.03409	0.969273
37	ISGRCop-1	38	647	1016	646	1015	649	1019	10	8.828427	4.38178	2.683282	-1.10715	0.790569
38	ISGRCop-1	39	673	4246	646	4221	699	4270	1157	169.131	65.10768	25.27602	-0.88376	0.921567
39	ISGRCop-1	40	649	3993	647	3992	652	3995	10	8.828427	5.444425	2.253495	-0.40882	0.910318
40	ISGRCop-1	41	649	2062	648	2060	652	2065	14	11.65685	4.505941	3.961881	0.847576	0.476347
41	ISGRCop-1	42	653	4008	649	4004	658	4014	64	28.14214	9.57109	8.537354	-1.30442	0.452047
42	ISGRCop-1	43	651	1509	651	1508	654	1511	7	6.828427	3.023716	2.799417	1.570796	0.377964
43	ISGRCop-1	44	651	1932	651	1932	652	1934	2	0	2	0	1.570796	1
44	ISGRCop-1	45	655	2286	651	2282	660	2292	65	28.14214	9.34746	8.852033	1.372432	0.321237
45	ISGRCop-1	46	705	1113	652	1070	765	1161	4269	512.4163	126.7348	62.60873	0.795259	0.869454
46	ISGRCop-1	47	654	3093	653	3092	656	3096	11	9.414214	4.34613	3.067356	-1.30776	0.708444

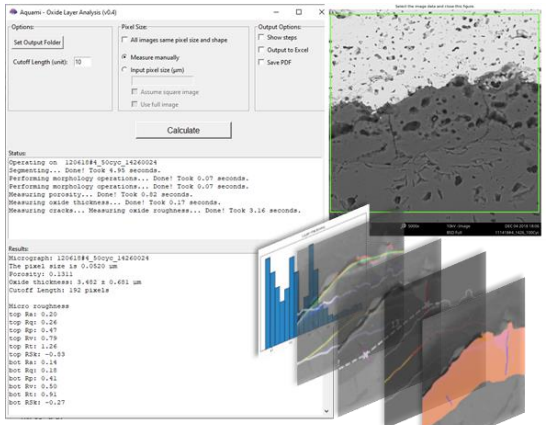






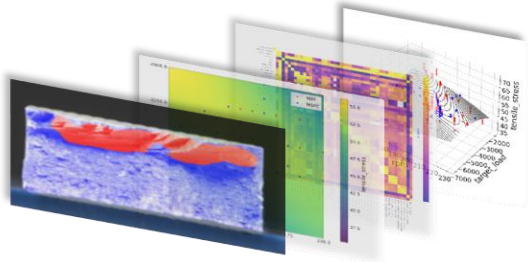


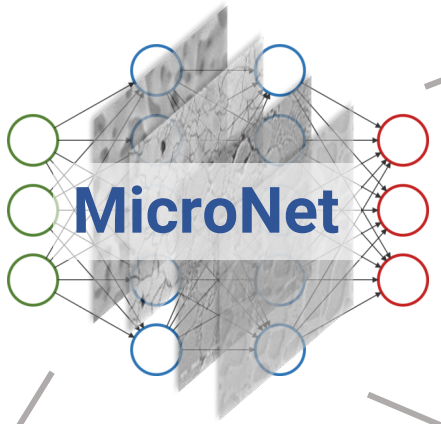
MicroNet



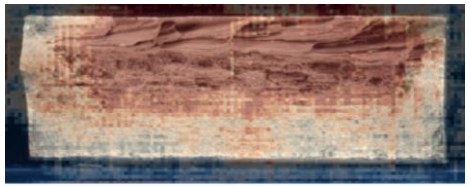
EBC TGO analysis software

SLS Core Stage Welds

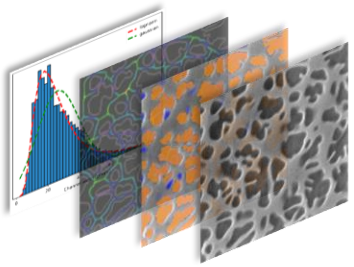




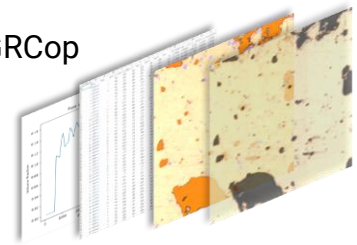
Direct regression and interpretability

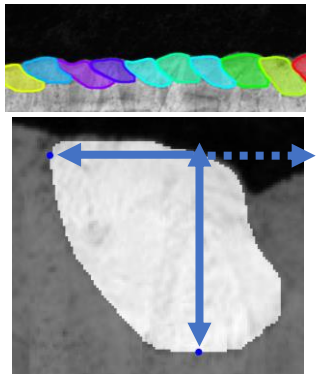


Ni-Superalloys



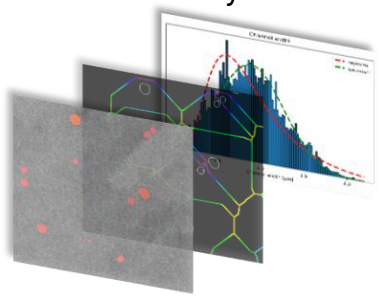
GRCop



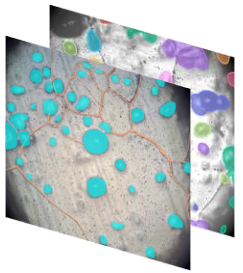


Automatic image analysis of melt pool geometry

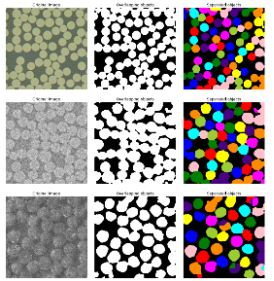
ODS Alloys



Wind tunnel Icing



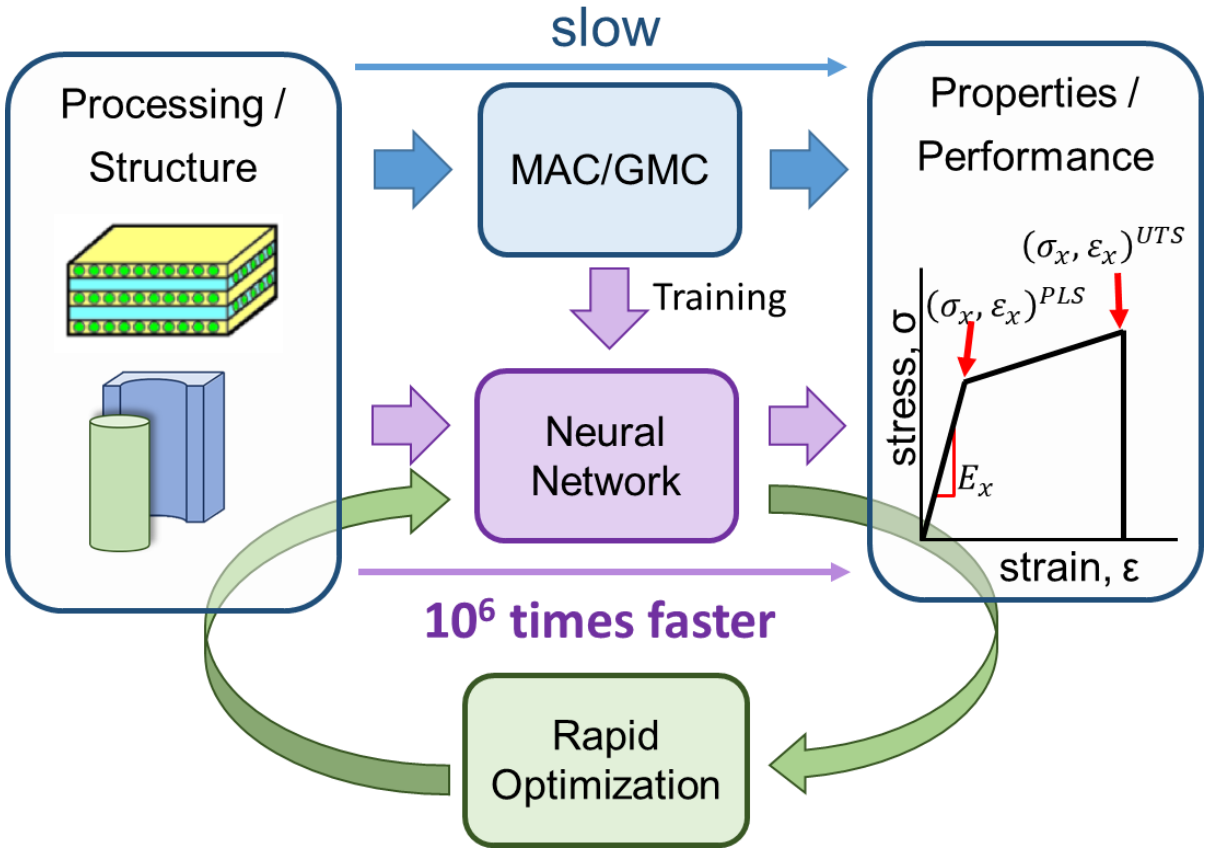
Composite Fibers



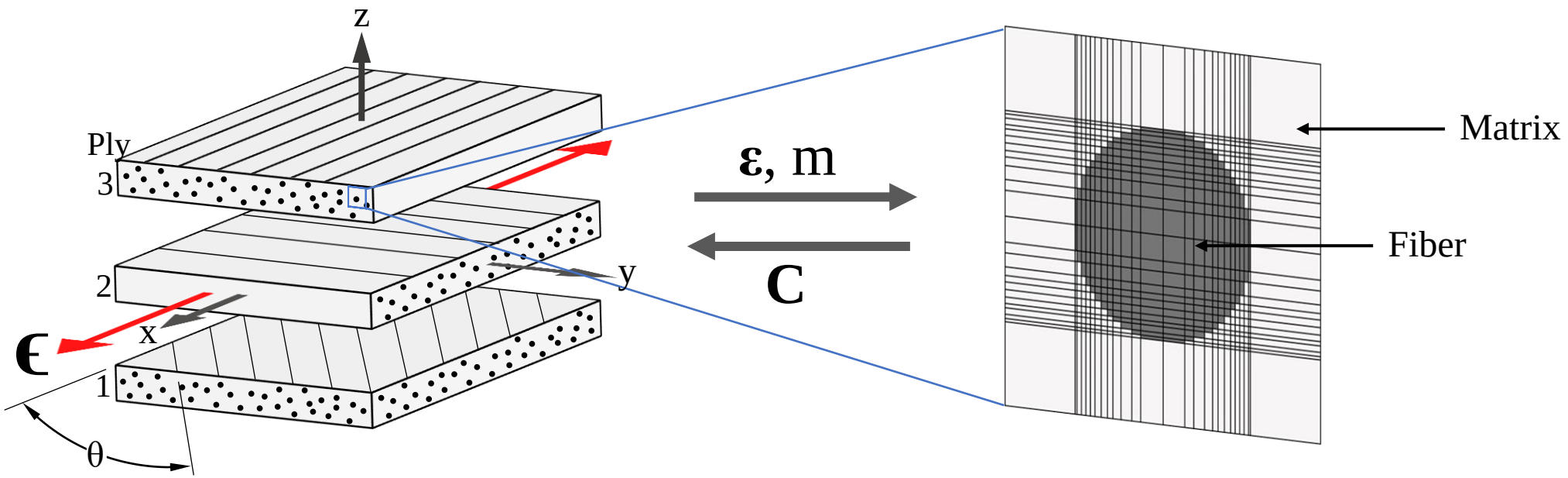
Surrogate Modeling

Modeling reduces the need for **expensive** physical experiments

Machine Learning reduces the need for **expensive** modeling



Surrogate Modeling



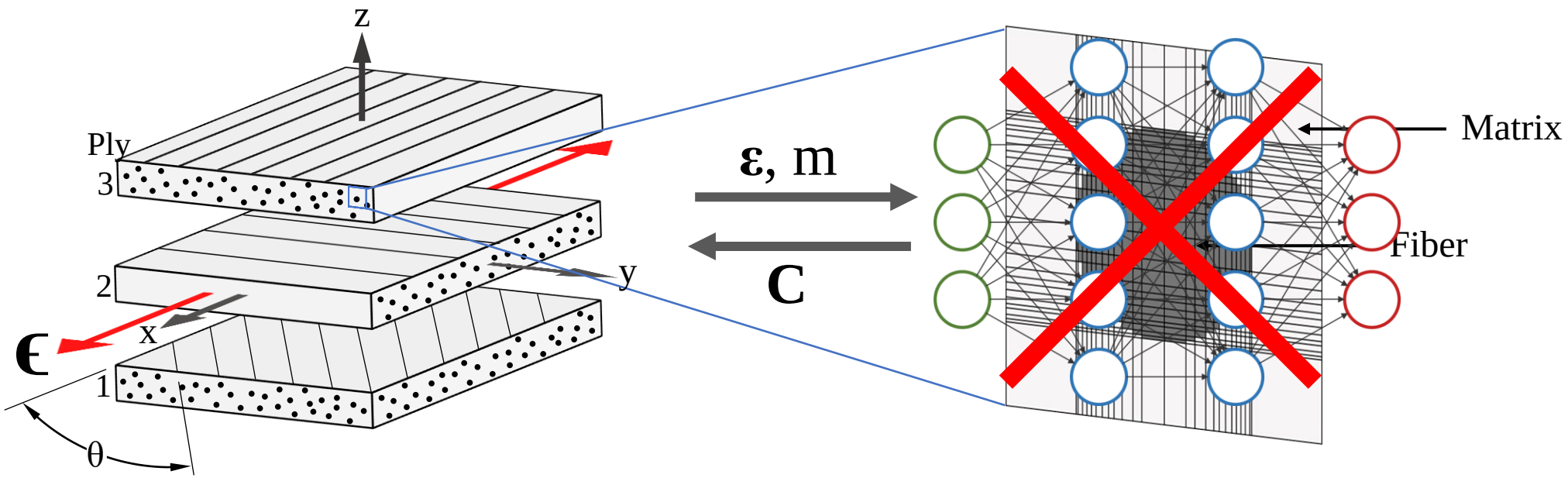
Inputs: strain increment (ϵ),
homogenized stiffness (C)

Outputs: global stress,
local strain (ε)

Inputs: local strain (ε)
Material properties (m)
Damage (d_n)

Outputs: homogenized stiffness (C)
Updated damage (d_{n+1})

Surrogate Modeling



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Material properties (m)
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Outputs: homogenized stiffness (C)
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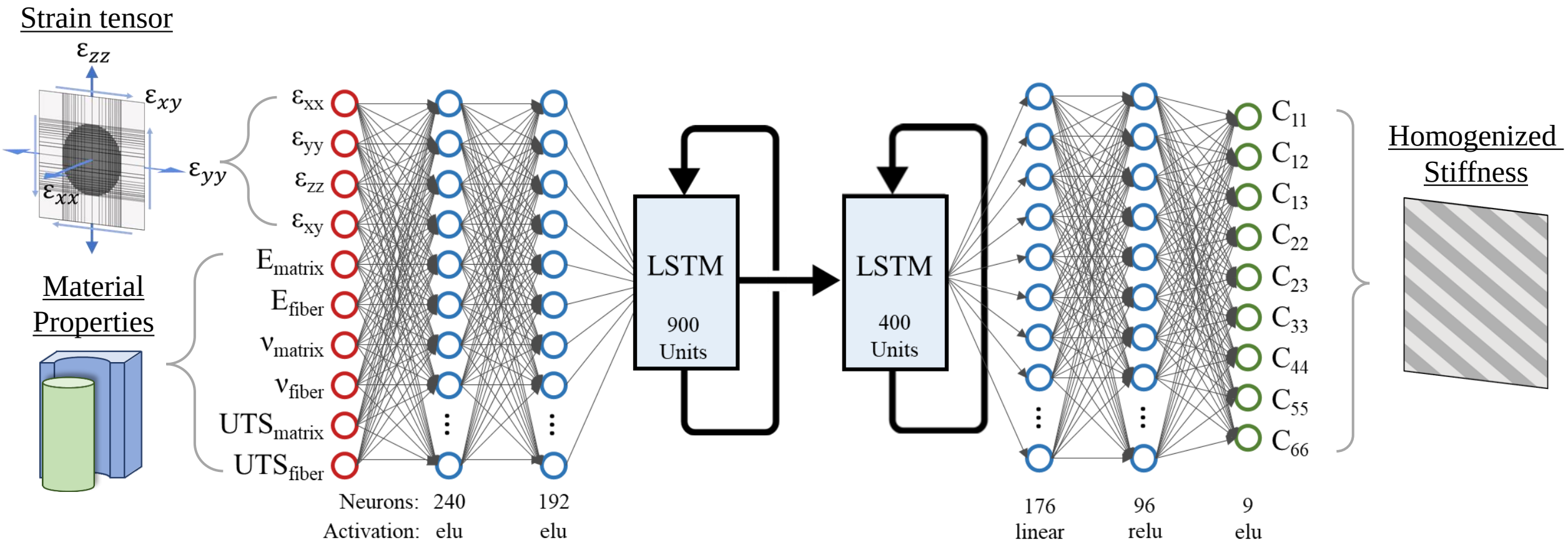
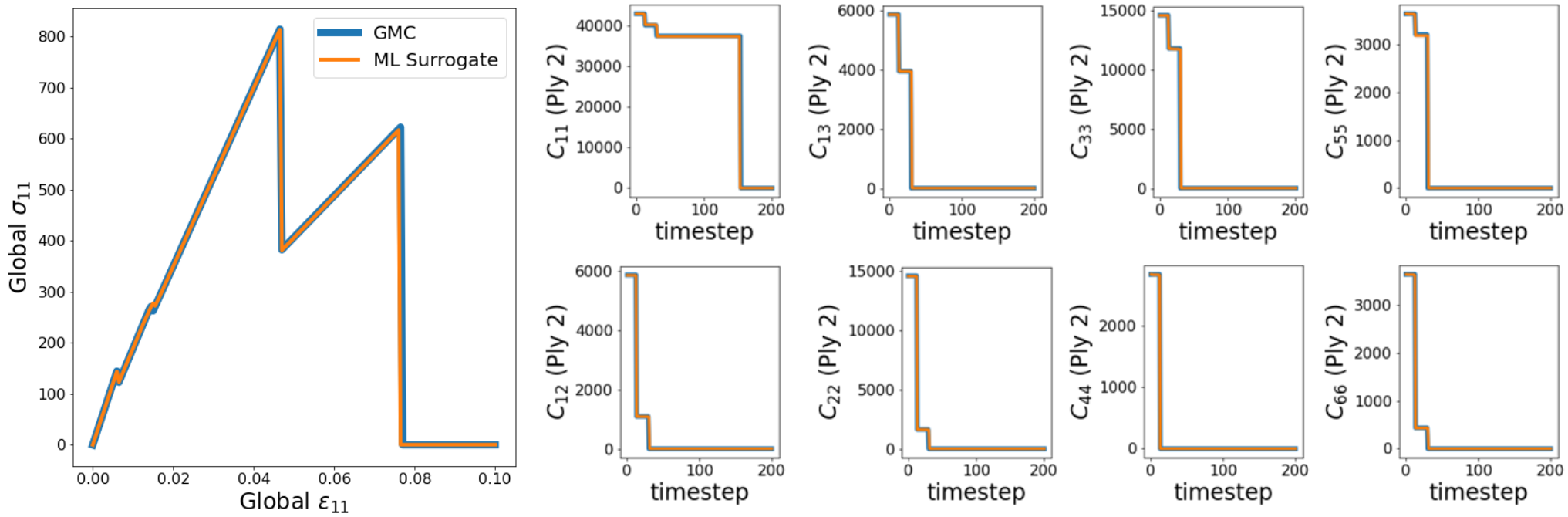
Surrogate Modeling



Surrogate Modeling

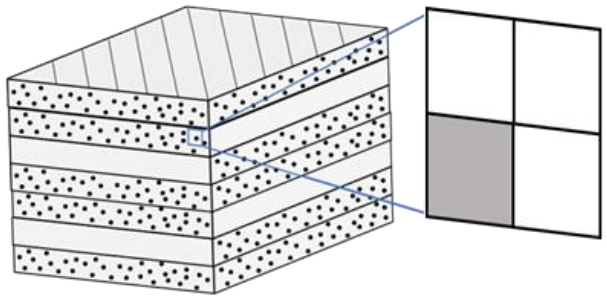
2 × 2 RUC [0°, 32.5°, -32.5°, 90 , 90, -32.5°, 32.5°, 0°]



Material Properties

	Fiber	Matrix
E	75 GPa	4 GPa
v	0.25	0.35
UTS	3,500 MPa	60 MPa

Laminate Configuration



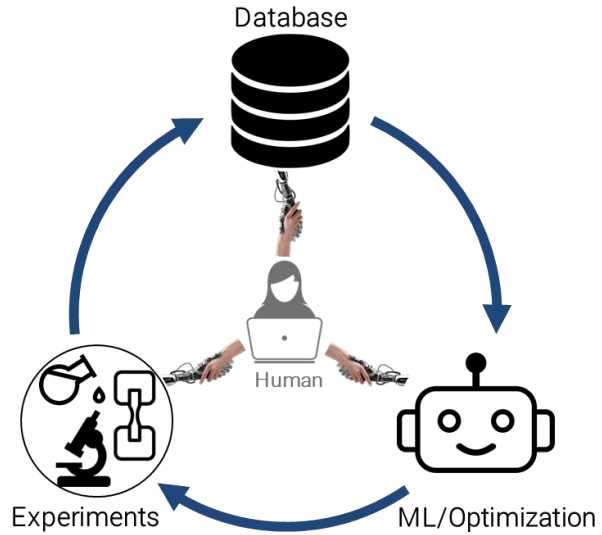
Accuracy Results

	MAE	R^2
Global Stress	8.6 MPa	0.96
Homogenized C	0.4 MPa	0.999997

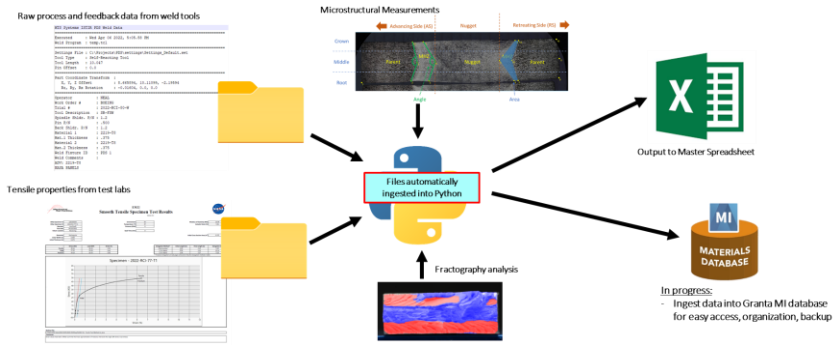
JARIMIS

"Just A Rather Intelligent Materials Interrogation System"

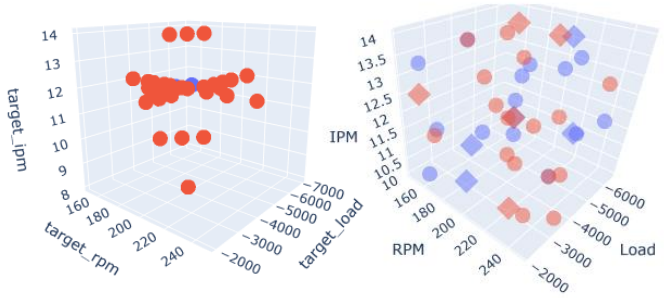
- A methodology and software framework that combines tools to efficiently apply materials informatics to more projects.
- Tools being applied to improve SLS weld quality.



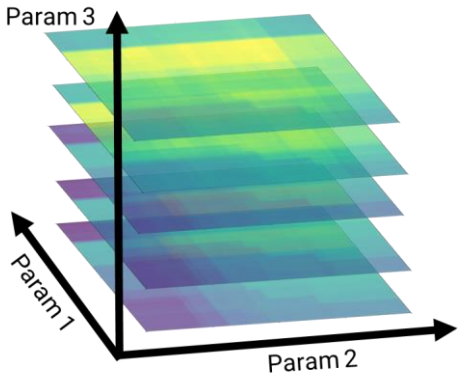
JARIMIS Framework



Automatic Data Ingestion



Space-filling DOE to capture non-linear effects



PSP Models

Conclusion

Most technology is limited by available materials

Batteries, jet engines, spaceships, processers, wind turbines, iron man suits

Accelerating materials development accelerates the future

Materials Informatics is accelerating materials development