Modelling of process-microstructure-properties relationships in aluminium components with advanced microstructural characterization and machine learning

Gagné, Marc-Olivier

Modelling of process-microstructure-properties relationships in aluminium components with advanced microstructural characterization and machine learning

Marc-Olivier Gagné
National Research Council Canada, Saguenay

Presentation Outline

- **Background**
- **Objective**
- **Implementing and leveraging a digital characterization workflow using optical microscopy**
  - Use case 1: High pressure vacuum die casting (HPVDC) with Aural™-2
    - Microstructure-properties model for HPVDC as-cast yield strength
  - Use case 2: Cold spray for additive manufacturing (CSAM) with AA6061
    - Process-microstructure relationship model to define safe process window for porosity size
- **Conclusion**

What is NRC

The **National Research Council** is the most important research organization of the government of Canada in science and technology.

The **Advanced Manufacturing Program** supports innovation in manufacturing technology. It host pre-competitive research clusters such as METALTec which feature an impressive industry-driven research portfolio.

The **Aluminium Technology Center** is one of 22 R&D sites across Canada. It focuses on aluminium transformation including casting, extrusion, hot/warm forming, welding, adhesive bonding, surface treatment and corrosion.

National Research Council Canada

Conseil national de recherches Canada

Acknowledgements

This project was conducted under the **METALTec industrial research and development group** managed by the NRC with the support of private members (+30) and public sponsors and collaborators.

This project was funded by the **Centre Québécois de Recherche et Développement de l'Aluminium (CQRDA)**.

MAJOR PRIVATE SPONSORS

PROVINCIAL FUNDING AGENCIES

INDUSTRIAL ASSOCIATIONS

ACADEMIC COLLABORATORS

GOVERNMENTS

ALUMINIUM AND IRON AND TITANIUM DIVISIONS

RAW MATERIAL SUPPLIERS

EQUIPMENT BUILDER

SECONDARY TRANSFORMATION

COMPONENTS/PRODUCTS MANUFACTURERS, TIERS 1/PART MANUFACTURERS

FINAL PRODUCTS, VEHICLE ASSEMBLY, OEM

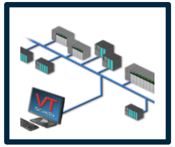
Objective: To integrate optical microscopy in a digital process workflow

For a successful transition toward digitalization, every part of the process should be included in the effort.

That include the characterization lab which might use optical microscopy (OM).

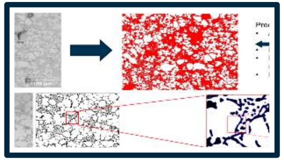
There are specific challenges related to OM when it comes to integrate it in a digital process.

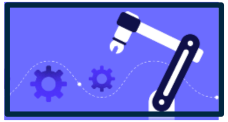
Image/Data Management

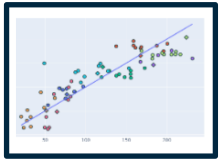

Connect the lab

Industry 4.0 integrated optical microscopy

Feature extraction & engineering




Automation


Leveraging the data

Integrating optical microscopy in a digital process workflow: 3 areas to focus on

From a typical standalone lab

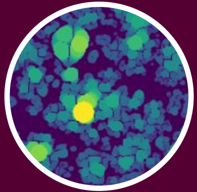
Scattered data
- Various Excel, CSV, TXT files
- No standardization, no centralisation

Partial/Manual image processing
- Fundamental microstructural components not systematically quantified
- No automation

Lack of AI-based data analysis
- No integrated tool to manipulate, visualize and process data
- No simple way to build and use ML models

To an "Industry 4.0" digital process workflow

Centralized data management



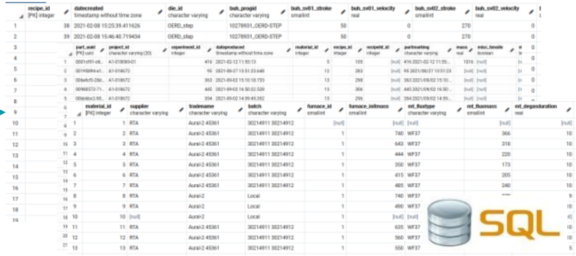
Automatic Image processing

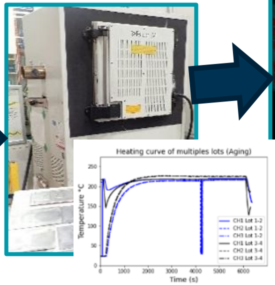
User-friendly data analysis and machine learning tool

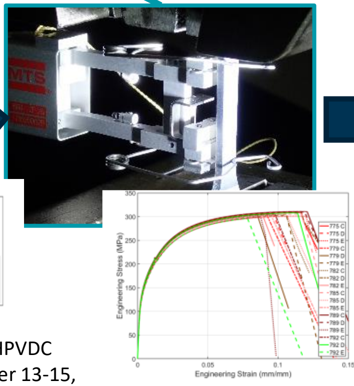
Artificial intelligence

Use case #1: HPVDC with Aural™-2 alloy

HPVDC stands for **H**igh **P**ressure **V**acuum **D**ie **C**asting: Common process, notably in the automotive industry used to produce large series of near net-shape, complex structural components.







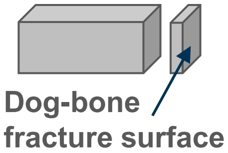
Related paper from 2022 NADCA conference: Gariépy A, Tu S, Gagné M-O and Samuel E, Local microstructure-properties model for HPVDC Aural(TM)-2 using image analysis and machine learning, North American Die Casting Congress and Tabletop, Lexington, KY, September 13-15, 2022

Use case #1: HPVDC with Aural™-2 alloy
Image acquisition and analysis

Manual | Automated

1) Metallographic sample preparation

Cutting



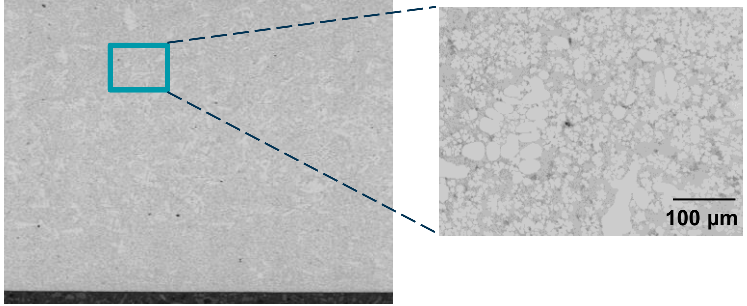
Mounting

Polishing

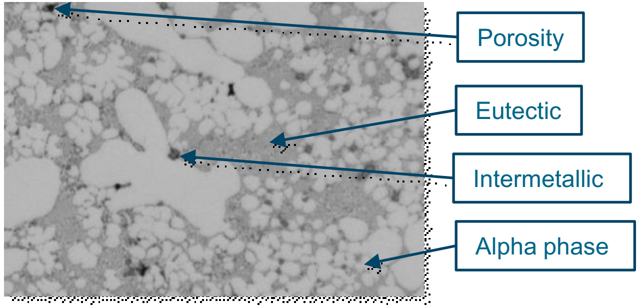
2) Image acquisition. HPVDC produces microstructural elements with various length scales.

Mosaic images

Close-up



3) Image analysis: systematic approach. Every microstructural component is thoroughly analysed.



Analysis parameters
Area, Area%
Morphology
Number
Position

FldNo	ObjId	Cat	AspRatio	Compactn	Roundnes	Perimeter	Area	XCent	YCent
n	n	n				mm	mm²	mm	mm
216	1	3	1.93443	0.46436	0.27701	0.10986	0.00022	10.891	-15.5895
216	2	3	1.79592	0.57314	0.36106	0.11575	0.00028	10.5292	-15.6182
216	3	3	1.32143	0.8283	0.69289	0.08869	0.00038	10.9103	-15.6204
216	4	3	1.40175	0.69847	0.53064	0.12333	0.00035	10.8414	-15.6218
216	5	3	1.88972	0.5494	0.32981	0.26956	0.00119	10.8874	-15.6419
216	6	3	1.78659	0.64728	0.39961	0.08176	0.00022	10.3849	-15.6204
216	7	3	1.40961	0.58679	0.44775	0.25866	0.00107	10.7797	-15.6426

Use case #1: HPVDC with Aural™-2 alloy
Data treatment & Feature engineering

4) Compile image analysis data

1 line per object (ex: porosities)

14	BpName	Routine	Mag	Unit	Calib	MeasType	MeasCnt	FieldCnt	ObjCnt	TotArea
15	Porosites	Siyu_A1-0	200X	Microns	0.299145	OBJ	10	1	1088	12269270
16										
17	FldNo	ObjId	Cat	AspRatio	Compactn	Roundnes	Perimeter	Area	XCent	YCent
18	n	n	n				µm	µm²	µm	µm
19	72	1	1	2	1	0	27	39	-13621	13574
20	72	2	1	2	1	0	15	15	-13711	13574
21	72	3	1	5	1	0	5	3	-13695	13573
22	72	4	1	6	0	0	6	3	-13959	13568
23	72	5	1	2	1	0	10	8	-13942	13567
24	72	6	1	6	0	0	6	3	-13944	13566
25	72	7	1	5	1	0	5	3	-14413	13546
26	72	8	1	6	0	0	6	3	-14982	13542
27	72	9	1	5	1	0	5	3	-13747	13539
28	72	10	1	2	1	1	20	32	-14908	13536
29	72	11	1	3	1	1	7	5	-14750	13538
30	72	12	1	5	1	0	5	3	-14859	13537
31	72	13	1	2	1	0	14	11	-15283	13534
32	72	14	1	2	1	1	12	14	-15014	13533
33	72	15	1	3	1	0	8	6	-15391	13534
34	72	16	1	5	1	0	5	3	-13514	13532
35	72	17	1	2	1	0	25	38	-15433	13528
36	72	18	1	2	1	1	14	15	-15491	13530
37	72	19	1	5	1	0	5	3	-14258	13530

Aggregate

Analysis parameters	Aggregated values
Porosities	**Mean size**
	Std size
	…
Intermetallic	**Mean size**
	Std size
	…

5) Perform feature engineering

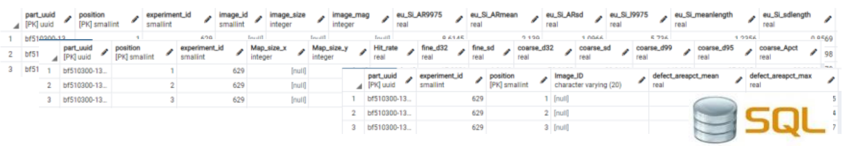
Engineer new features from the original ones

- Alternative size estimation (ex: D32 $\frac{\sum d^3}{\sum d^2}$)
- Edge cases (top 5 or top 1 percentile)
- Split skin and core
- …

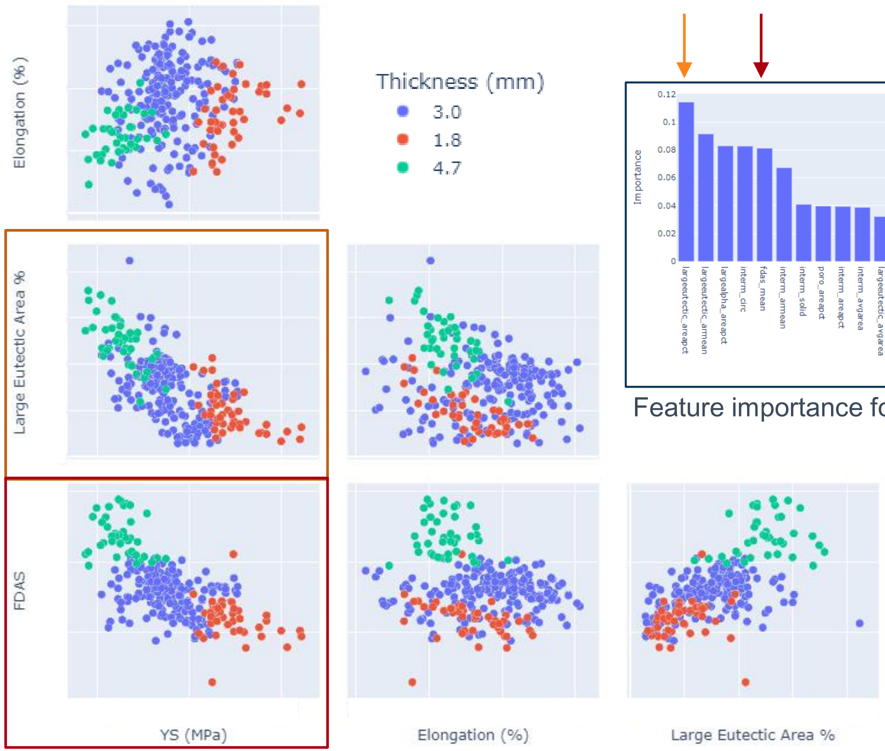
Final microstructural dataset with up to 70 features

1	specimen	experime	position	ymin	ymax	metallo_t	thickness	offsetys	uts	elongatio	breakinsic	areareduc	largealph	largealpha	largealpha	largealpha
2	348A_F	348	A	86.049	2930.512	2844.463	1.8	149.7	306.8	7.266	TRUE	12.1145	19.418	553.717	0.422	0.793
3	348B_F	348	B	76.341	1835.707	1759.366	1.8	152	309.9	7.525	TRUE	11.0177	12.405	592.888	0.439	0.802
4	348C_F	348	C	86.931	2900.064	2813.133	3	136.2	297.4	10.421	TRUE	14.7137	13.765	540.767	0.408	0.787
5	348D_F	348	D	84.725	2847.994	2763.269	3	144.9	303	13.914	TRUE	15.3295	14.143	560.22	0.411	0.79
6	348E_F	348	E	82.96	2883.296	2800.336	3	130.8	286.6	8.47	FALSE	12.6464	14.839	598.053	0.447	0.807
7	348F_F	348	F	85.607	4547.788	4462.181	4.7	127.3	265.8	6.946	FALSE	11.8858	17.735	586.217	0.418	0.793
8	348G_F	348	G	72.811	4535.432	4462.621	4.7	127.7	272	8.382	TRUE	11.8241	19.432	612.631	0.392	0.781
9	351A_F	351	A	78.547	1798.64	1720.093	1.8	152.4	316.1	10.361	TRUE	15.4229	8.632	552.651	0.426	0.791
10	351B_F	351	B	81.636	1788.932	1707.296	1.8	155.8	318.8	10.224	FALSE	13.8317	8.001	520.773	0.429	0.791
11	351C_F	351	C	80.312	2879.766	2799.454	3	139.3	294.4	11.244	TRUE	14.4335	17.104	544.06	0.437	0.8
12	351D_F	351	D	81.195	2904.477	2823.282	3	135.6	296.7	9.679	TRUE	13.9735	17.693	587.298	0.443	0.804
13	351E_F	351	E	87.814	2837.403	2749.589	3	136.8	290.6	10.866	TRUE	16.6798	13.925	510.488	0.422	0.791

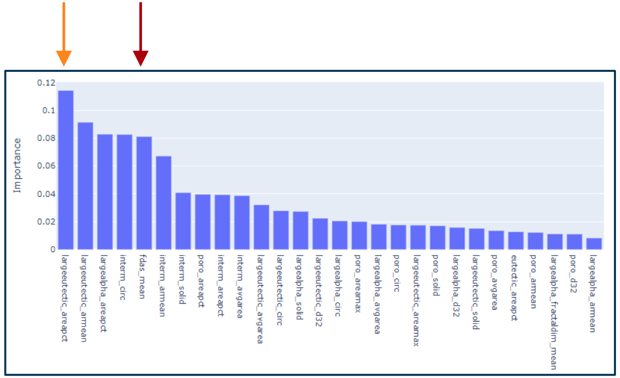
For each sample, there is thousands of objects analysed. Automating the data treatment is a crucial step to create an efficient characterization workflow.



Use case #1: HPVDC with Aural™-2 alloy
Using microstructural features to predict yield strength (YS)

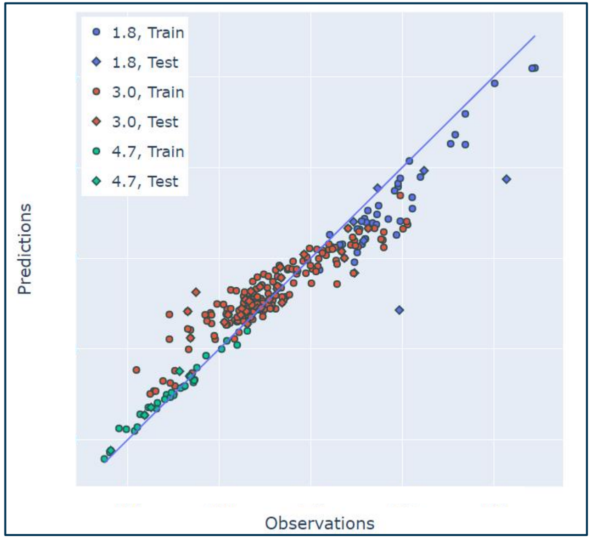


Relationship between microstructural features and mechanical properties for *as-cast* samples



Feature importance for the extra tree regressor YS model

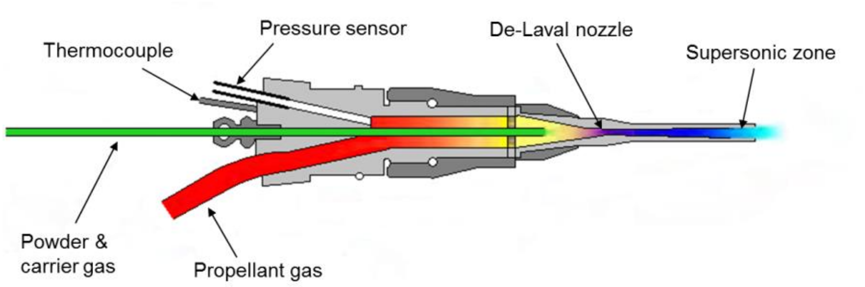
Machine learning model leverages the relationships between the microstructural features and the yield strength



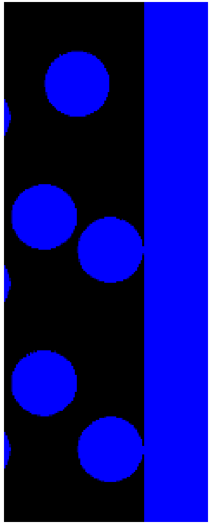
Extra tree regressor fit for the YS. Split by thicknesses and train/test

Set	RMSE	R^2
Training set	2.67	0.90
Test set	4.17	0.77

Use case #2: Cold Spray for Additive Manufacturing (CSAM) with AA6061 alloy



Particles are accelerated in the gas stream to high speed



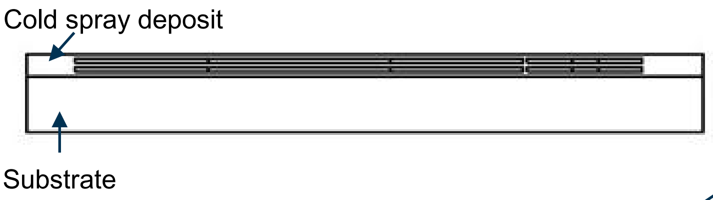
H. Assadi, www.modares.ac.ir/eng/ha10003/CGS.htm

Process parameters

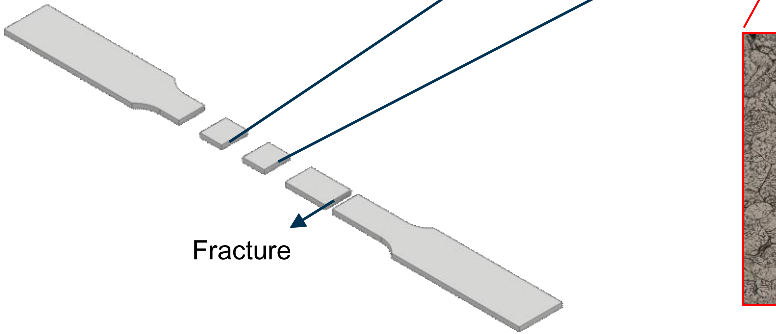
Gas pressure, Gas temperature,
Standoff distance, Spray angle,
Gun traverse speed
Nozzle shape + material,
Particle shape, size, material
Substrate material, surface condition
+ surface temperature

Use case #2: CSAM with AA6061 Characterization workflow

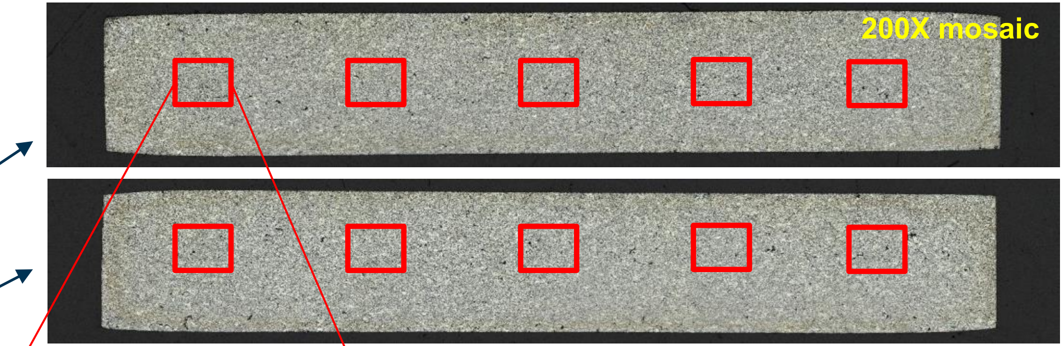
1) Extract tensile coupons from deposit

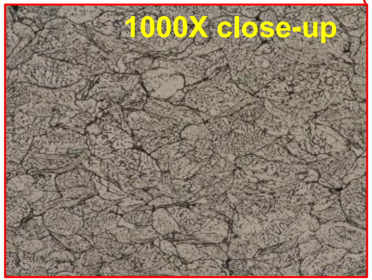


2) Extract metallography coupons from tensile coupons

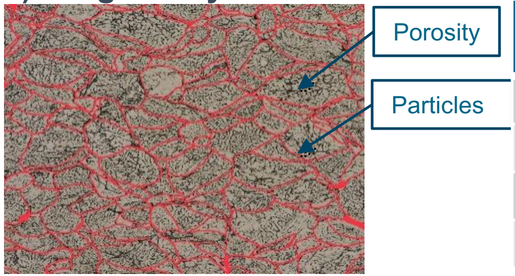


3) Image acquisition (mosaics and close-ups)





4) Image analysis

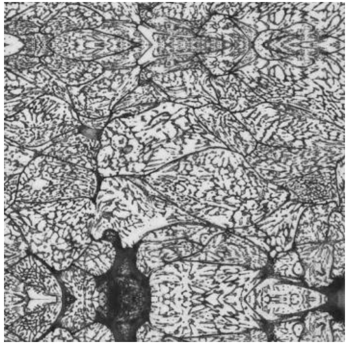


Analysis parameters
Area, Area%
Morphology
Number
Position

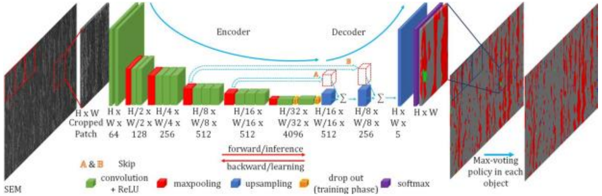
Use case #2: CSAM with AA6061
The challenge of particle segmentation

Problem: Particles segmentation in cold spray microstructure images is challenging due to the strong internal contrast within the particles.

Solution: train a transfer learning convolutional neural network (CNN) model to perform the segmentation using the images acquired in the project.



Strong internal contrast of microstructure



Encoder → Decoder

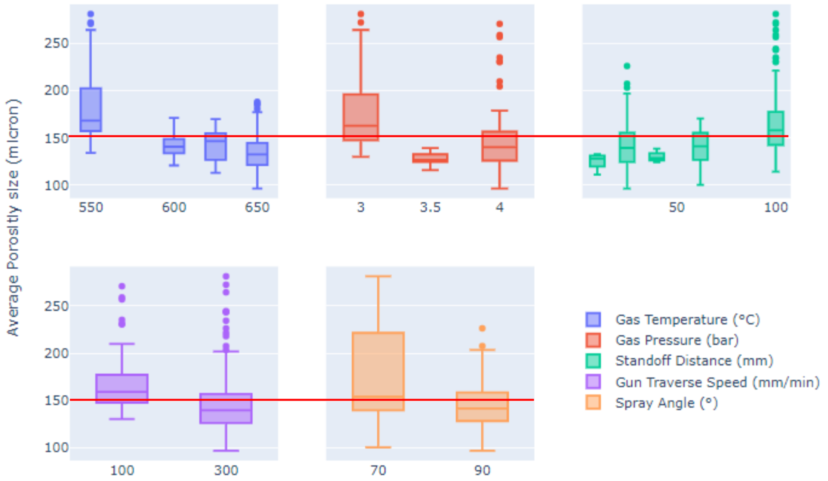
Model output: Mask of the particle boundaries

python

Segmentation Models

TensorFlow

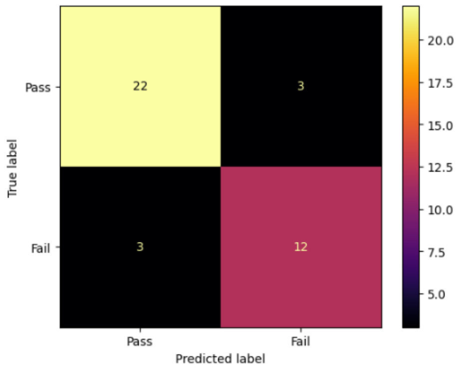
Use case #2: CSAM with AA6061
Process-microstructure relationships



Relationships between process parameters and average porosity size of <u>*as-sprayed*</u> deposits

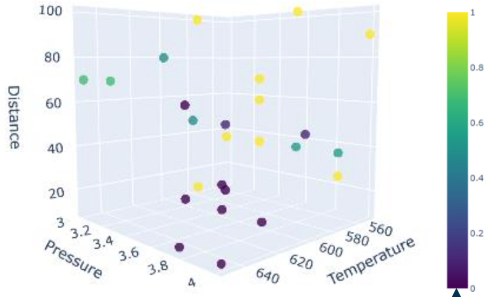
Hypothetical use case: The application require the porosity size to stay below 150 µm

Create a decision tree model that maps the process parameters to the average porosity size using the threshold (150 µm)



metric	score
Accuracy	85%
Precision*	80%
Recall*	80%

** Fail class*

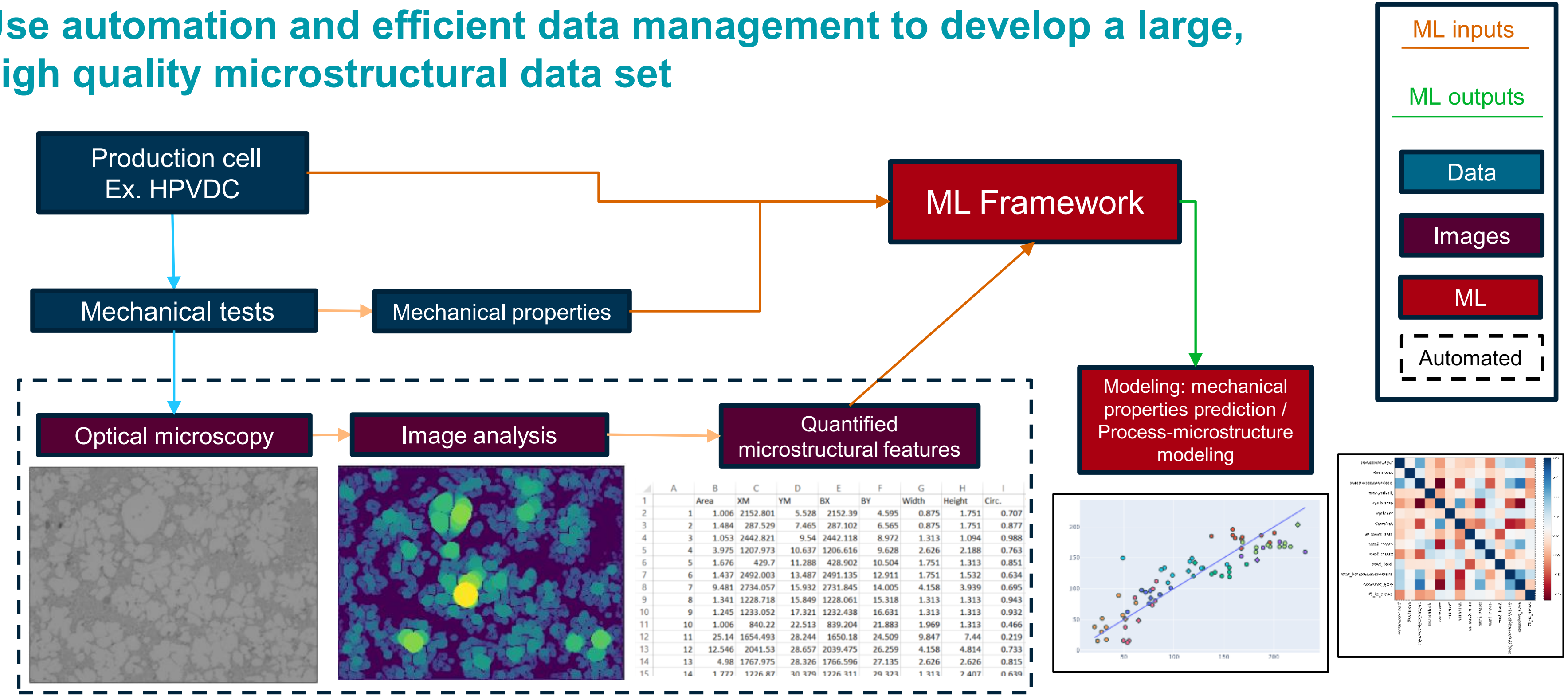


Probability to get an average porosity size above 150 µm

Define “safe” process window. Unlock the capacity to predict if porosity will be an issue for a given set of parameters.

Development workflow
Acquire data and train various models

Use automation and efficient data management to develop a large, high quality microstructural data set



	A	B	C	D	E	F	G	H	I
1		Area	XM	YM	BX	BY	Width	Height	Circ.
2	1	1.006	2152.801	5.528	2152.39	4.595	0.875	1.751	0.707
3	2	1.484	287.529	7.465	287.102	6.565	0.875	1.751	0.877
4	3	1.053	2442.821	9.54	2442.118	8.972	1.313	1.094	0.988
5	4	3.975	1207.973	10.637	1206.616	9.628	2.626	2.188	0.763
6	5	1.676	429.7	11.288	428.902	10.504	1.751	1.313	0.851
7	6	1.437	2492.003	13.487	2491.135	12.911	1.751	1.532	0.634
8	7	9.481	2734.057	15.932	2731.845	14.005	4.158	3.939	0.695
9	8	1.341	1228.718	15.849	1228.061	15.318	1.313	1.313	0.943
10	9	1.245	1233.052	17.321	1232.438	16.631	1.313	1.313	0.932
11	10	1.006	840.22	22.513	839.204	21.883	1.969	1.313	0.466
12	11	25.14	1654.493	28.244	1650.18	24.509	9.847	7.44	0.219
13	12	12.546	2041.53	28.657	2039.475	26.259	4.158	4.814	0.733
14	13	4.98	1767.975	28.326	1766.596	27.135	2.626	2.626	0.815
15	14	1.772	1226.87	30.379	1226.311	29.323	1.313	2.407	0.639

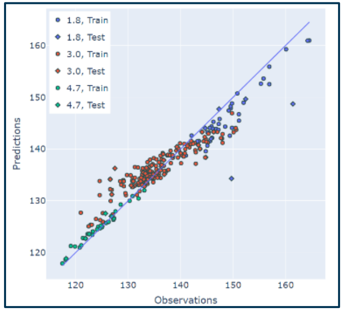
Production workflow
Use trained model to predict new cases

Leverage tuned models to predict key material properties when developing new parts

Production cell
Ex. HPVDC

Tuned ML models

Mechanical properties prediction



Microstructural quality classification

Optical microscopy

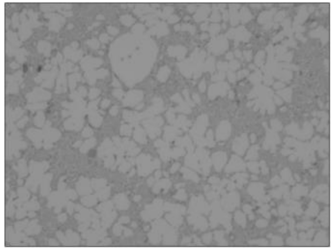
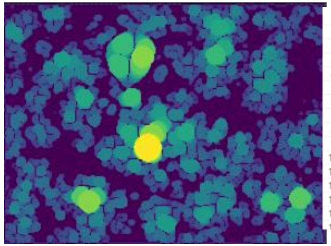
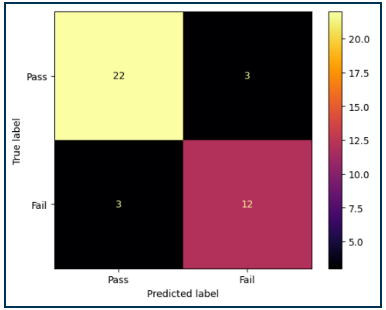


Image analysis



Quantified microstructural features

	A	B	C	D	E	F	G	H	I
1		Area	XM	YM	BX	BY	Width	Height	Circ.
2	1	1.006	2152.801	5.528	2152.39	4.595	0.875	1.751	0.707
3	2	1.484	287.529	7.465	287.102	6.565	0.875	1.751	0.877
4	3	1.053	2442.821	9.54	2442.118	8.972	1.313	1.094	0.988
5	4	3.975	1207.973	10.637	1206.616	9.628	2.626	2.188	0.763
6	5	1.676	429.7	11.288	428.902	10.504	1.751	1.313	0.851
7	6	1.437	2492.003	13.487	2491.135	12.911	1.751	1.532	0.634
8	7	9.481	2734.057	15.932	2731.845	14.005	4.158	3.939	0.695
9	8	1.341	1228.718	15.849	1228.061	15.318	1.313	1.313	0.943
10	9	1.245	1233.052	17.321	1232.438	16.631	1.313	1.313	0.932
11	10	1.006	840.22	22.513	839.204	21.883	1.969	1.313	0.466
12	11	25.14	1654.493	28.244	1650.18	24.509	9.847	7.44	0.219
13	12	12.546	2041.53	28.657	2039.475	26.259	4.158	4.814	0.733
14	13	4.98	1767.975	28.326	1766.596	27.135	2.626	2.626	0.815
15	14	1.772	1226.87	30.379	1226.311	29.323	1.313	2.407	0.639



ML inputs

ML outputs

Data

Images

ML

Automated

Conclusions
Benefits of a digital characterization workflow

- **Automation largely reduces the effort required to build a microstructural dataset (up to a factor 10!);**

- **Digitalization of the metallography lab allows to integrate microstructural data in a digital process workflow creating new possibilities for process development and quality control. In this project, leveraging the microstructural data using machine learning resulted in:**

Use case 1 (HPVDC):

- Good microstructure-mechanical properties models to predict yield strength (RMSE: 4.2 MPa, R^2: 0.77 on test set);

- Unsatisfactory ductility model for HPVDC (R^2 ~ 0.35) (not presented herein). Possible cause: Missing feature from OM dataset and/or very local properties that led to failure?

Use case 2 (CSAM):

- Good microstructure-mechanical properties models to predict the fracture stress of the CSAM deposits (R^2 ~ 0.80) (not presented herein);

- Process-microstructure relationships and models such as the porosity size classification model (Acc: 85%, prec: 80%, recall: 80%).

THANK YOU

Marc-Olivier Gagné • Research Council Officer

Marc-Olivier.Gagne@nrc-cnrc.gc.ca