Prediction of optical signatures and their influence on part performance: a model system using 316L stainless steel

William Kunkel, Dan J. Thoma

University of Wisconsin-Madison

ETI Annual Workshop

February 20 – 21, 2024, Golden, CO

National Nuclear Security Administration

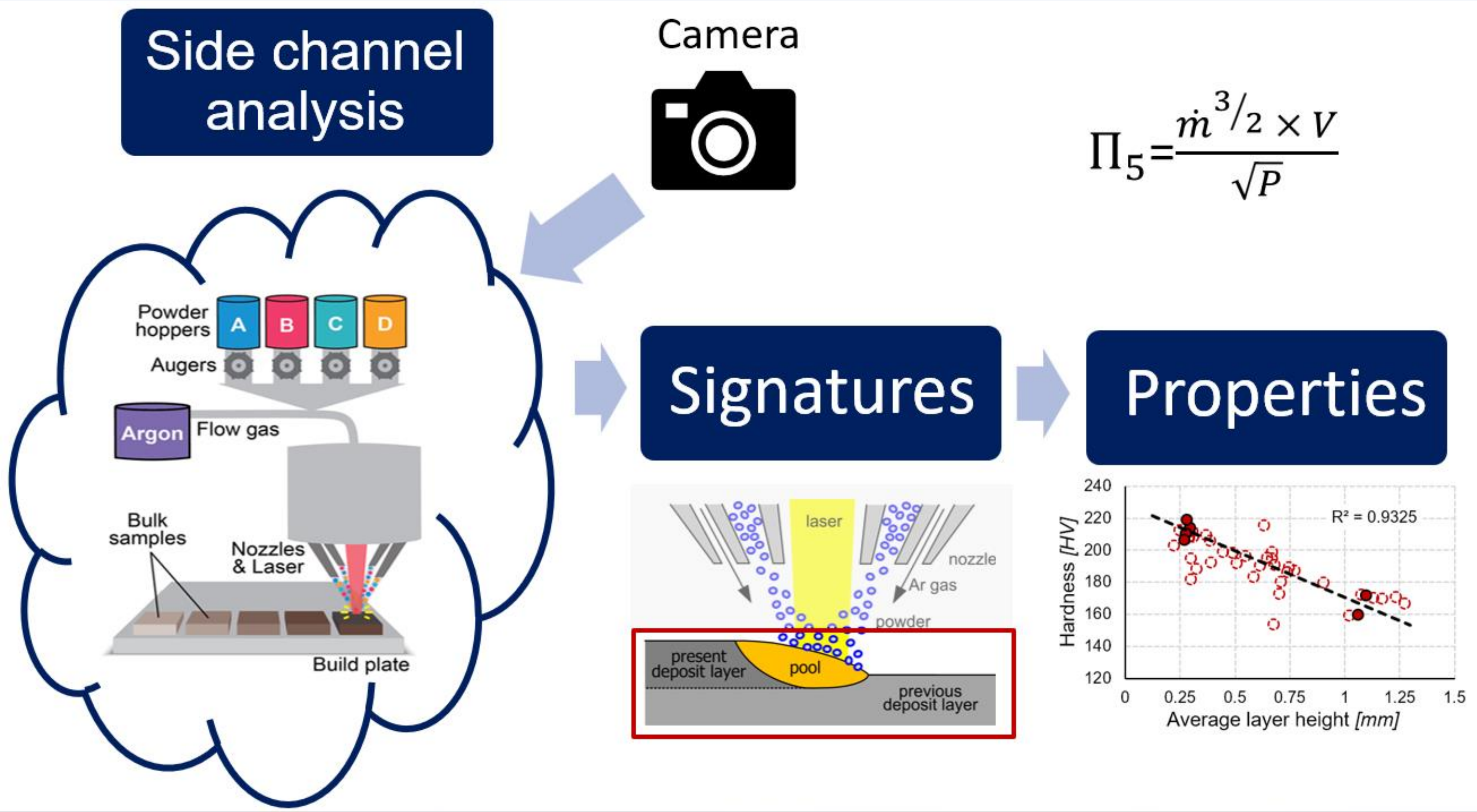
Consortium for Enabling Technologies & Innovation

Outline – signatures for verification and safeguarding of AM

1. Need for safeguards and verification in AM
2. Introduction to directed energy deposition (DED)
3. Existing predictive models for DED
4. Analytical and ML methods to predict signatures
5. Linking signatures to part performance
6. Summary

National Nuclear Security Administration

Overview of using signatures for verification and safeguarding of AM



Develop reduced order model to predict signatures

Outline – signatures for verification and safeguarding of AM

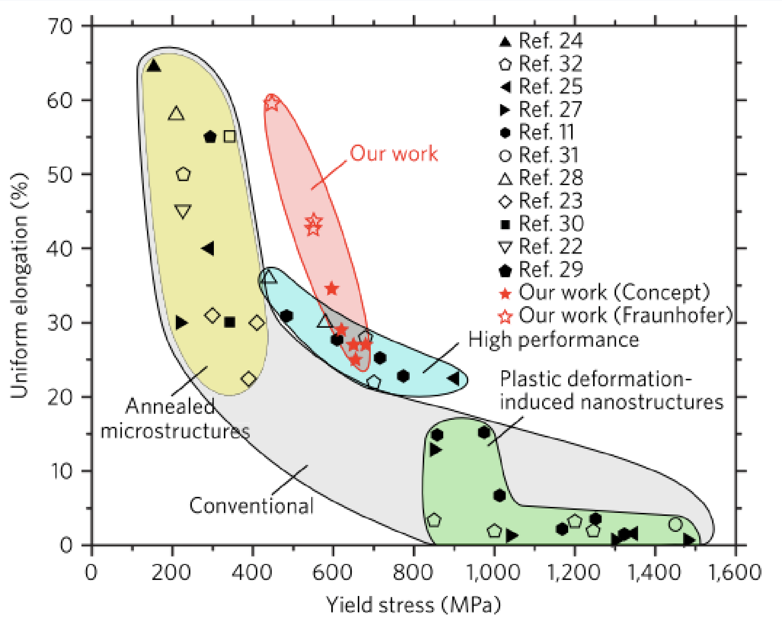
1. **Need for safeguards and verification in AM**
   - **Process any material**
2. Introduction to directed energy deposition (DED)
3. Existing predictive models for DED
4. Analytical and ML methods to predict signatures
5. Linking signatures to part performance
6. Summary

National Nuclear Security Administration

Process any material in complex geometries

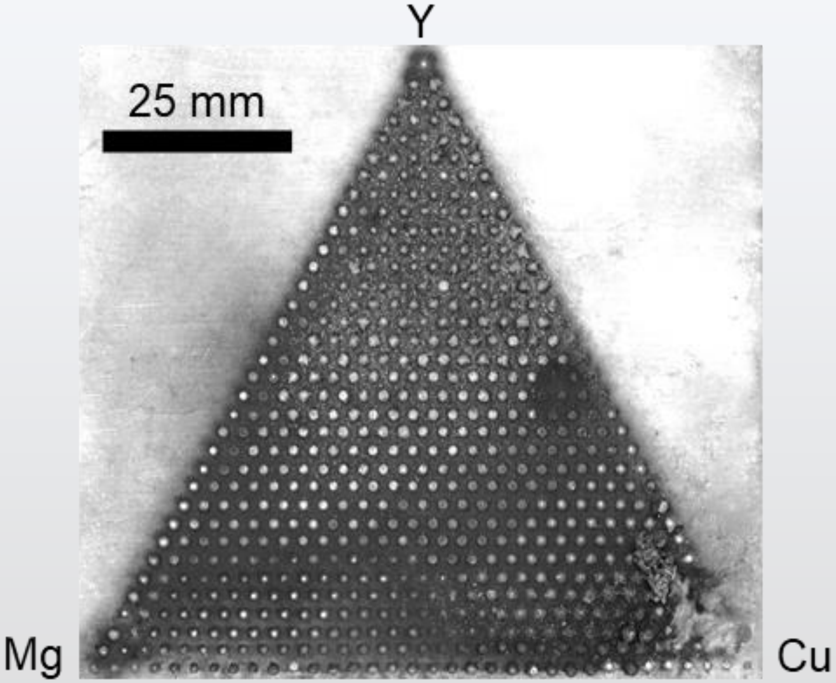
Enhanced materials properties

Dense materials

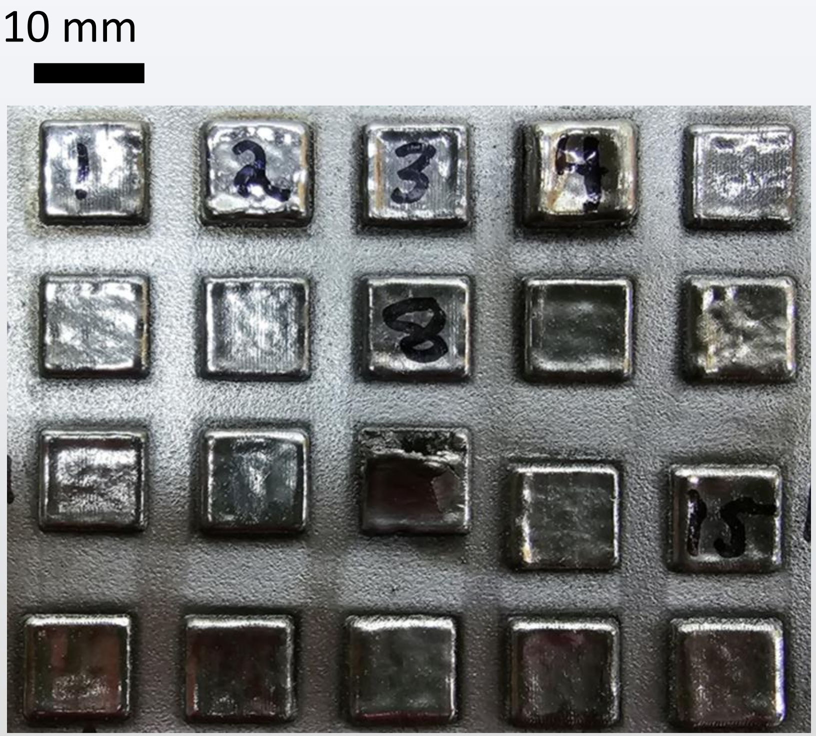


Enhanced strength/ductility ratio [2]

Other examples of superior properties include corrosion [3], irradiated-assisted stress corrosion cracking [4]



Mg-Cu-Y Metallic Glass [1]



Niobium based HEA

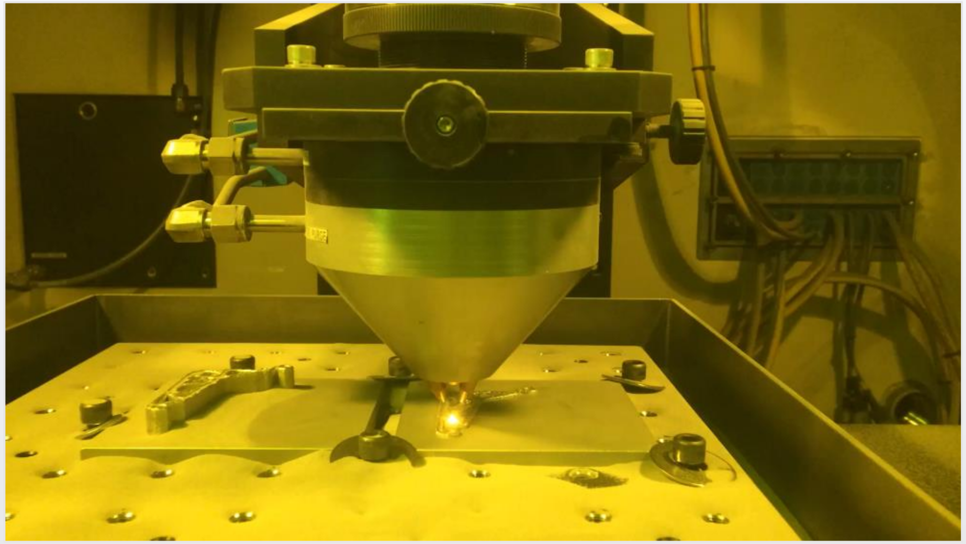
[1] Thoma, Dan J., et al. *Metals* 13.7 (2023): 1317
[2] Y.M. Wang et al., Additively manufactured hierarchical stainless steels with high strength and ductility, Nat. Mater. 17 (2018) 63–70.
[3] Q. Chao et al., On the enhanced corrosion resistance of a selective laser melted austenitic stainless steel, Scr. Mater. 141 (2017) 94–98.
[4] M. Song et al., Radiation damage and irradiation-assisted stress corrosion cracking of additively manufactured 316L stainless steels, J. Nucl. Mater. 513 (2019) 33–44.

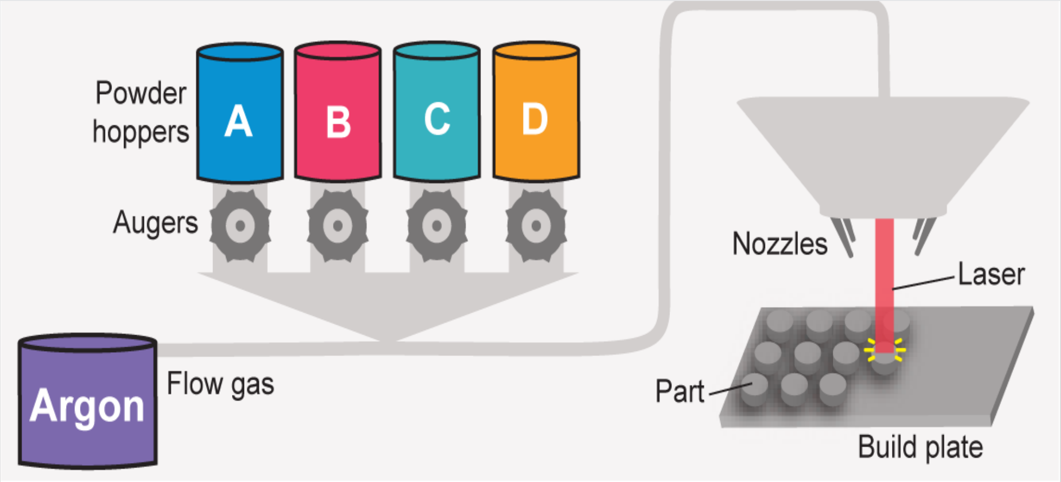
National Nuclear Security Administration

Outline – signatures for verification and safeguarding of AM

1. Need for safeguards and verification in AM
2. **Introduction to directed energy deposition (DED)**
   - **Processing-Structure-Property Relationships (*Conventional*)**
   - **Signature-Property Relationships *(New)***
3. Existing predictive models for DED
4. Analytical and ML methods to predict signatures
5. Linking signatures to part performance
6. Summary

Directed Energy Deposition (DED) process





Common uses

- Functionally graded materials
- Repair and cladding

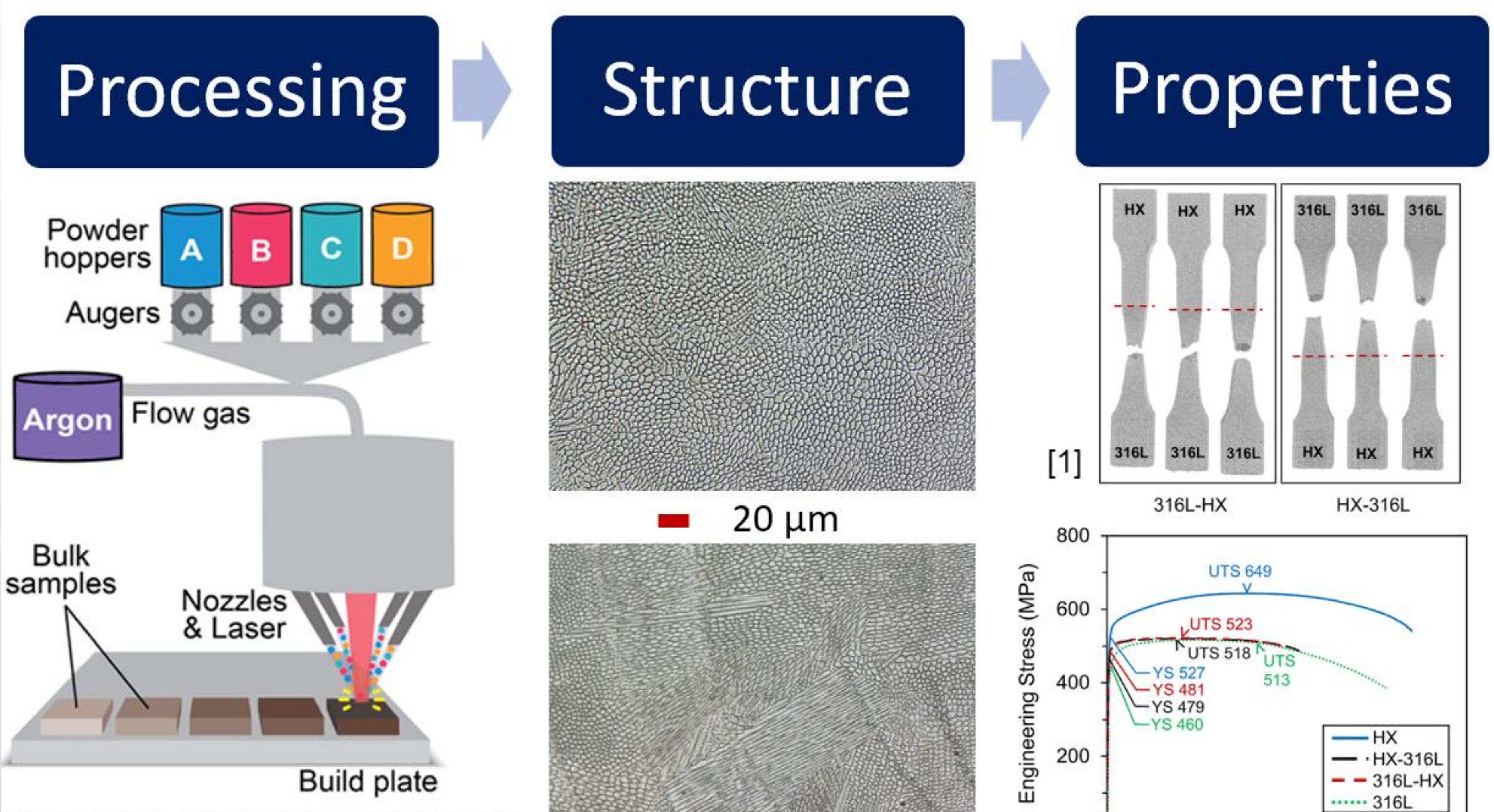
Challenges to nonproliferation

- 100 + variables

Need reduced order model

National Nuclear Security Administration

Conventional understanding of AM parts

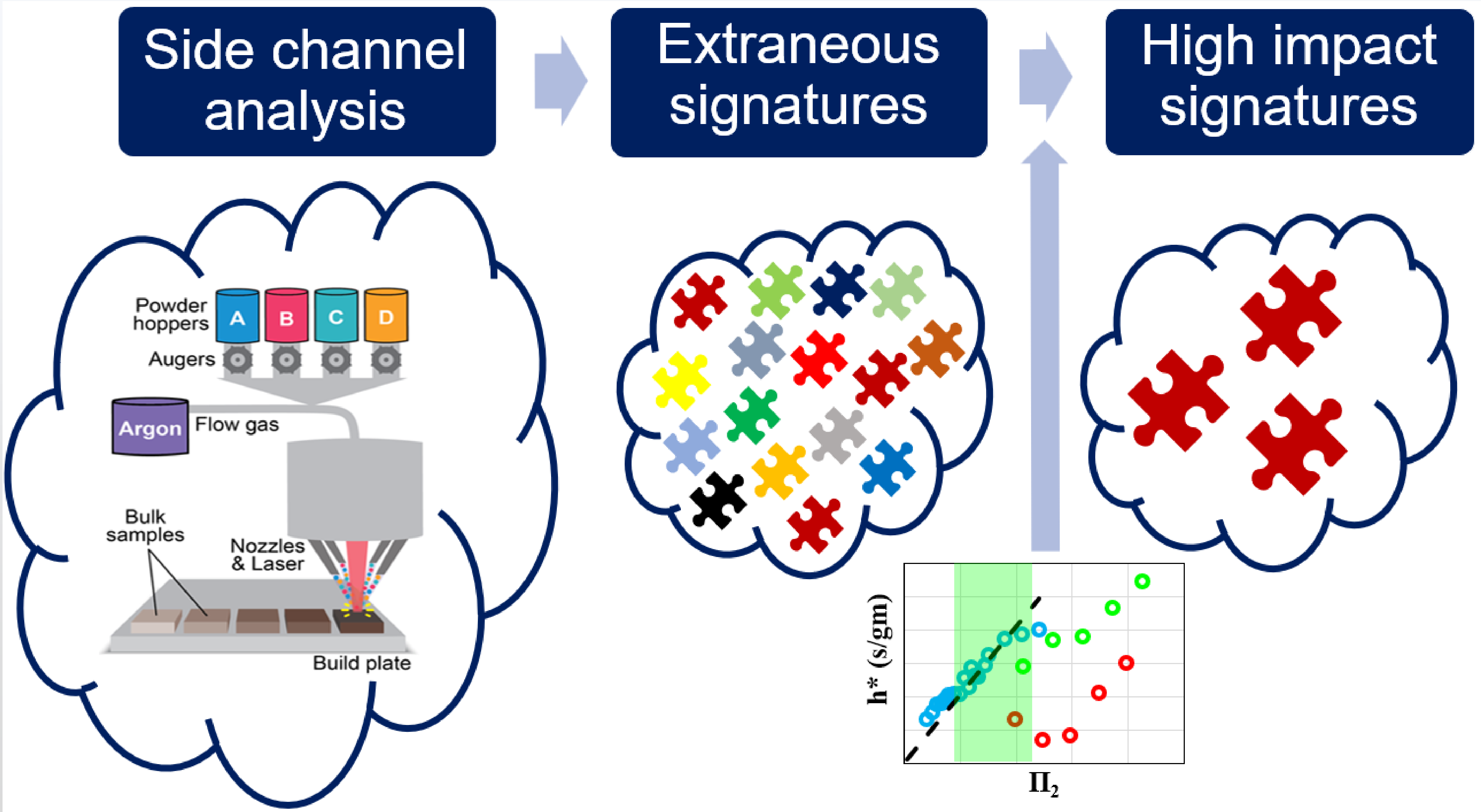


[1] Rankouhi, Behzad, et al. "Characterization of multi-material 316L-Hastelloy X fabricated via laser powder-bed fusion." *Materials Science and Engineering: A* 837 (2022): 142749.

Direct access to:
- Parts
- MFG information

Need link from processing to properties

Dimensional analysis provides a pathway to identify the important information to extract

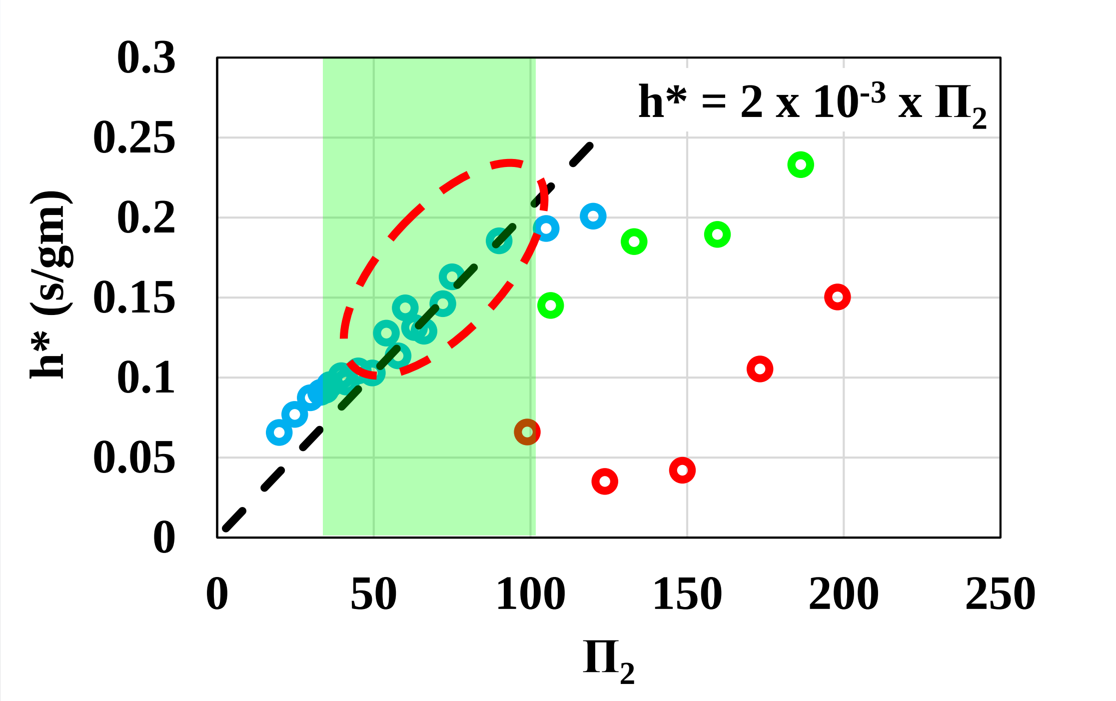


Outline – signatures for verification and safeguarding of AM

1. Need for safeguards and verification in AM
2. Introduction to directed energy deposition (DED)
3. **Existing predictive models for DED**
   - **Predict process parameters for any material**
   - **Model optical signatures**
   - **Developed using dimensional analysis**
4. Analytical and ML methods to predict signatures
5. Linking signatures to part performance
6. Summary

National Nuclear Security Administration

Background: Dimensional analysis to identify process parameters



$$h^* = \frac{h_{actual}}{(n \times Z) \times \dot{m}}$$

$$\Pi_2 = \frac{E_g \times \alpha}{\dot{m} \times H} \times \frac{Z}{h} = \frac{P \times \alpha}{v \times D_l \times \dot{m} \times H} \times \frac{Z}{h}$$

- Uses electronic signatures, laser spot size and material properties
- **Works across material systems**
- 316L ss, Cr-Fe-Mn-Ni MPEA, Mo-4Si-6B

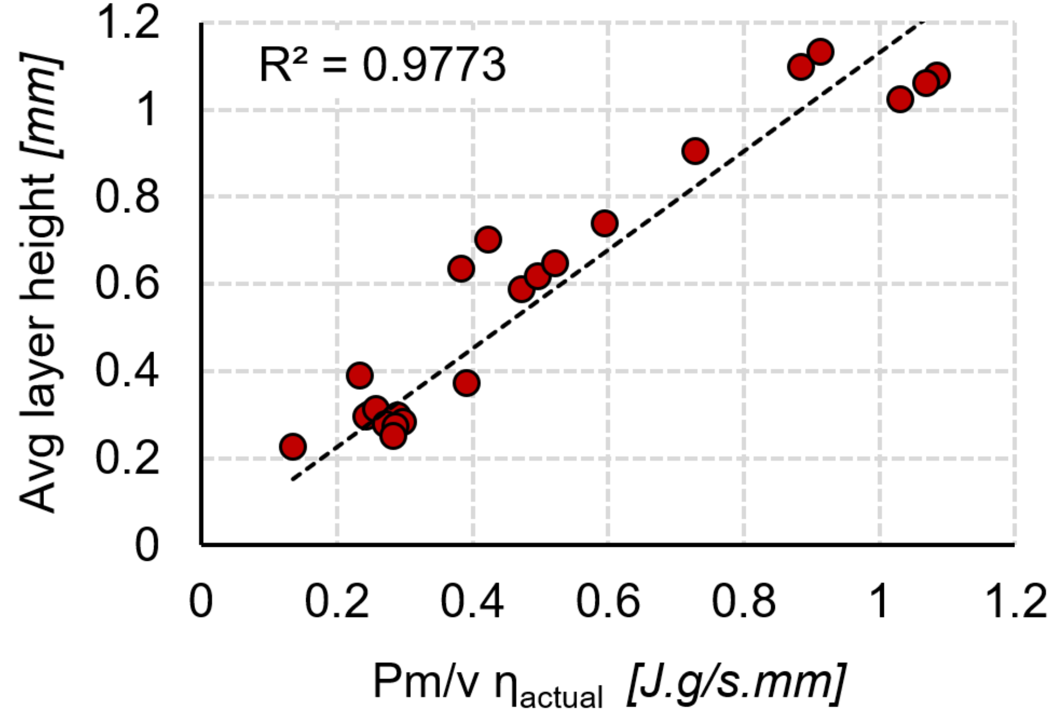
Quality builds follow $h^* = 2 \text{ x } 10^{-3} \text{x } \pi_2$

[2] Z. Islam et al., Applied Physics Letters 119.23 (2021): 231901.

[3] Z. Islam et al., "Reactive Synthesis in Additive Manufacturing of an Ultrahigh Temperature MoSiB Alloy" *(Accepted)*

National Nuclear Security Administration

Model: Average layer height (Optical signature)



$$\frac{\text{Power} \times \text{Mass flow rate}}{\text{Scanning speed}} \times \eta_{\text{actual}}$$

- Build geometry and capture efficiency are coupled [4],[5]
- Average layer height can be precited from process information and capture efficiency
- $\boldsymbol{\eta_{actual}}$ **is a measured value**

[4] S. Donadello et a, *Opt. Lasers Eng.*, vol. 149, p. 106817, Feb. 2022, doi: 10.1016/j.optlaseng.2021.106817.

[5] R. Koike et al, S.*Procedia CIRP*, vol. 78, pp. 133–137, Jan. 2018, doi: 10.1016/j.procir.2018.09.061.

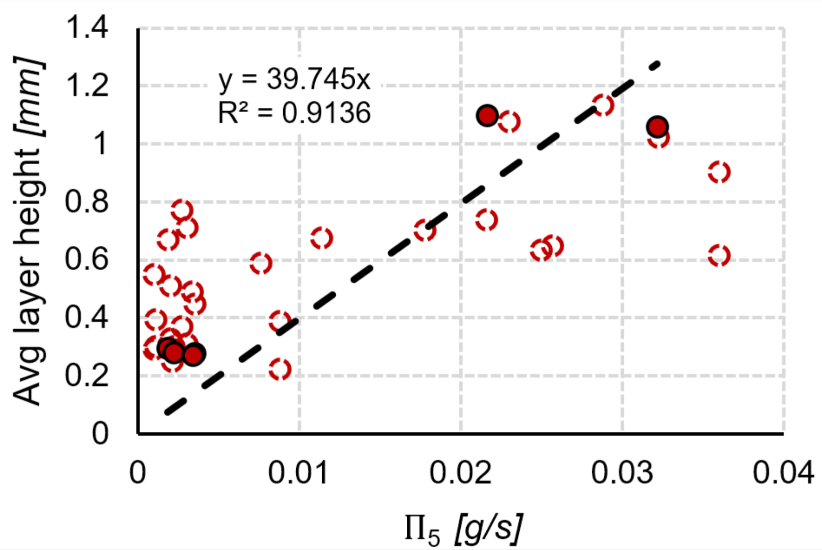
National Nuclear Security Administration

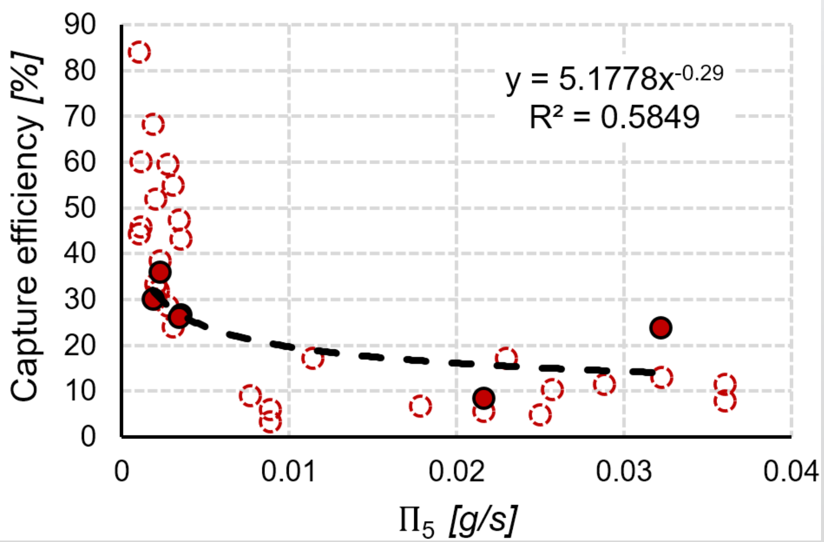
Outline – signatures for verification and safeguarding of AM

1. Need for safeguards and verification in AM
2. Introduction to directed energy deposition (DED)
3. Existing predictive models for DED
4. **Analytical and ML methods to predict signatures**
    - **Using reduced order modeling, ML and analytical agree**
5. Linking signatures to part performance
6. Summary

National Nuclear Security Administration

Model for capture efficiency and average layer height





Defects

No defects

$$\Pi_5 = \frac{\dot{m}^{3/2} \times V}{\sqrt{P}}$$

- Buckingham Pi Theory for dimensional analysis
  - Scaled by $\dot{m}$

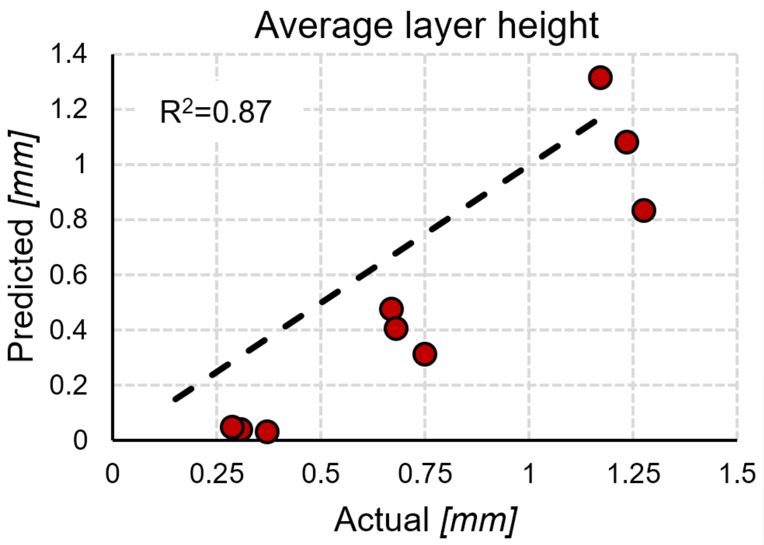
- **Capture efficiency is high at high powers (low pi)**
- Capture efficiency is lower at high flow rates

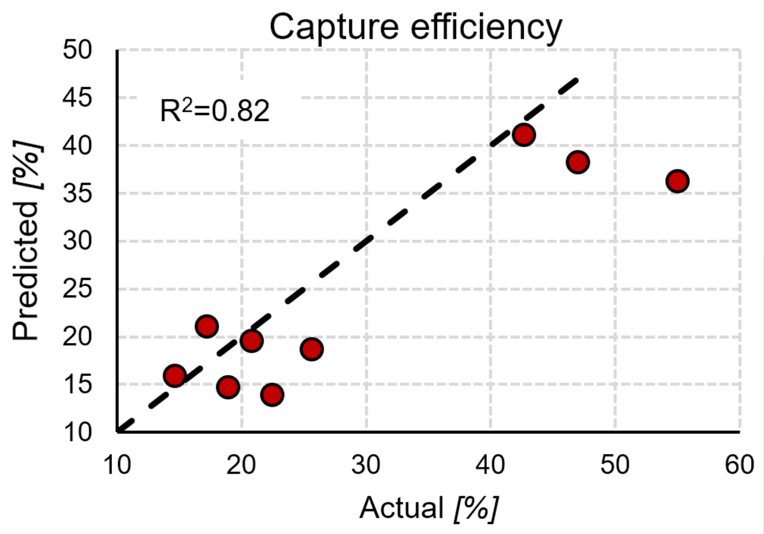
- Layer height increases with mass flow rate
- **Layer height decreases with high powers (spreading)**

Signatures give information about processing !!!!

National Nuclear Security Administration

Predicting signatures using analytical models

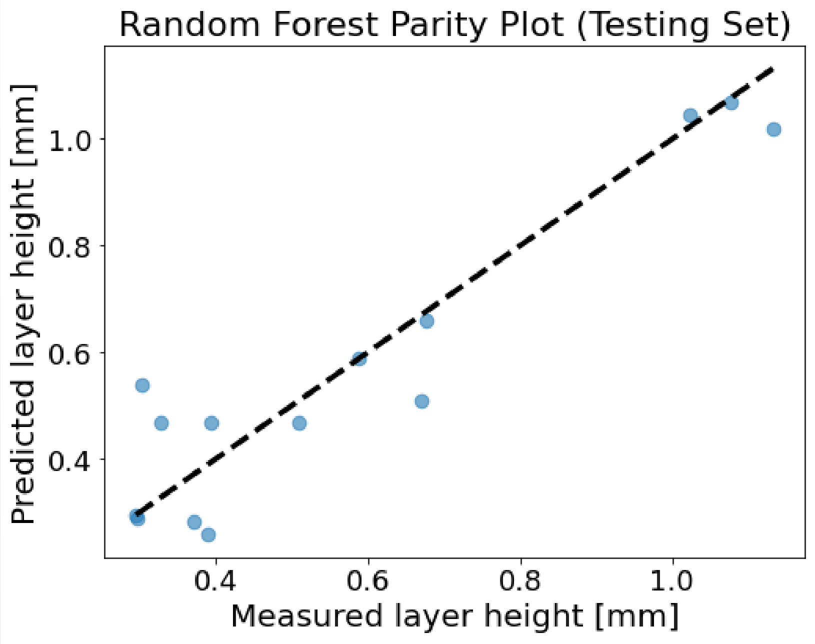


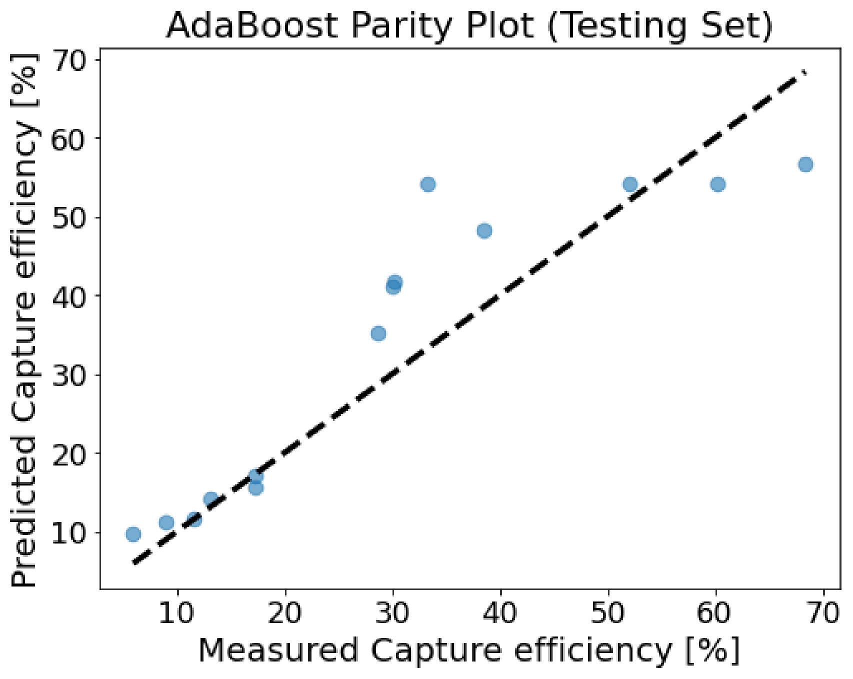


$$\boxed{\Pi_5 = \frac{\dot{m}^{3/2} \times V}{\sqrt{P}}}$$

- Optical signatures were predicted
  - *Predictions were underestimated*
- Simple model → complex phenomena
- **Pathway from optical signatures to processing conditions**

Predicting signatures using ML methods





ML Methods

Agrees with analytical

Used:
$\dot{m}$, P, V, Z

Model	(Layer height) MSE	(Layer height) R^2	(Efficiency) MSE	(Efficiency) R^2
Random forest	0.1	**0.88**	11.71	0.61
Gradient boosting	0.14	0.78	15.88	0.29
Adaptive boosting	0.21	0.49	8.59	**0.79**

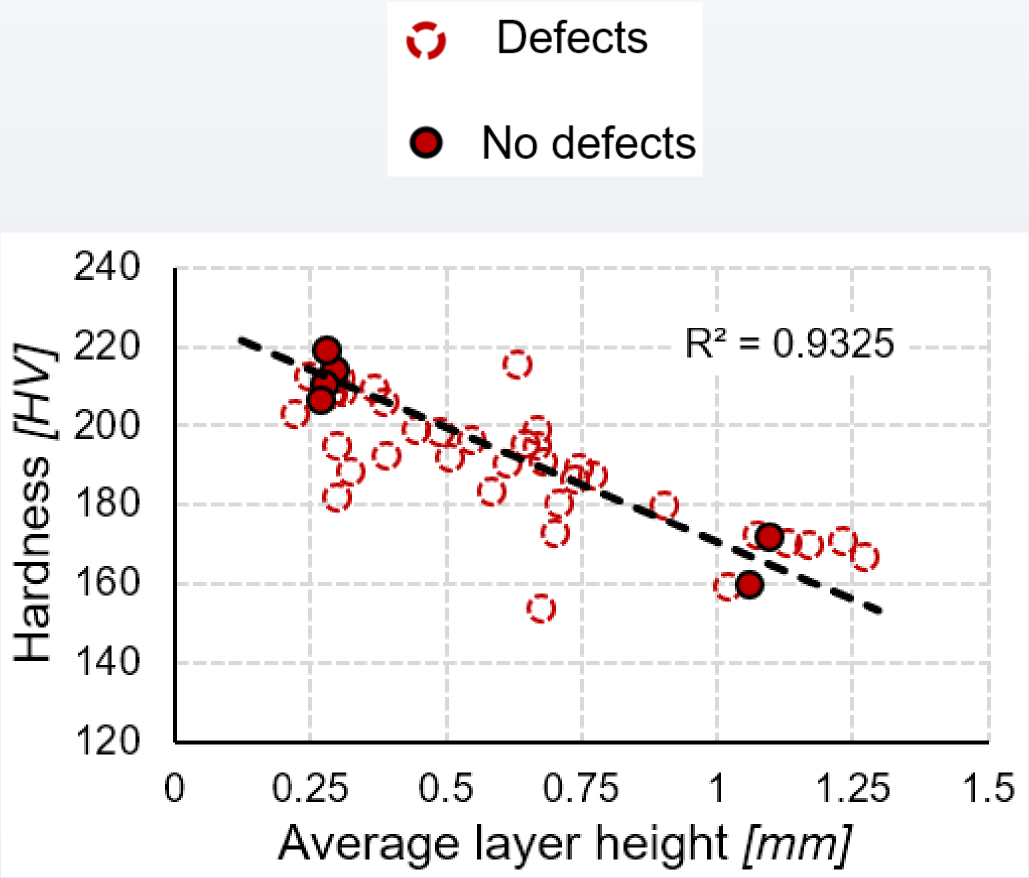
National Nuclear Security Administration

Outline – signatures for verification and safeguarding of AM

1. Need for safeguards and verification in AM
2. Introduction to directed energy deposition (DED)
3. Existing predictive models for DED
4. Analytical and ML methods to predict signatures
5. **Linking signatures to part performance**
    - **Optical signatures are predictive of material properties**
6. Summary

National Nuclear Security Administration

Influence of optical signatures on performance (Structure and properties)



Optical signatures ←→	**Performance**
Δ Height 279%	Δ Hardness 27%

- **Optical signatures scale with performance**
- Hall-Petch relationship links DAS and Hardness
- DAS (cooling rate)→ governing mechanism
  - Likely other features

National Nuclear Security Administration

Outline – signatures for verification and safeguarding of AM

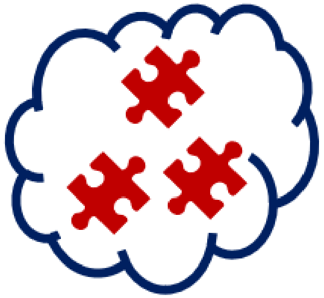
1. Need for safeguards and verification in AM
2. Introduction to directed energy deposition (DED)
3. Existing predictive models for DED
4. Analytical and ML methods to predict signatures
5. Linking signatures to part performance
6. **Summary**

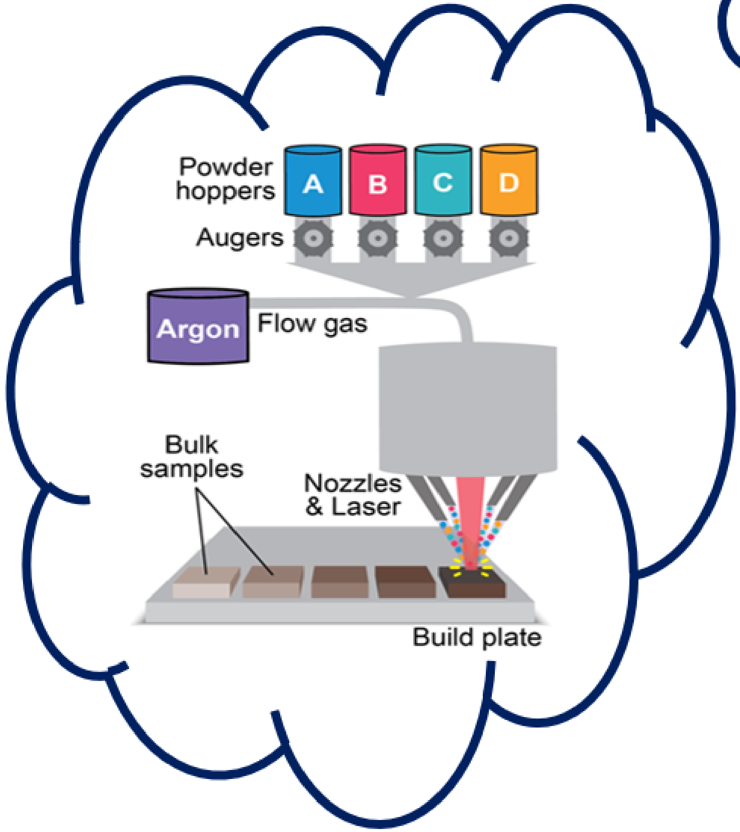
National Nuclear Security Administration

Summary →Optical signatures predict performance

Side channel analysis

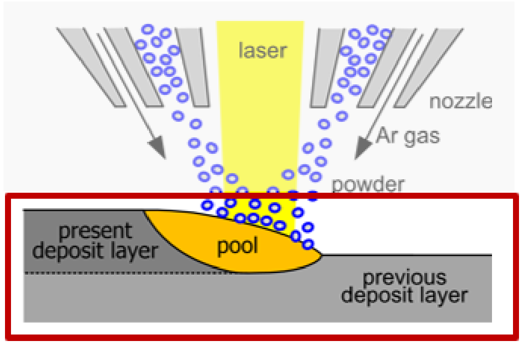
$$\Pi_5 = \frac{\dot{m}^{3/2} \times V}{\sqrt{P}}$$

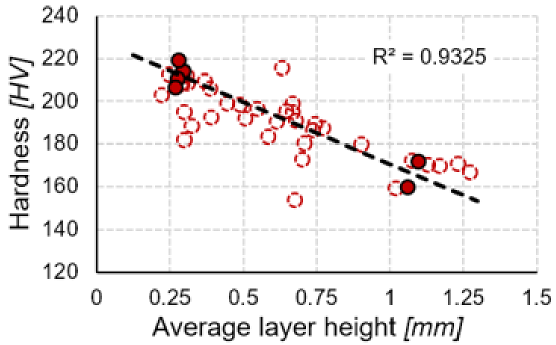




Signatures

Properties





Reduced order model and ML predict performance

ACKNOWLEGEMENTS

This material is based upon work supported by the Department of Energy / National Nuclear Security Administration under Award Number(s) DE-NA0003921.

NNSA
National Nuclear Security Administration

Consortium for
ENABLING TECHNOLOGIES & INNOVATION