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Materials Design for Advanced Systems

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Materials Design for Advanced Systems

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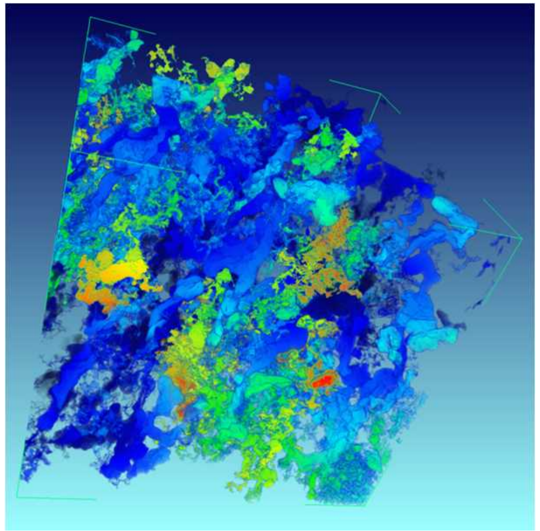
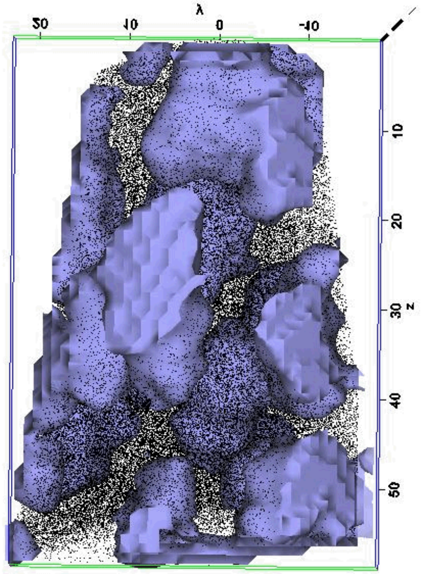
Materials Science and Engineering

FY 2018





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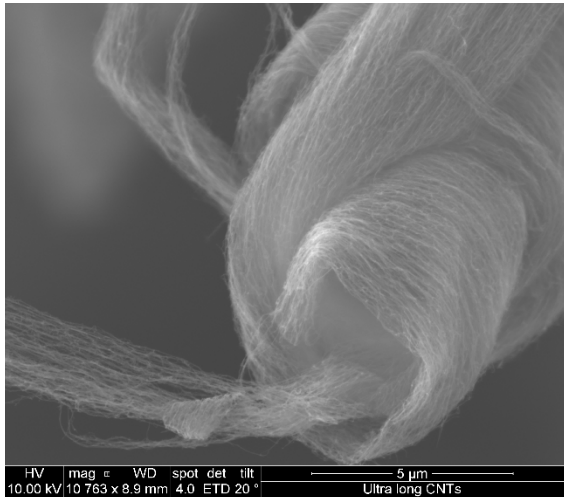
What Happens When you Mix Carbon Nanotubes with Alloys

Ultra Long Chain Carbon Nano-Tubes



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Al

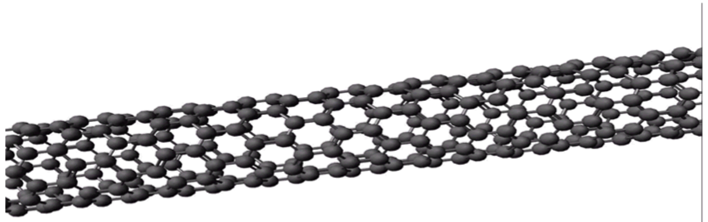
=

Metal Matrix Composites

0.2% Vol CNT additions can result in:

- >75% increase in yield strength
- >50% increase in tensile strength
- ~45% increase in hardness (Hv)

- **Highly anisotropic material**
- **Ultra-light material-** ***~1.5 g/cm^3***
- **Ultra-high specific strength-** ***~100X > steel (tensile)***
- **High specific surface area-** ***~1300 m^2/g***
- **Ultra-high thermal conductivity-** ***4X-9X > Cu***
- **Ultra-high current densities-** ***~10^{6}X > copper***



Challenges
Engineering Anisotropy
Engineering Microstructure

These CNT MMC can be engineered with directional anisotropy to:

- Effectively increase thermal conductivity along a desired direction
- Decreasing thermal conductivity in a perpendicular direction
- Employed where Lightweight and directional conductivity is essential

Carbon nanotube (CNT) reinforced Aluminum Metal Matrix Composites (MMC):

Carbon nanotubes are an amazing class of carbon nanomaterials. Nominally they have a:
density of ~1.5 g/cm^3 or less making them a light weight material
high specific strength (tensile) ~100X greater than steel
high specific surface areas up to ~1300 m^2/g
high thermal conductivity 4X-9X greater than copper
These excellent properties have led to their use as additives in polymers and specialized coatings to enhance the base properties of the parent material.
CNT-reinforced MMCs have been investigated as a means to enhance mechanical, thermal, and electrical properties over the base metal matrix. They may be of considerable interest for vehicle light-weighting applications because CNTs can be used in relatively small amounts to invoke a considerable change in properties over the base metal matrix [1] (see Table 1 [2]). While hypothetically attractive, this emerging class of materials has not been adopted by industry. This is likely due to a lack of practical processing techniques to allow use in current industrial infrastructure while addressing the issues of:
CNT dispersion within the metal matrix
Adhesion of CNTs to the metal matrix and its interfacial properties
Addressing these issues are critical to producing a high performance CNT-reinforced MMC [1].

Carbon nanotube (CNT) reinforced Aluminum Metal Matrix Composites (MMC):

Table 1: *Mechanical properties listed for an induction cast CNT-reinforced high purity aluminum metal matrix composite.*

Using the values from Table 1 [2], and current market pricing for high quality single-wall CNTs [3], the added materials cost of the CNTs added on a per pound basis is less than $1/lb$_m$ aluminum.

Vol % CNTs	Elastic Mod. (GPa)	Yield Strength (MPa)	Tensile Strength (MPa)	Elongation (%)	Hardness (H_v)
0%	64±1.5	65±5	82±4	2.15±0.35	27±4
0.1%	65±2.1	105±4	112±3	2.35±0.40	34±4
0.2%	67±2.9	115±5	125±3	3.10±0.55	39±5

A brief survey of the available literature on CNT-reinforced Aluminum MMCs, suggests **the majority of research efforts have focused on high purity aluminum**. While of scientific interest, pure aluminum is not directly applicable to the automotive industry. A handful of research articles were found on the following alloys A356, 2014, 2024, 6061, 6082, and 7075 [4-8]. A majority of these efforts incorporated CNTs directly via stir casting or used ball milling to "mechanically alloy" CNTs with alloy powder before consolidation. No CNT-reinforced Al-alloy MMC work within the U.S. was found from the brief literature survey.

Carbon nanotube (CNT) reinforced Aluminum Metal Matrix Composites (MMC):

Additionally, no information was found on the effects of carbon nanotubes on the formability or malleability of the resulting composites. While no direct information was given, some of the references provided below at least indirectly suggest that the CNT-reinforced Al alloy MMC could be formed and shaped via routine methods.

INL Funded Seed Project:

INL has currently invested a small quantity of internal research dollars towards the investigation of CNT-reinforced Al MMCs. The composition of the Al alloy is very similar to A356. This work is specifically focused on the use of an induction casting method. As some Aluminum alloys have paramagnetic properties, the electromagnetic field generated from induction coils can induce a flow in the Al melt. This in turn leads to inherent mixing of CNTs into the melt and ideally maximizes CNT dispersion within the metal matrix.

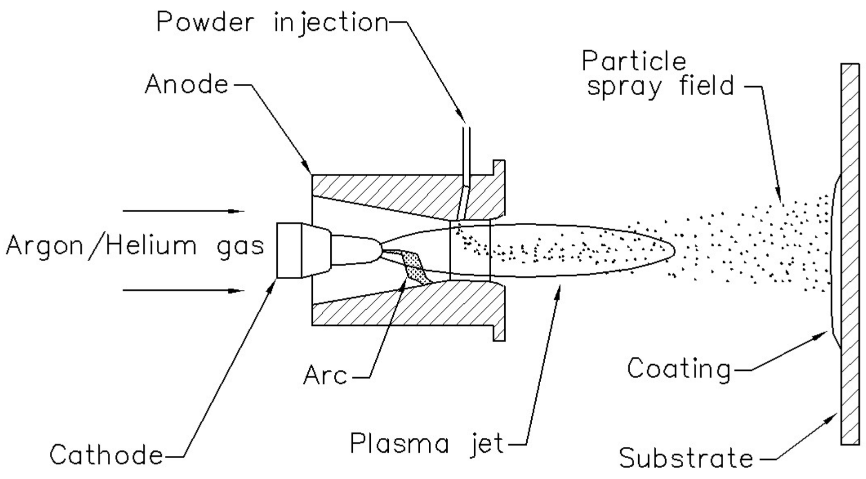
[1] S.R. Bakshi, D. Lahiri, and A. Agarwal, Carbon nanotube reinforced metal matrix composites – a review, International Materials Reviews 55(1) (2010) 41-64
[2] M. Mansoor, M. Shahid, Carbon nanotube-reinforced aluminum composite produced by induction melting, J. App Res Tech. 14(4) (2016) 215-224.
[3] OCSiAl General Price Reference Sheet https://ocsial.com/assets/documents/TUBALL_Price_List_General_1.pdf
[4] H.H. Kim, J.S.S. Babu, C.G. Kang, Fabrication of A356 aluminum alloy matrix composite with CNTs/Al_2O_3 hybrid reinforcements, Mat Sci Eng A 573 (2013) 92-99.
[5] R. Perez-Bustamante, M.J. Gonzalez-Ibarra, J. Gonzalez-Cantu, I. Estrada-Guel, J.M. Herrera-Ramirez, M. Miki-Yoshida, et al, AA2024-CNTs composites by milling process after T6-temper condition, J Alloys and Compounds 536S (2012) S17-S20.
[6]X. Zhu, Y. Zhao, M. Wu, H. Wang, Q. Jiang, Fabrication of 2014 aluminum matrix composites reinforced with untreated and carboxyl-functionalized carbon nanotubes, J Alloys and Compounds 674 (2016) 142-152.
[7] A.A. Najimi, H.R. Shahverdi, Effect of milling methods on microstructures and mechanical properties of Al6061-CNT composite fabricated by spark plasma sintering, Mat Sci Eng A 702 (2017) 87-95.
[8] A. Basithrahman, S. Abirami, Tribological behavior of AA 7075 Hybrid Composite using Stir Casting Method, International Journal of Engineering Research and Technology, 6(1) (2017).

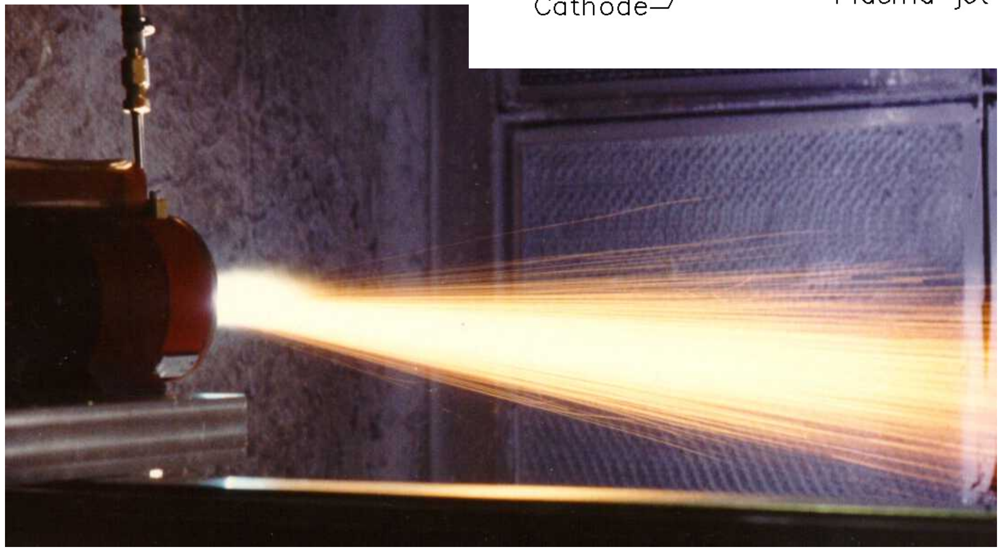
Coating Technologies Value Proposition: Development of Coating for Multi-Product Pipelines

- Currently, the oil industry transports crude oil, petroleum products and natural gas because it is energy efficient, safe and convenient. Ultimately, this results in reduced costs in getting products and streams from the site of origin or manufacture to point where it is needed.
- Typically there are dedicated pipelines for each type of stream being transported through the pipelines. Imagine a scenario where depending on compatibility, a single pipeline system can be used to transport multiple types of products. Such a pipeline would have to be engineered to withstand not only the external perturbations pipelines are exposed to (e.g., digging), but also mechanical stresses and corrosion and degradation, both external (due to soil or environment) and internal (caused by the characteristics of the product being transported).
- **Value Proposition:** A single pipeline will reduce initial capital expenditure for infrastructure, and will likely reduce overall operating expenditure since maintenance will be limited to a single pipeline, instead of multiple ones.
- In order to achieve this goal, it is proposed that materials and/or coating be developed for the multi-product pipelines. We propose to use modeling and simulations to screen and design materials for coatings and/or suitable piping materials. One of the many tools at our disposal include the use of Neural Network Potentials, coupled with Artificial Intelligence and Machine learning to identify material that can suitably be used for these multi-stream pipelines. INL also has world class coating capability to apply coatings using the formulations determined to be the most suitable.

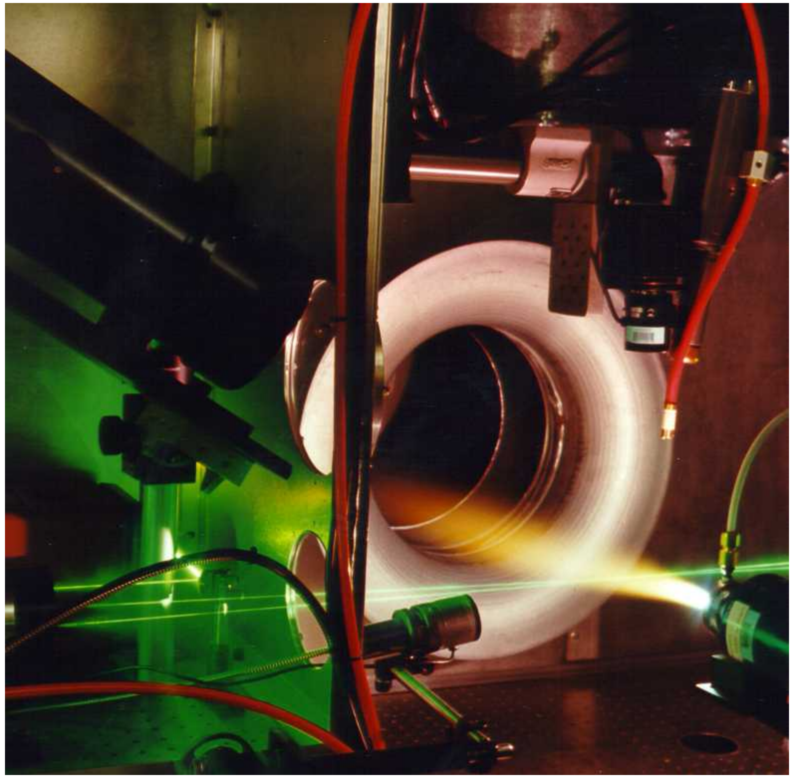
INL Has World Class Metallic Coating Capabilities

Key…consistently deliver particles with the “right” velocity, temperature, melt fraction, and chemistry to a properly prepared substrate.



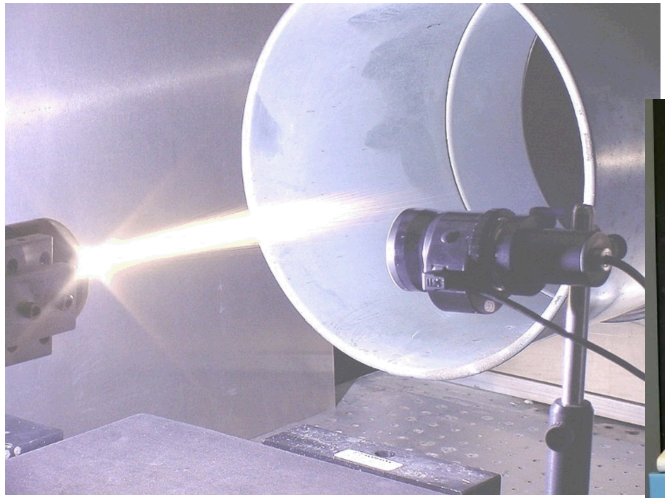


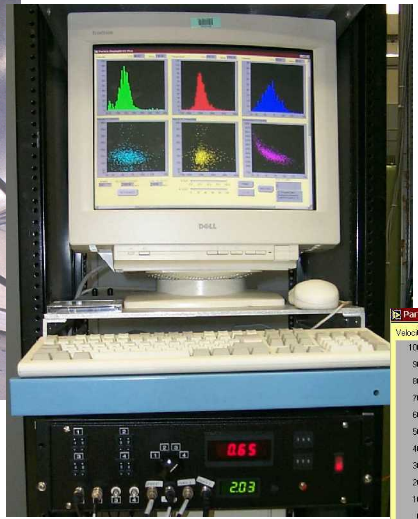
INL World Class Spray Diagnostics and Coating Development



- 15 years of thermal spray research with over 50 publications.
- Laser based measurement of particle velocity, size and temperature.
- Passive spray monitoring of particle state with active feedback control of spay parameters.

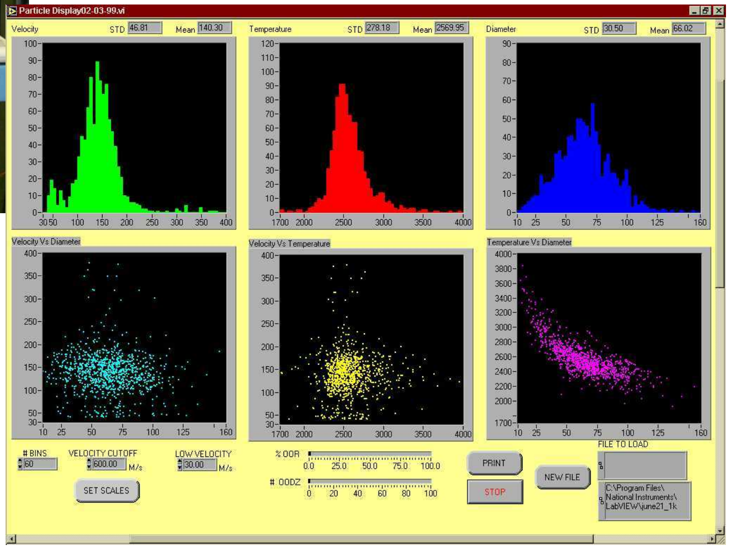
Spray Diagnostics: In-flight Particle Monitor





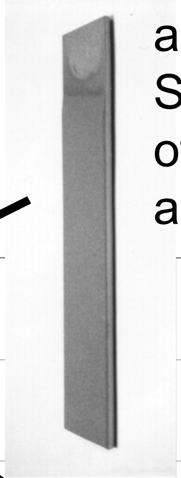
Passive measurement of individual sprayed particle velocity, size and temperature as a function of process parameters.

For consistent coating quality the sprayed particles must be delivered with the “right” velocity, temperature and melt fraction…

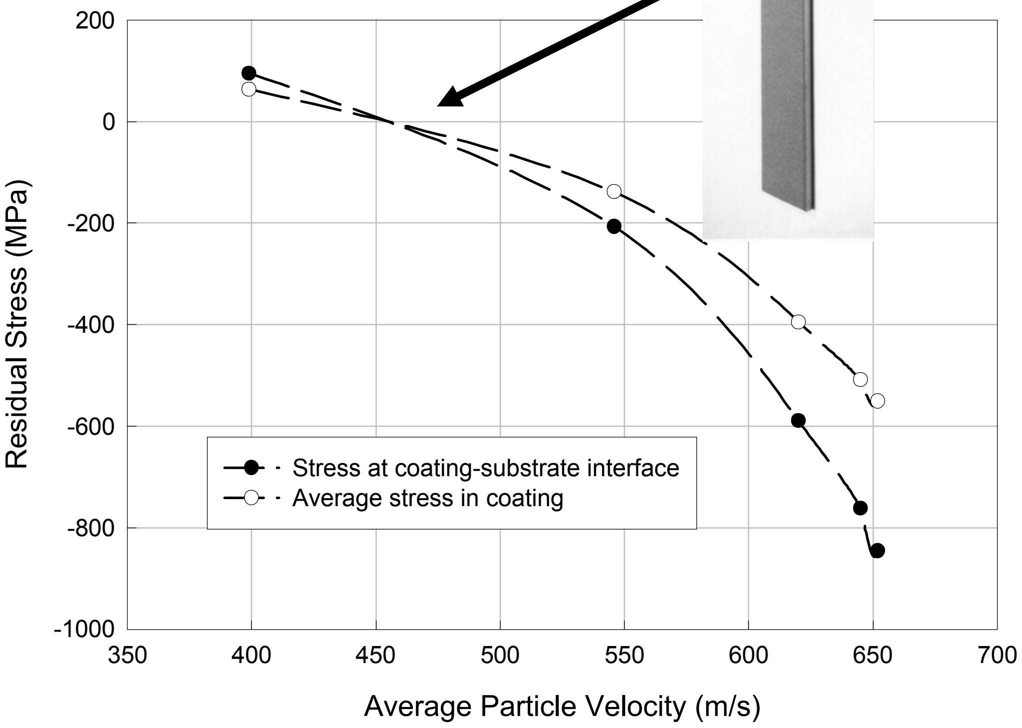


Control of Residual Stress By Controlling Sprayed Particle Velocity

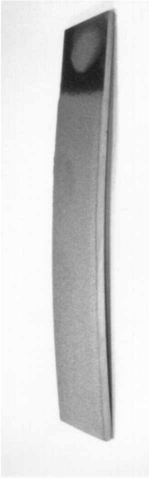
TENSILE



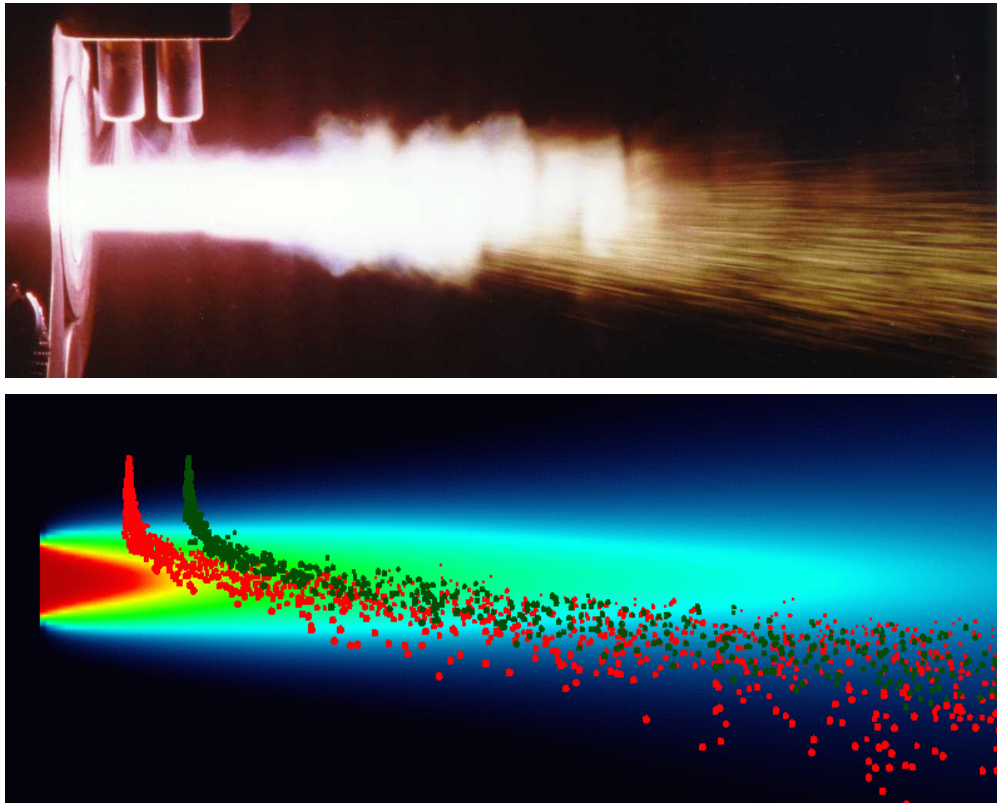
NEUTRAL residual stress can be achieved through the PEENING STRESS by measurement and control of the sprayed particle temperature and velocity



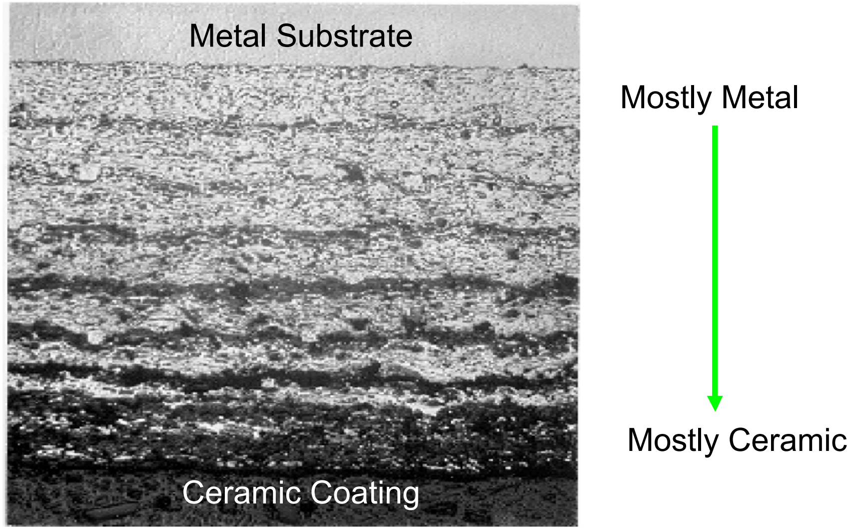
COMPRESSIVE



Control of CTE Mismatch through the Formation of Functionally Graded Materials with Dual Injection Plasma Spray



Metal and ceramic particulate precursors are injected individually through separate locations.

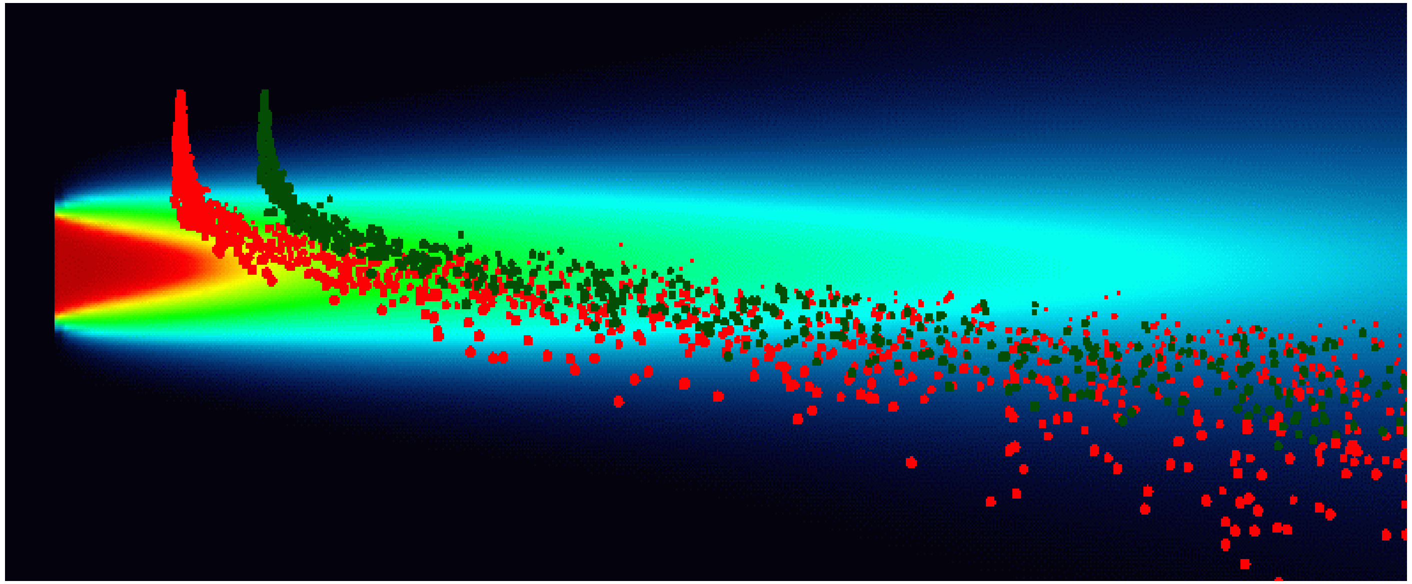


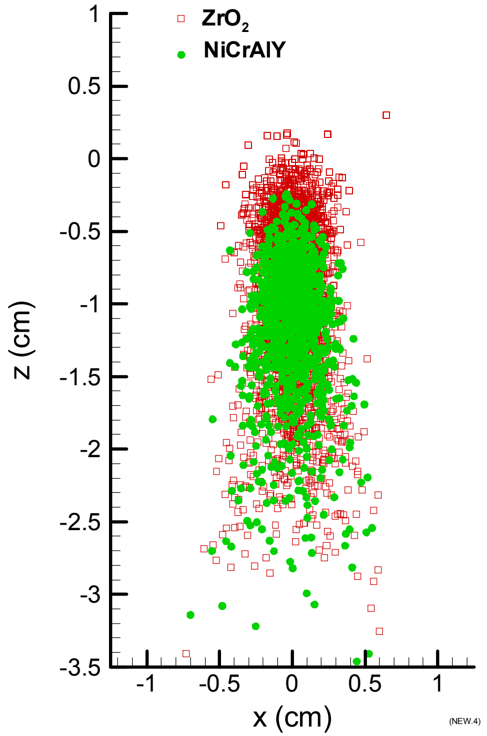
Graded coating with coefficient of thermal expansion match at the substrate interface graded to hard protective ceramic on the outer surface.

Thermal Spray Processing of Functionally Gradient Materials

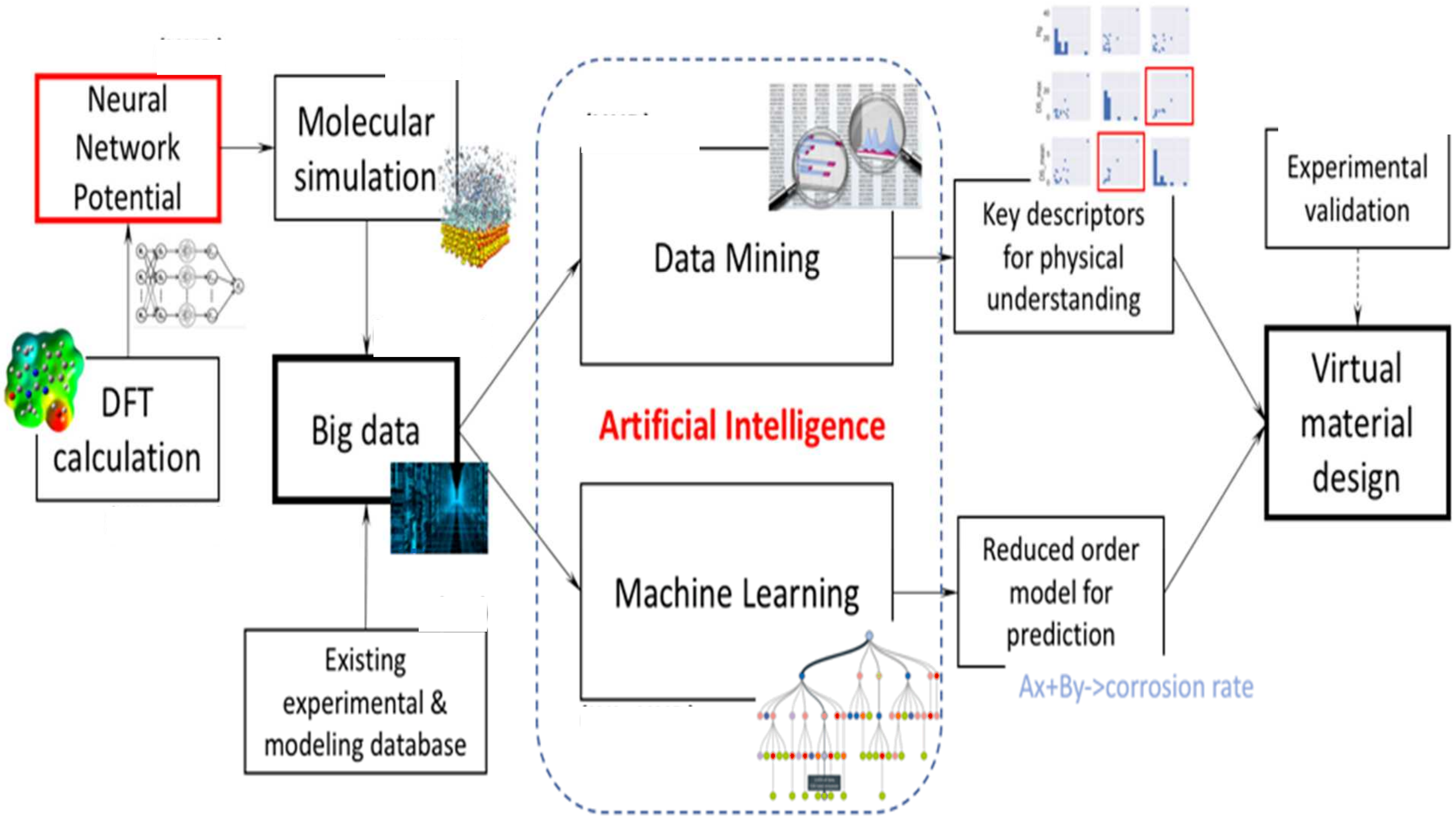
Successful thermal spray processing of FGMs requires that radically different particle types be delivered to the substrate with appropriate temperature, molten fraction, velocity, and with the same trajectory.

- Control of particle trajectory through the hot gas stream.





Extensible Artificial Intelligence Framework for Understanding and Design of Corrosion-Resistant Alloys



Proto-Data → Multi-Scale Modeling Data → Meta-Data → Knowledge

DFT, Experiment | Atomistic, Meso-Scale, CALPHAD, FE | Data about Data | Invent, Build, Design