# Past, present and future of Metallurgy: towards sustainable Metallurgy

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# Metallurgy: where we came from, where we are and where we need to go

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- Metallurgy (what is this?).
- Metallurgy in the past.
- Metallurgy today, through some numbers
- Some of the problems metallurgy faces today as a result of its success
- Tools available for metallurgy today.
- What about the future?.
- Some final remarks.

Metallurgy is a pseudo-science, that deals with inaccurate assumptions, undefined theories and untestable hypotheses. Based on unreliable information, uncertain measurements and incomplete data. Obtained from unconvincing experiments, indiscriminate investigations and non-reproducible operations. Using instruments, equipment and utensils of dubious precision, insufficient resolution and inadequate sensitivity, by unreliable people, unknown affiliation and questionable intelligence.

A “friend”

Metallurgy is a domain of materials science and engineering that studies the physical and chemical behavior of metallic elements, their inter-metallic compounds, and their mixtures, which are known as alloys. Metallurgy encompasses both the science and the technology of metals; that is, the way in which science is applied to the production of metals, and the engineering of metal components used in products for both consumers and manufacturers. Metallurgy is distinct from the craft of metalworking. Metalworking relies on metallurgy in a similar manner to how medicine relies on medical science for technical advancement. A specialist practitioner of metallurgy is known as a metallurgist.

Wikipedia

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# Metallurgy, at the heart of human development. Some important milestones.

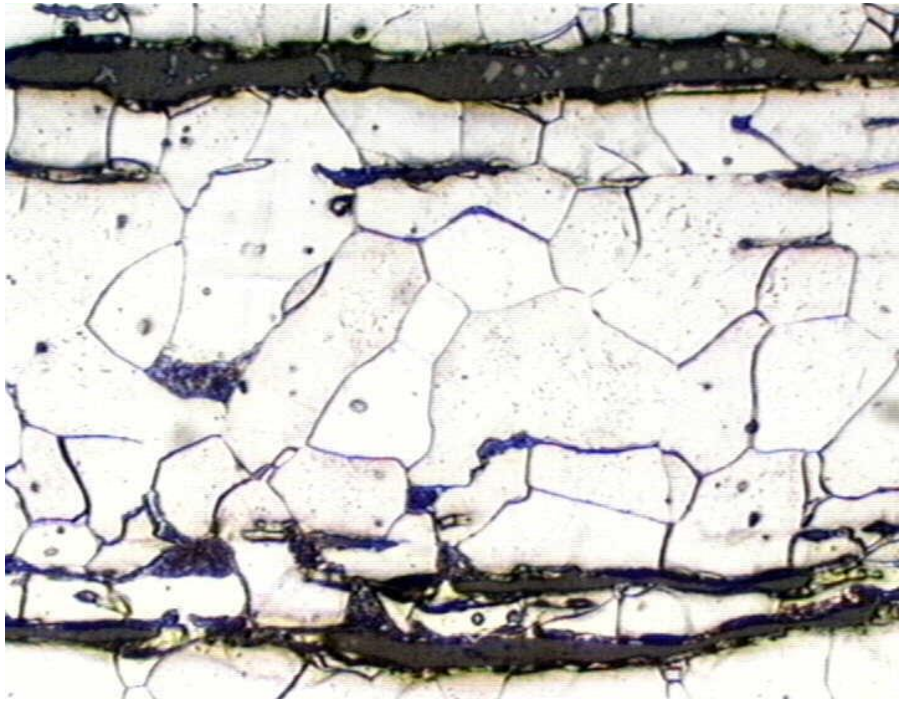
3500 BC. The Egyptians cast iron (possibly as a product of copper refining) for the first time, in small quantities and for ornaments and ceremonial purposes.

"iron from the sky"

**First 'big processing secret' of the material that has dominated the world for centuries: steel.**

## Metallurgy, at the heart of human development. Some important milestones.

300 BC In southern India, Wootz steel is made from sponge iron in a crucible.

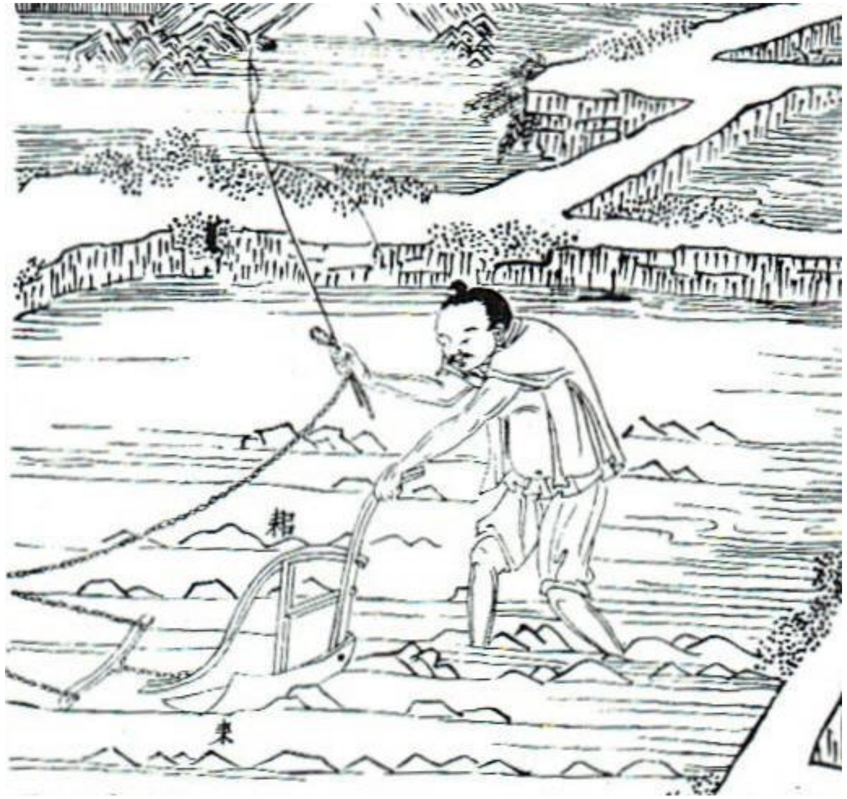


Hundreds of years later, Damascus swords were made from this type of steel, which inspired blacksmiths, artists and metalworkers for many generations.

# Metallurgy, at the heart of human development. Some important milestones.

200 BC. In China, iron is cast (iron foundry).

**For the first time complex iron parts are made, and iron smelting begins in history.**



## Metallurgy, at the heart of human development. Some important milestones.

1450: Johannes Gutenberg develops a lead-tin-antimony alloy which he cast with copper and produces type suitable for his printing press.

**The possibility of mass communication is established.**

## Metallurgy, at the heart of human development. Some important milestones.

1709: Abraham Darby I discovers that coke can efficiently replace charcoal in the smelting furnaces of iron smelting.

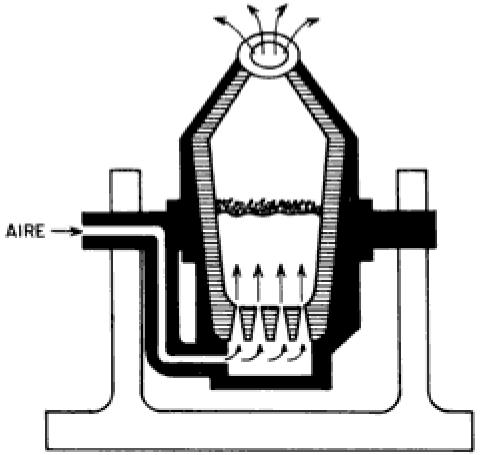
Sedgley, Staffordshire

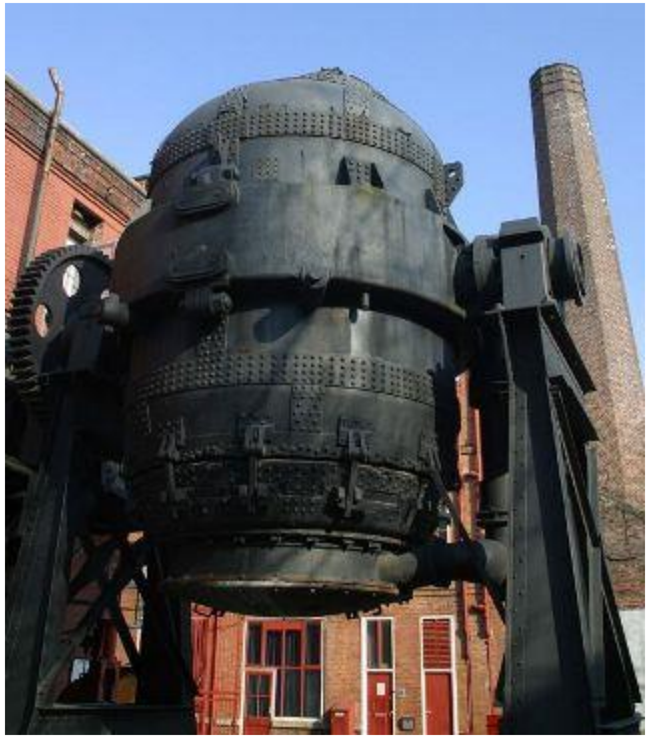
**It drastically reduces the cost of smelting (enabling mass production) and saves huge regions from deforestation.**

# Metallurgy, at the heart of human development. Some important milestones.

1856: Henry Bessemer patents a bottom-blown low-carbon steel converter.

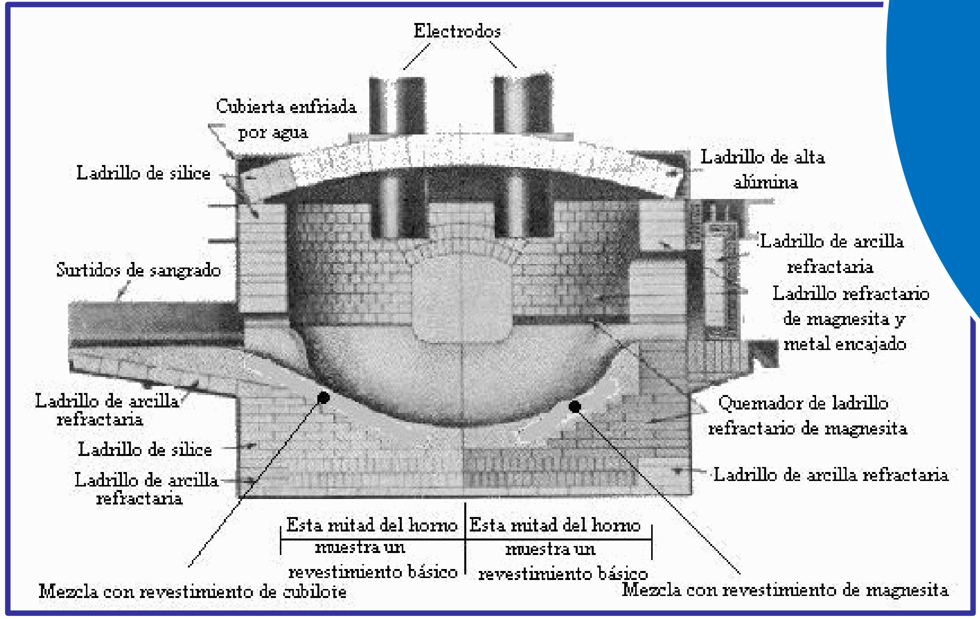
It ushers in an era of massive use of cheap steel in transport, construction and general industry.



# Metallurgy, at the heart of human development. Some important milestones.

1878: William Siemens patents the electric arc furnace.



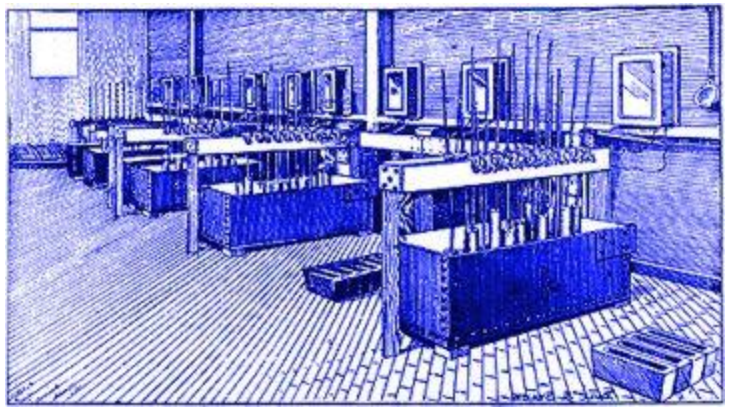

**The predecessor of the modern electric arc furnace, which is the foundation of modern steel production and many other alloys.**

# Metallurgy, at the heart of human development. Some important milestones.

1886: Charles Martin Hall and Paul Héroult independently and simultaneously discover the reduction of alumina to aluminium.

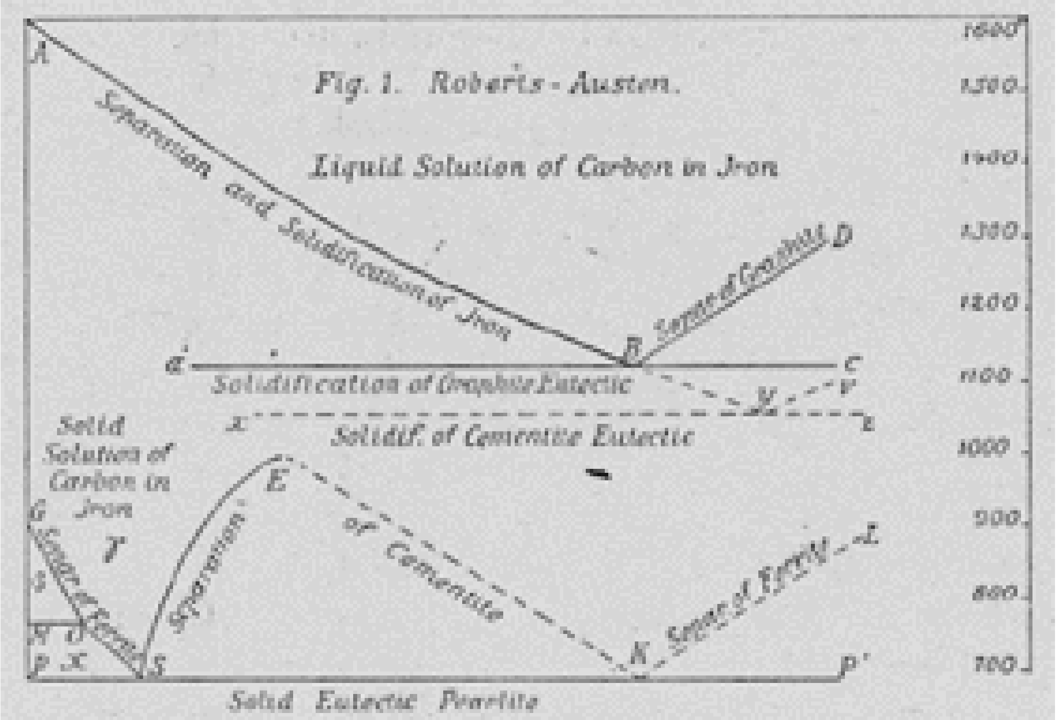
**The beginning of the use of aluminium for commercial purposes is encouraged.**

ALCOA



# Metallurgy, at the heart of human development. Some important milestones.

1898: William Roberts-Austen develops the Fe-C phase diagram.




**Initial work on the most crucial phase diagram in metallurgy lays the foundation for an indispensable tool in many other material systems.**

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# Metallurgy today, through some numbers


All the Metals We Mined in 2019. Visual Capitalist; 2019. https://www.visualcapitalist.com.

https://elements.visualcapitalist.com/sand-steel-and-cement-the-annual-production-of-the-worlds-building-blocks/

# Metallurgy today, through some numbers


| Rank | HS code | Product description | Value (million USD) |
|---|---|---|---|
| 1 | 260300 | Copper ores and concentrates | 1432.65 |
| 2 | 730890 | Structures and parts of structures, iron or steel, ne | 1192.79 |
| 3 | 710812 | Gold in unwrought forms non-monetary | 1090.84 |
| 4 | 790111 | Zinc, not alloyed, unwrought, >99% pure | 1075.96 |
| 5 | 740311 | Copper cathodes and sections of cathodes unwrought | 725.66 |
| 6 | 760429 | Bars, rods and other profiles, aluminium alloyed | 646.54 |
| 7 | 740400 | Copper/copper alloy waste or scrap | 646.45 |
| 8 | 760612 | Aluminium alloy rectangular plate/sheet/strip,t >0.2m | 643.11 |
| 9 | 721632 | Sections, I, iron or non-alloy steel, nfw hot-roll/drawn/extruded > 80m | 608.23 |
| 10 | 740811 | Wire of refined copper > 6mm wide | 577.14 |
| 11 | 470329 | Chem wood pulp, soda/sulphate, non-conifer, bleached | 422.00 |
| 12 | 760120 | Aluminium unwrought, alloyed | 417.38 |
| 13 | 721633 | Sections, H, iron or non-alloy steel, nfw hot-roll/drawn/extruded > 80m | 400.25 |
| 14 | 760421 | Profiles, hollow, aluminium, alloyed | 352.03 |
| 15 | 730820 | Towers and lattice masts, iron or steel | 347.59 |
| 16 | 701090 | Glass containers nes for packing or conveyance goods | 330.29 |
| 17 | 721420 | Bar/rod, iron or non-alloy steel, indented or twisted, nes | 322.08 |
| 18 | 281820 | Aluminium oxide, except artificial corundum | 321.76 |
| 19 | 740200 | Unrefined copper, copper anodes, electrolytic refinin | 316.72 |
| 20 | 710813 | Gold, semi-manufactured forms, non-monetary | 314.41 |

Total exports of raw material commodities: **27738** million USD

**Main non-food, non-energy raw material commodities exported by Spain**

Data source: DESA/UNSD, United Nations Comtrade database

# Metallurgy today, through some numbers


| Rank | HS code | Product description | Value (million USD) |
|---|---|---|---|
| 1 | 260300 | Copper ores and concentrates | 2330.91 |
| 2 | 721049 | Flat rolled iron or non-alloy steel, coated with zinc, width >600mm, ne | 1253.69 |
| 3 | 760120 | Aluminium unwrought, alloyed | 1028.65 |
| 4 | 260800 | Zinc ores and concentrates | 999.48 |
| 5 | 711291 | Waste and scrap of precious metals; of gold, including metal clad with gold but excluding sweepings containing other precious metals | 877.27 |
| 6 | 720449 | Ferrous waste or scrap, nes | 730.55 |
| 7 | 740311 | Copper cathodes and sections of cathodes unwrought | 588.08 |
| 8 | 740400 | Copper/copper alloy waste or scrap | 581.73 |
| 9 | 760612 | Aluminium alloy rectangular plate/sheet/strip,t >0.2m | 562.98 |
| 10 | 270112 | Bituminous coal, not agglomerated | 479.49 |
| 11 | 760110 | Aluminium unwrought, not alloyed | 450.25 |
| 12 | 701090 | Glass containers nes for packing or conveyance goods | 441.05 |
| 13 | 720421 | Waste or scrap, of stainless steel | 370.47 |
| 14 | 260111 | Iron ore, concentrate, not iron pyrites,unagglomerate | 341.15 |
| 15 | 722530 | Hot rolled alloy-steel, coils width >600mm, nes | 338.43 |
| 16 | 470321 | Chem wood pulp, soda or sulphate, conifer, bleached | 333.37 |
| 17 | 730890 | Structures and parts of structures, iron or steel, ne | 324.24 |
| 18 | 470329 | Chem wood pulp, soda/sulphate, non-conifer, bleached | 316.60 |
| 19 | 720711 | Rectangular iron or non-alloy steel bars, <.25%C, width< twice thicknes | 284.42 |
| 20 | 310520 | Nitrogen-phosphorus-potassium fertilizers, pack >10kg | 270.33 |

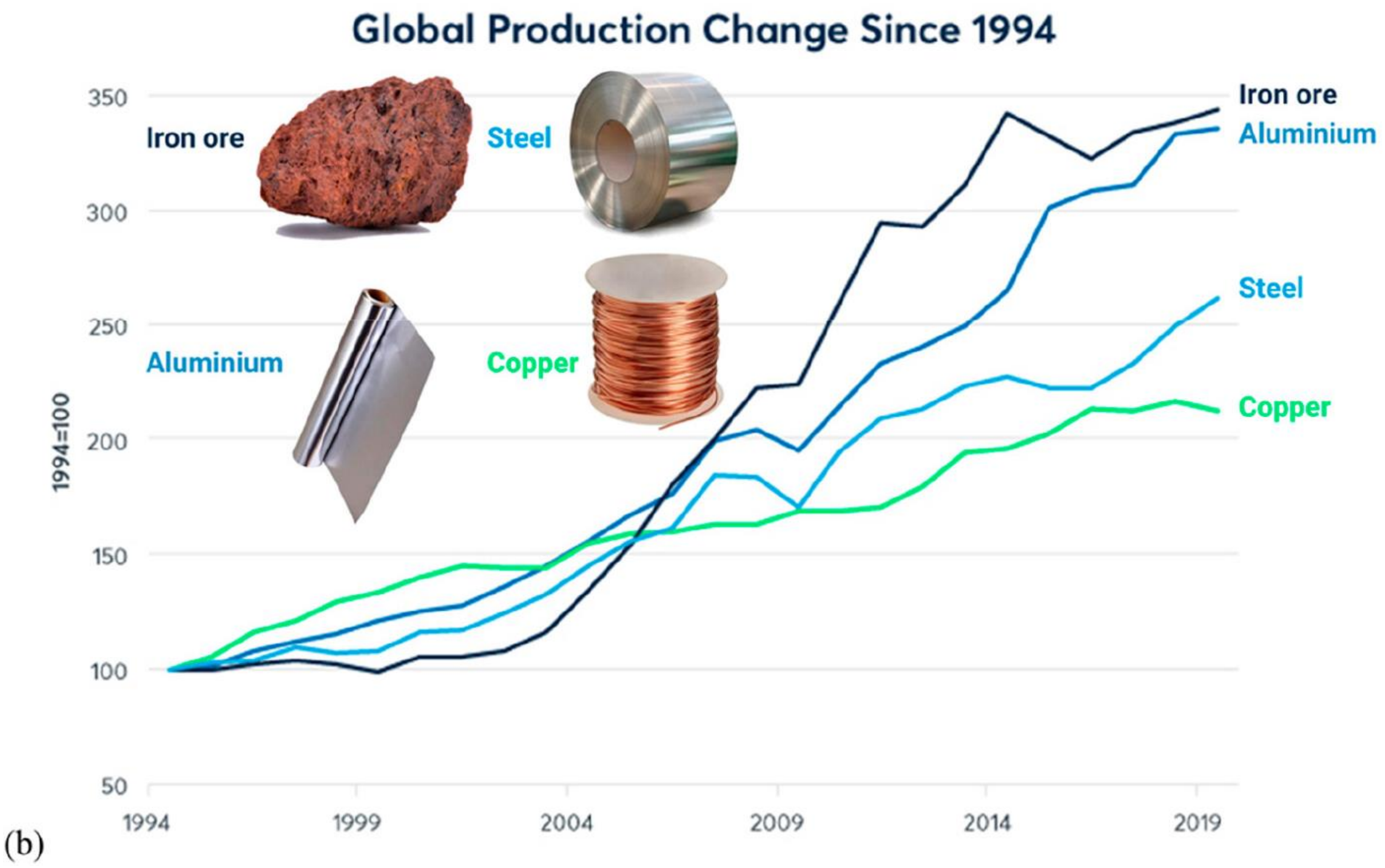
Total imports of raw material commodities: **28996** million USD

**Main non-food, non-energy raw material commodities imported by Spain**

**Export: 27738 million USD**
**Import: 28996 million USD**

Data source: DESA/UNSD, United Nations Comtrade database

# Metallurgy today, through some numbers




OECD. Global Material Resources Outlook to 2060: Economic Drivers and Environmental Consequences; OECD Publishing: Paris, 2019.

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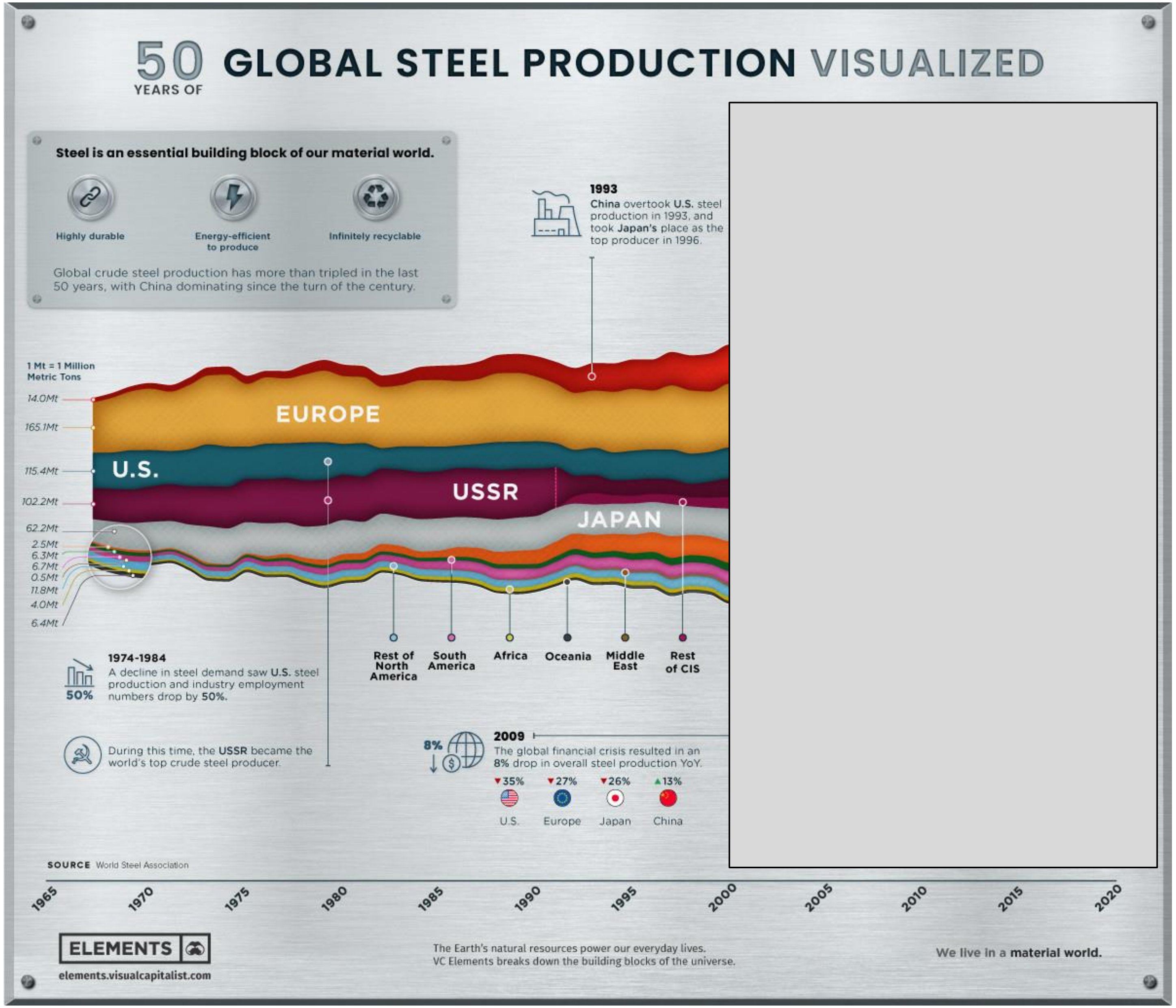


World Economic Forum report 2019

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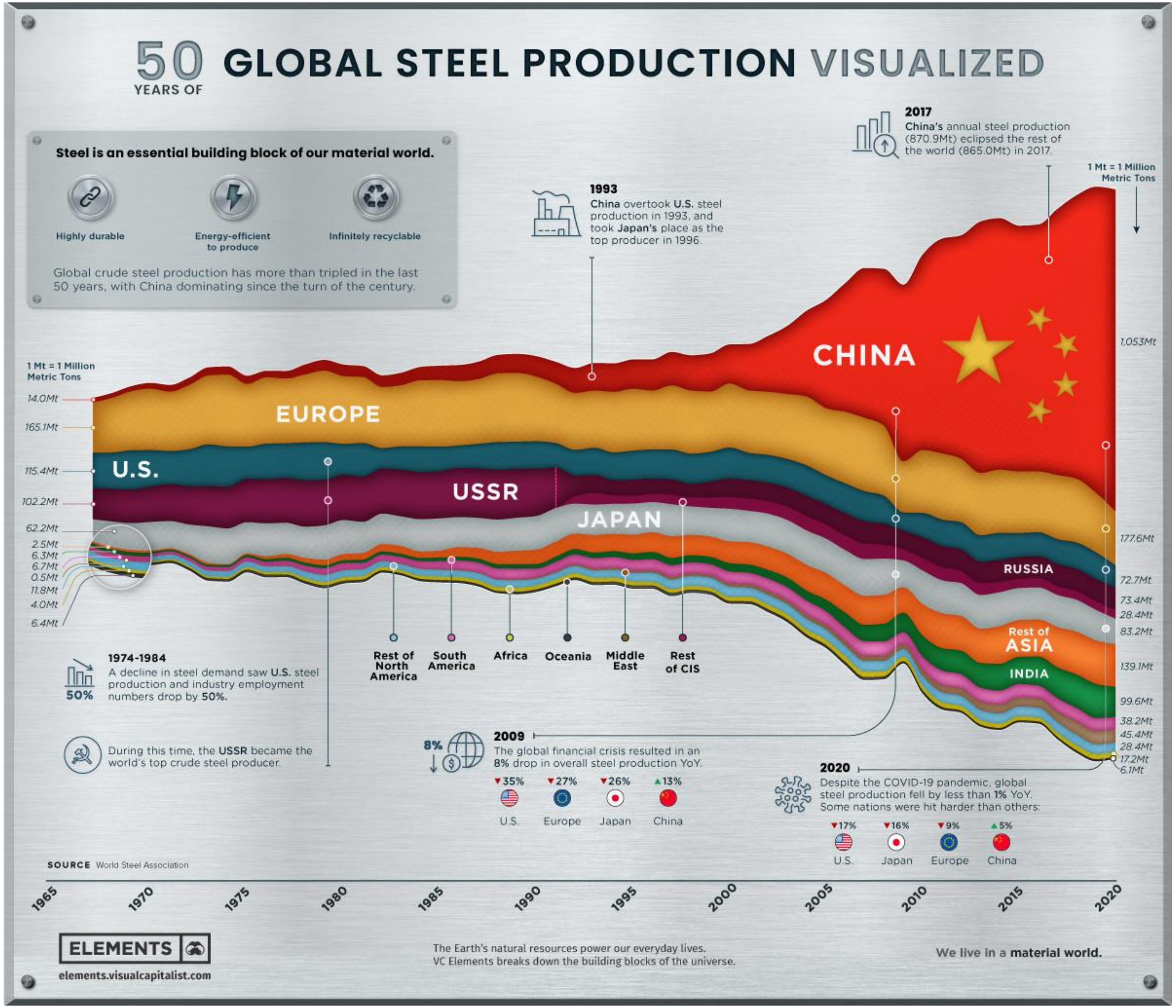


World Economic Forum report 2019

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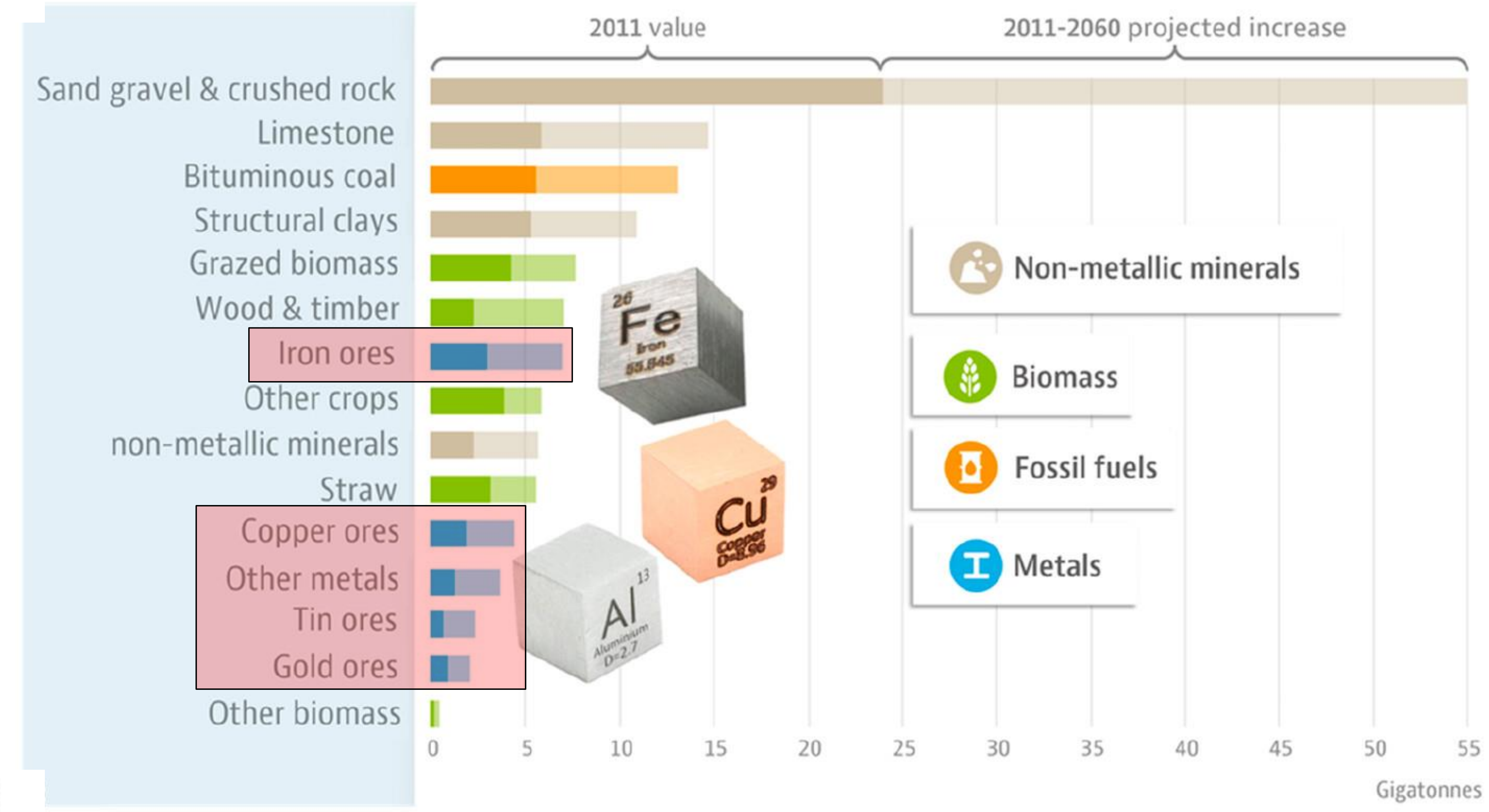


OECD. Global Material Resources Outlook to 2060: Economic Drivers and Environmental Consequences; OECD Publishing: Paris, 2019.

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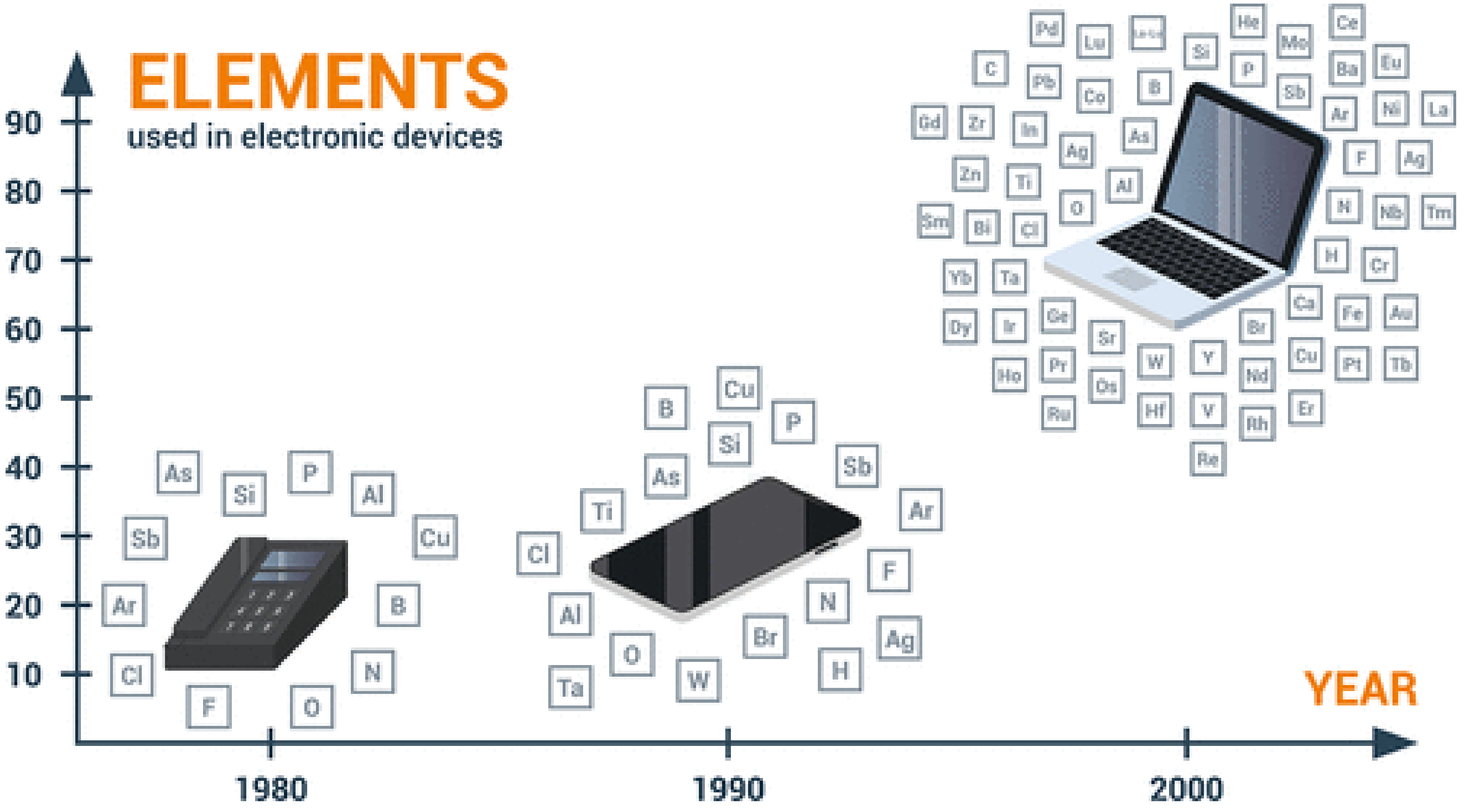


Christian, B. et al.Elemental Compositions of over 80 Cell Phones. J. Electron. Mater. 2014, 43, 4199−4213.

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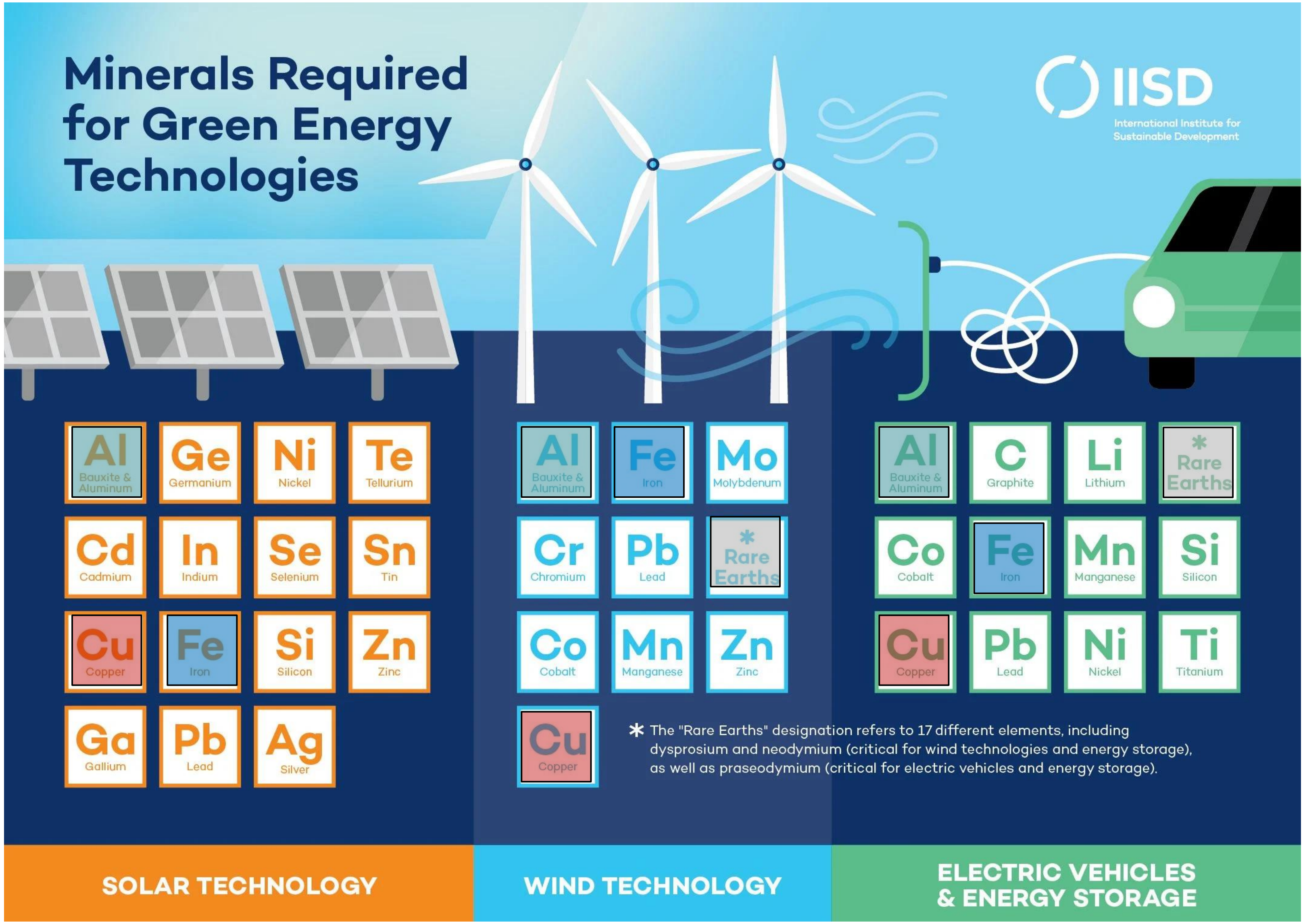


Clare Church and Alec Crawford, International Institute for Sustainable Development, July 2019 “The fuels of conflict in the transition to a low-carbon economy”

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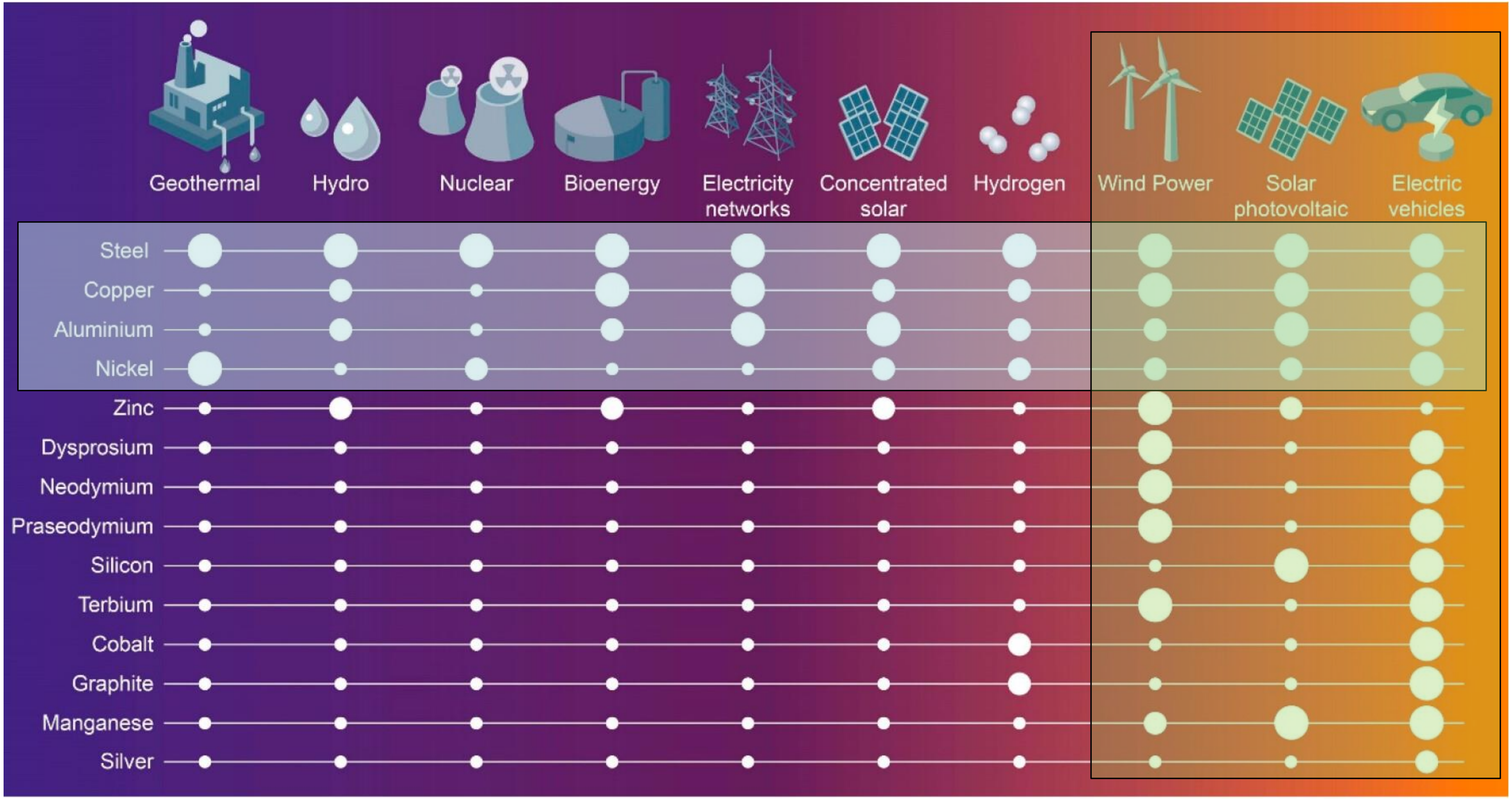


de Pee, A.; Pinner, D.; Occo, R.; Somers, K.; Witteveen, M. Decarbonization of Industrial Sectors: The next Frontier; McKinsey Co., 2018; pp 1−68.

# Metallurgy today, through some numbers

| Supply Risk | Raw material | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 4.8 | Gallium | | | | | | ● | | | ● | ● | ● | | ● | ● | ● |
| 4.1 | Magnesium | | | ● | | | | | | | ● | ● | ● | ● | ● | ● |
| 4.0 | REE (magnets) | | ● | ● | ● | ● | | ● | | ● | ● | ● | | ● | ● | ● |
| 3.8 | Boron | | ● | ● | ● | ● | ● | ● | | ● | ● | ● | | ● | ● | ● |
| 2.7 | PGM | | ● | ● | | | | | | ● | ● | ● | | ● | ● | ● |
| 1.9 | Lithium | ● | | | | | | | | ● | | ● | | ● | ● | ● |
| 1.8 | Germanium | | | | | | ● | | | ● | ● | ● | | | | ● |
| 1.8 | Natural graphite | ● | ● | ● | | | | | ● | ● | | ● | | ● | ● | |
| 1.7 | Cobalt | ● | ● | ● | | | | | | ● | | ● | ● | ● | ● | ● |
| 1.6 | Titanium metal | | | | | | | | | | | ● | ● | ● | ● | ● |
| 1.4 | Silicon metal | | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● |
| 1.2 | Manganese | ● | ● | ● | ● | | | ● | ● | ● | ● | ● | ● | ● | ● | ● |
| 1.2 | Aluminium | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● |
| 0.5 | Nickel | ● | ● | ● | ● | | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● |
| 0.1 | Copper | ● | ● | ● | ● | ● | ● | ● | | ● | ● | ● | ● | ● | ● | ● |
| 5.3 | HREE (rest) | | ● | ● | | | | | | ● | ● | ● | ● | ● | ● | ● |
| 4.4 | Niobium | | | ● | ● | | | | | ● | | | ● | | ● | ● |
| 3.5 | LREE (rest) | | ● | ● | | | | | | ● | | ● | | ● | ● | ● |
| 3.3 | Phosphorus | ● | | | | | ● | | ● | | | | | | | |
| 2.6 | Strontium | | ● | ● | | | | | | ● | | ● | | | | |

Source: Joint Reseearch Center, UE

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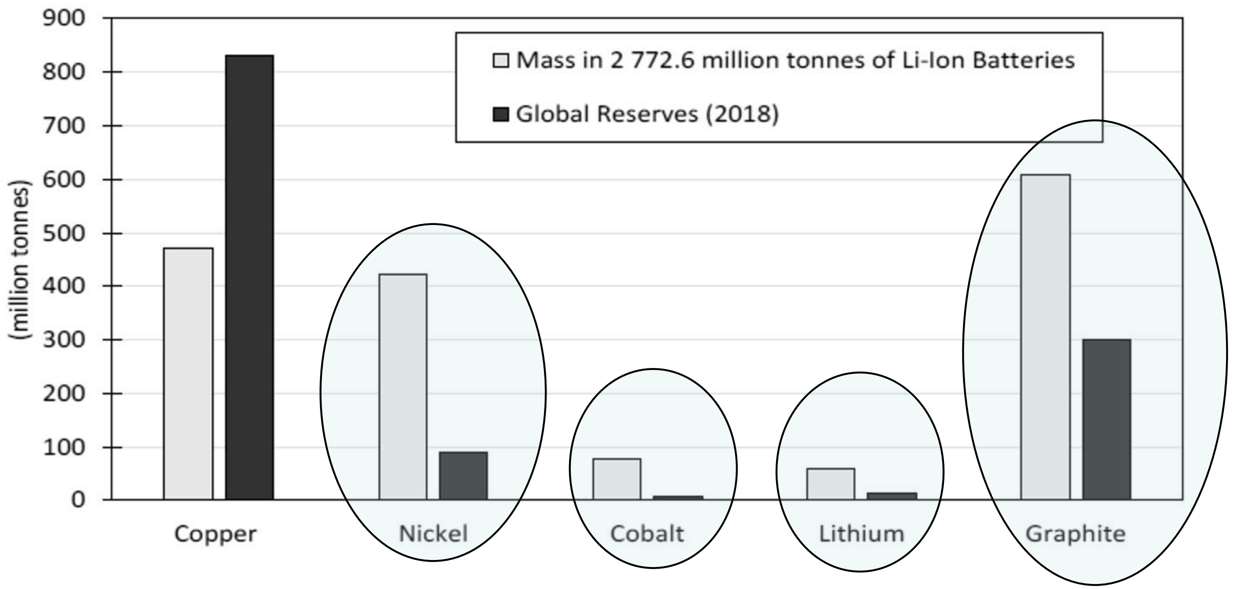


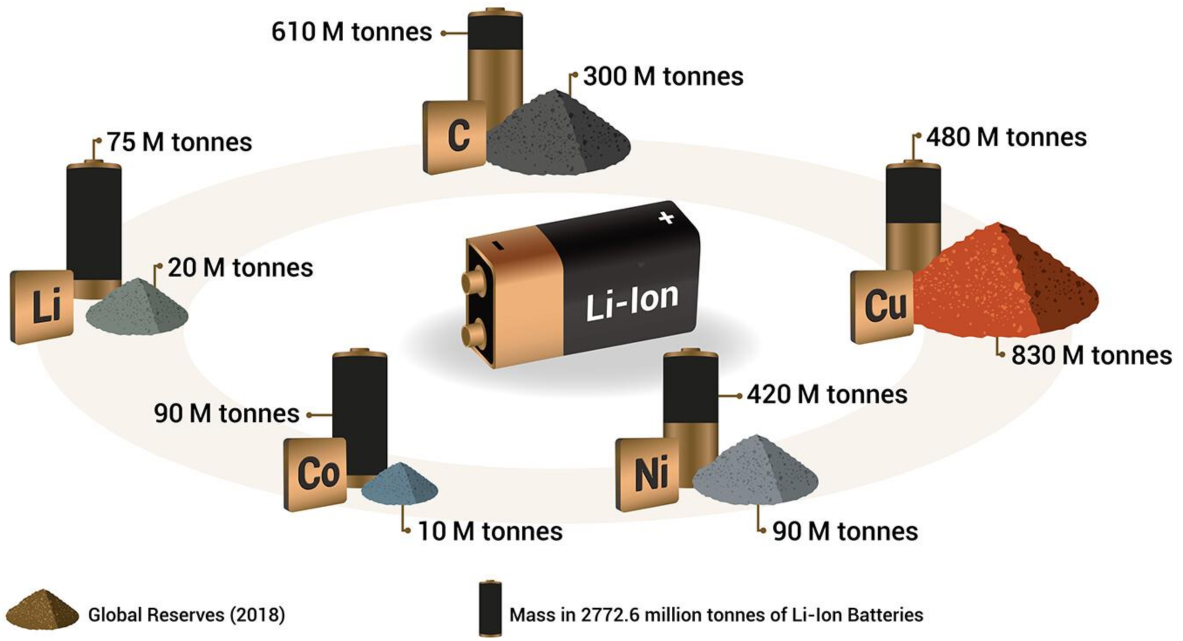


## The transition to the green energy

D. Raabe "The Materials Science behind Sustainable Metals and Alloys" Chemical Reviews 2023 123 (5), 2436-2608 DOI: 10.1021/acs.chemrev.2c00799

https://countercurrents.org/2022/08/is-there-enough-metal-to-replace-oil

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# Some of the problems metallurgy faces today as a result of its success


**Steel is the largest single industrial contributor to global warming through its massive $CO_2$ emissions which primarily stem from the use of fossil reductants in blast furnaces, a route which stands for about 70% of the global steel production**

Holappa, L. A General Vision for Reduction of Energy Consumption and CO2 Emissions from the Steel Industry. Metals (Basel) 2020, 10, 1117.

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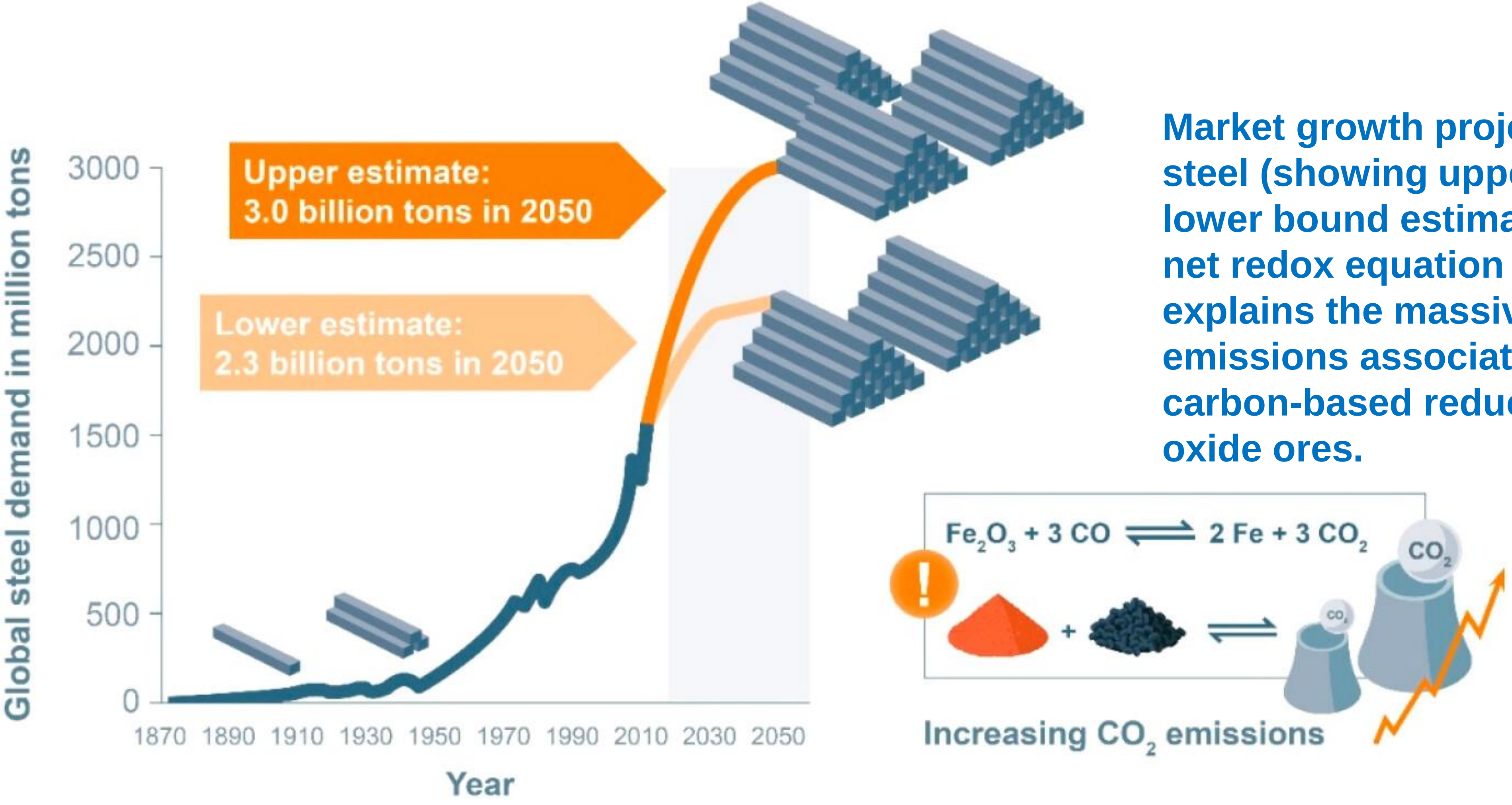


**Market growth projections for steel (showing upper bound and lower bound estimates) and the net redox equation which explains the massive $CO_2$ emissions associated with the carbon-based reduction of iron oxide ores.**


Mercier, F.; Decarvalho, A.; Hijikata, T.; Ozturk, B.; Morenghi D.; Mattera, G.; Giua, L. OECD Data on Global Steel Market Developments; Global Steel Market Developments.

D. Raabe "The Materials Science behind Sustainable Metals and Alloys" Chemical Reviews 2023 123 (5), 2436-2608 DOI: 10.1021/acs.chemrev.2c00799

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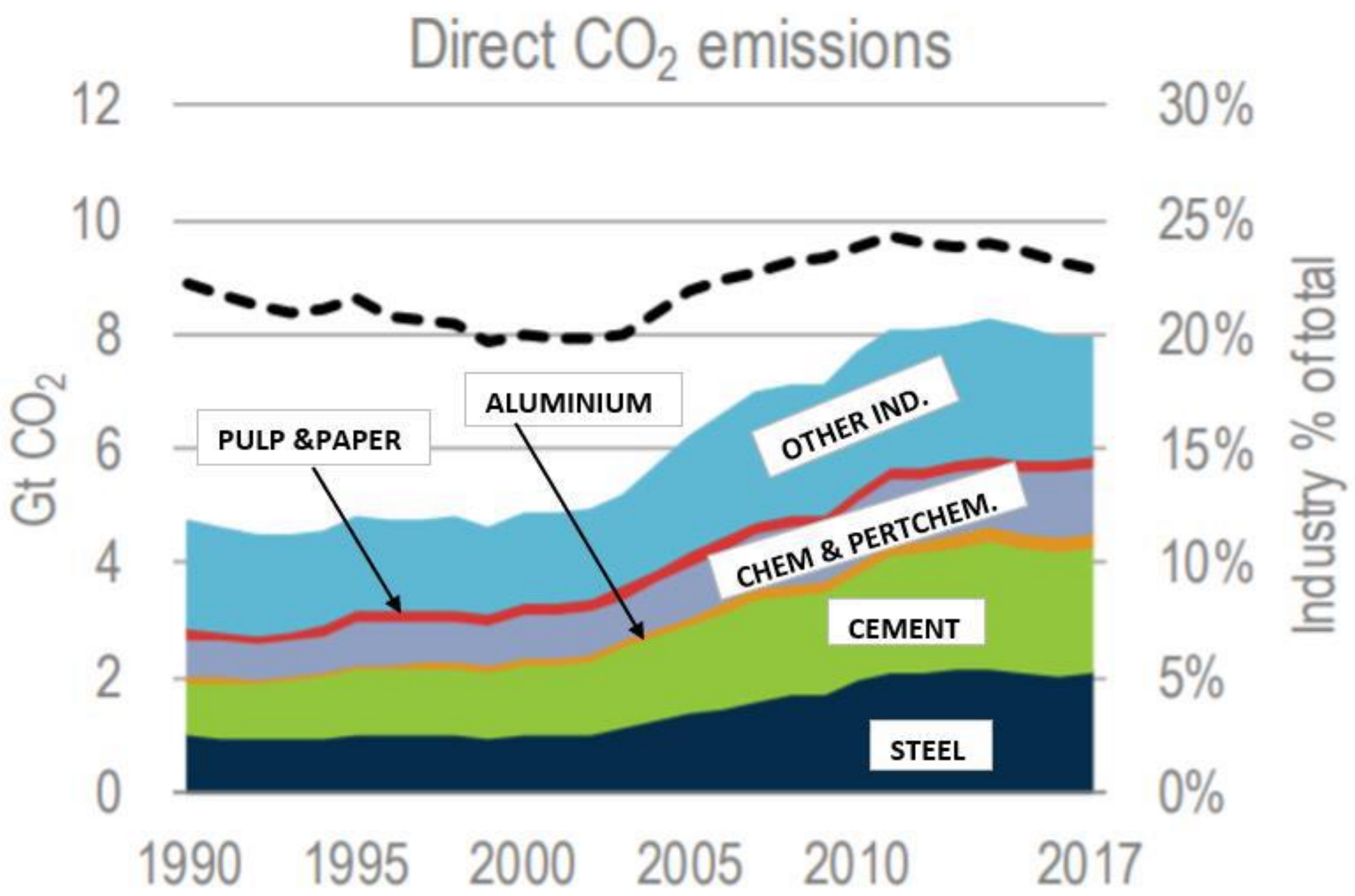


**The steel industry is the single largest source of industrial $CO_2$ emissions**

**The steel industry is responsible for around 5% of $CO_2$ emissions in the EU and 7% globally**


Reduction of Greenhouse Gas Emissions in Steel Production, Final Report, Dr Jai Kant Pandit, Dr Max Watson & Dr Abdul Qader, March 2020, CO2CRC Report No: RPT20-6205 IEA. (2020). Iron and Steel Technology Roadmap

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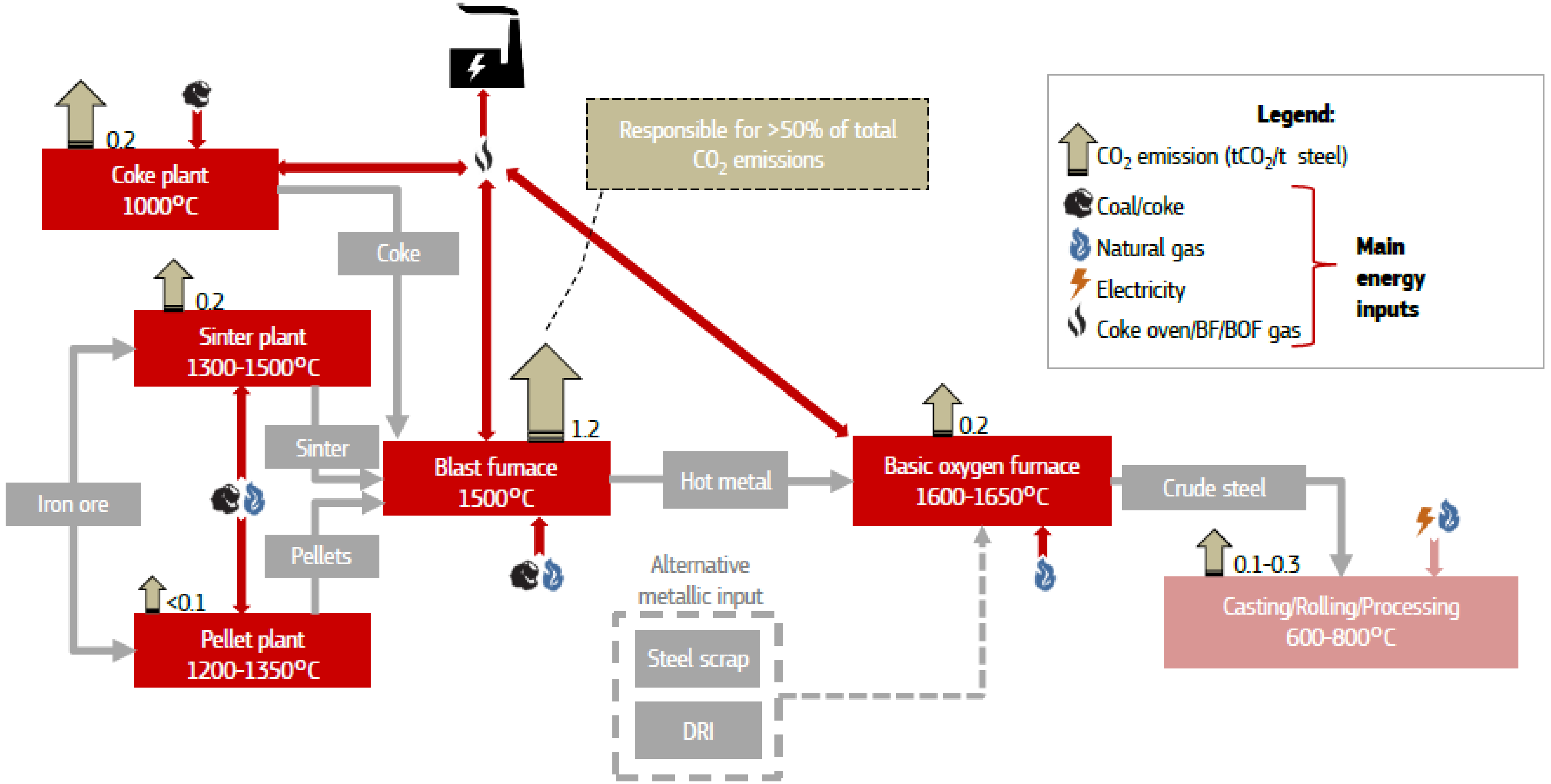


Simplified flow diagram and CO2 emissions of the BF-BOF route

Technologies to decarbonise the UE Steel industry. 2022. Joint Research Centre UE

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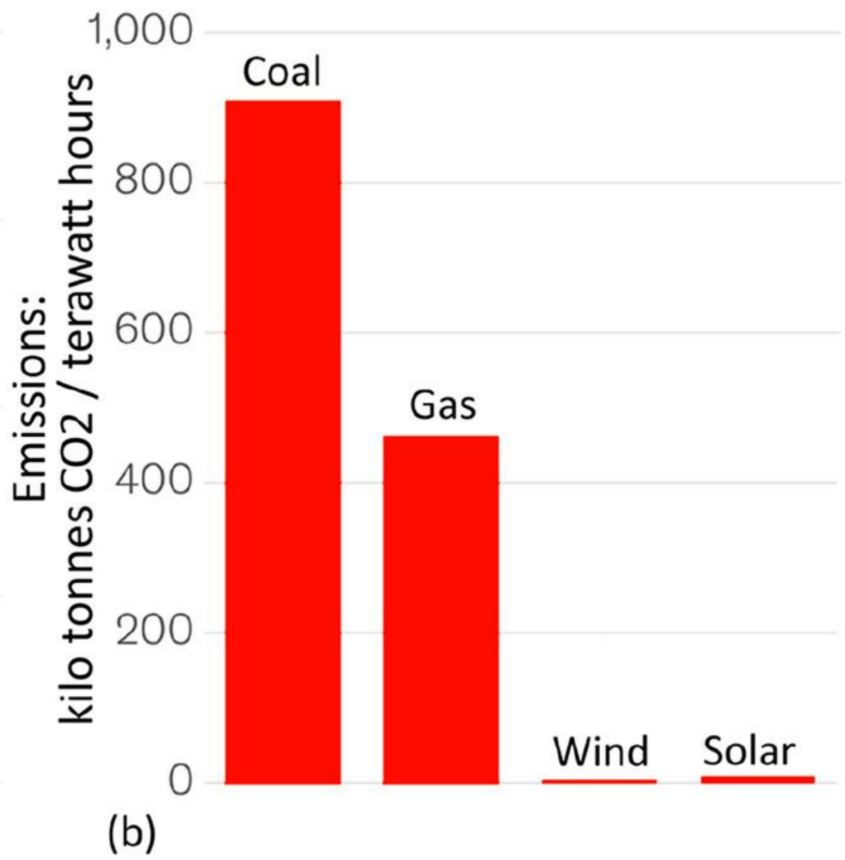


Rebound effect in the metallurgical sector for the case of power generation.

D. Raabe "The Materials Science behind Sustainable Metals and Alloys" Chemical Reviews 2023 123 (5), 2436-2608 DOI: 10.1021/acs.chemrev.2c00799

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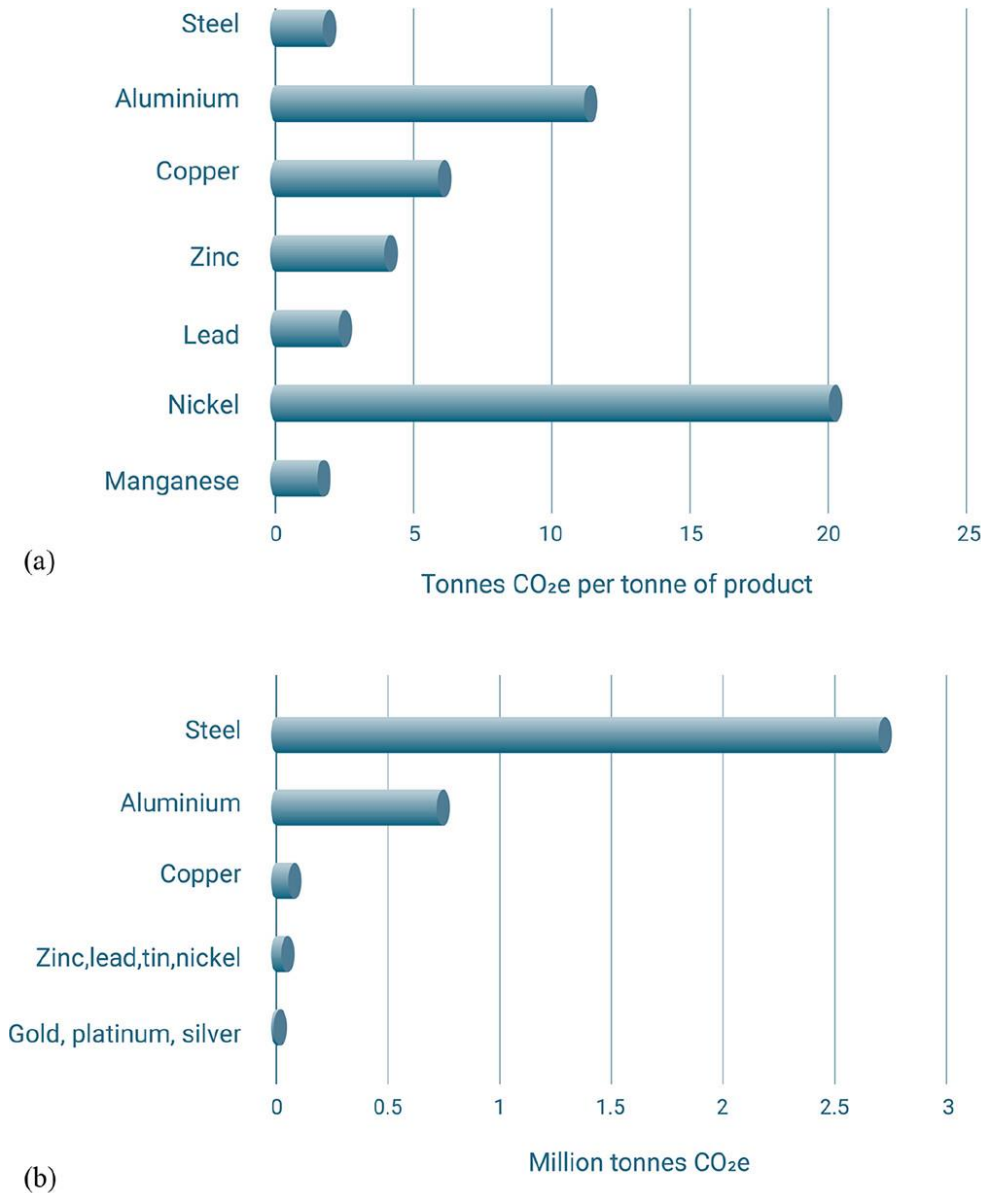


(a)

(b)

a) $CO_2$ emissions for different metals per tonne of product.
b) Total amount of $CO_2$ emissions for different metals, scaled by their respective total production volumes.

Van der Voet, E.; Van Oers, L.; Verboon, M.; Kuipers, K. Environmental Implications of Future Demand Scenarios for Metals: Methodology and Application to the Case of Seven Major Metals. *J. Ind. Ecol.* 2019, *23*, 141.

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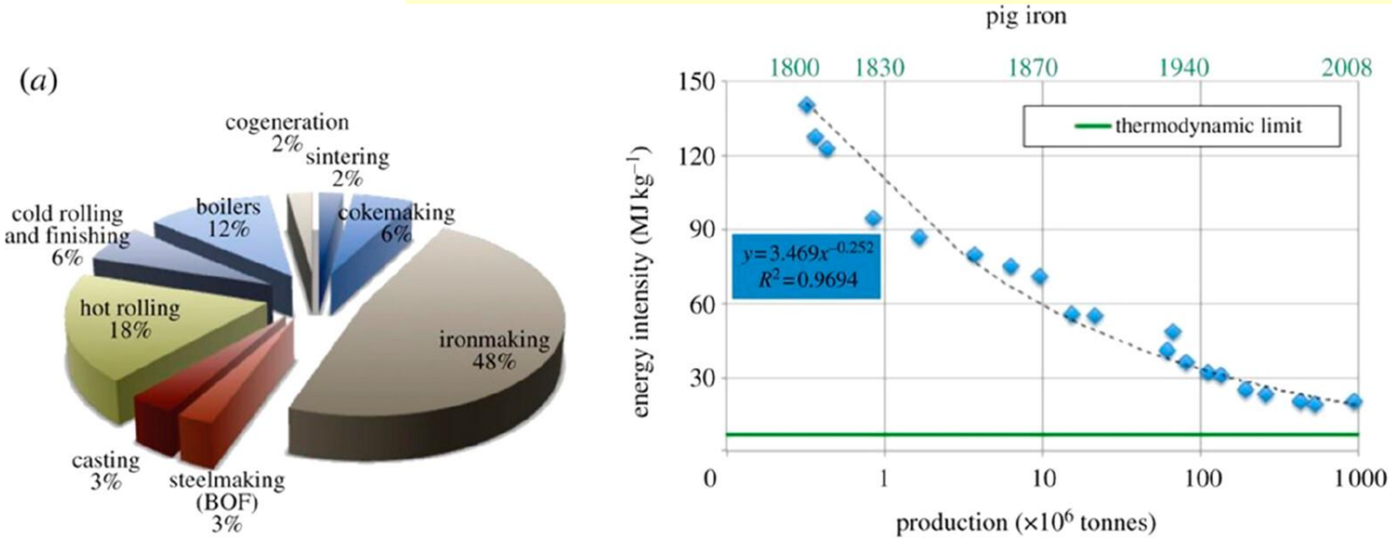
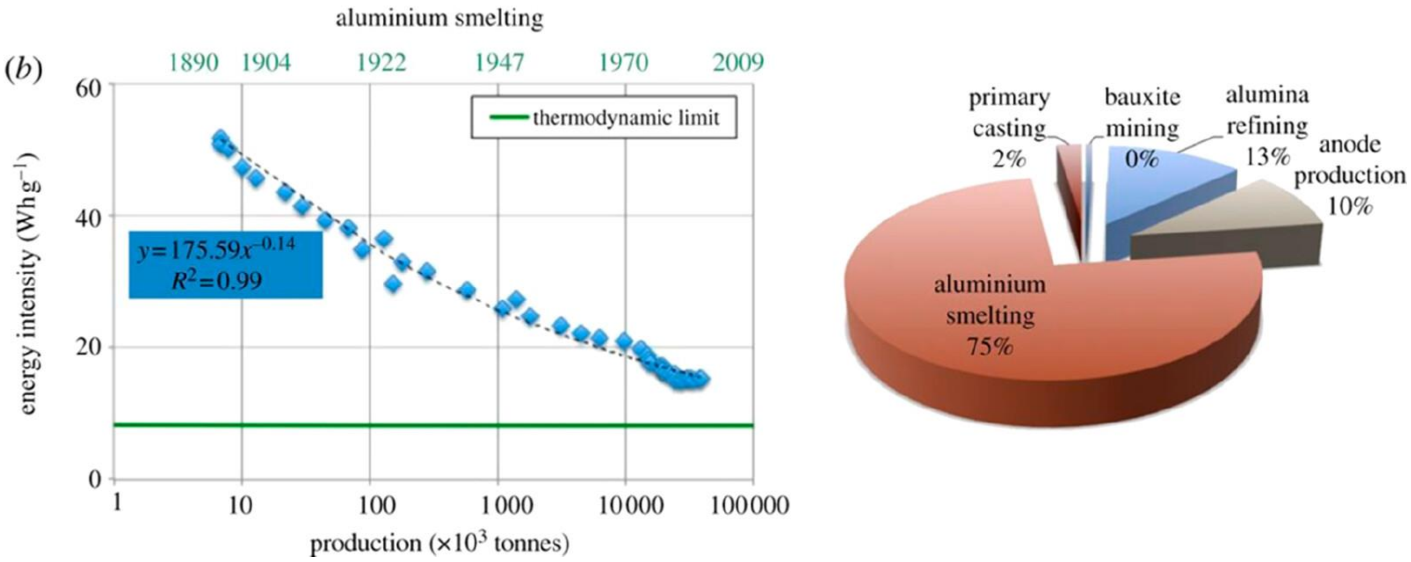



**Pig iron production from hematite oxide by using coke as reductant**




**Aluminum production by using electricity in the molten salt electrolysis process**

Gutowski, T. G.; et al The Energy Required to Produce Materials: Constraints on Energy-Intensity Improvements, Parameters of Demand. Philos. Trans. R. Soc. A Math. Phys. Eng. Sci. 2013, 371, 20120003.

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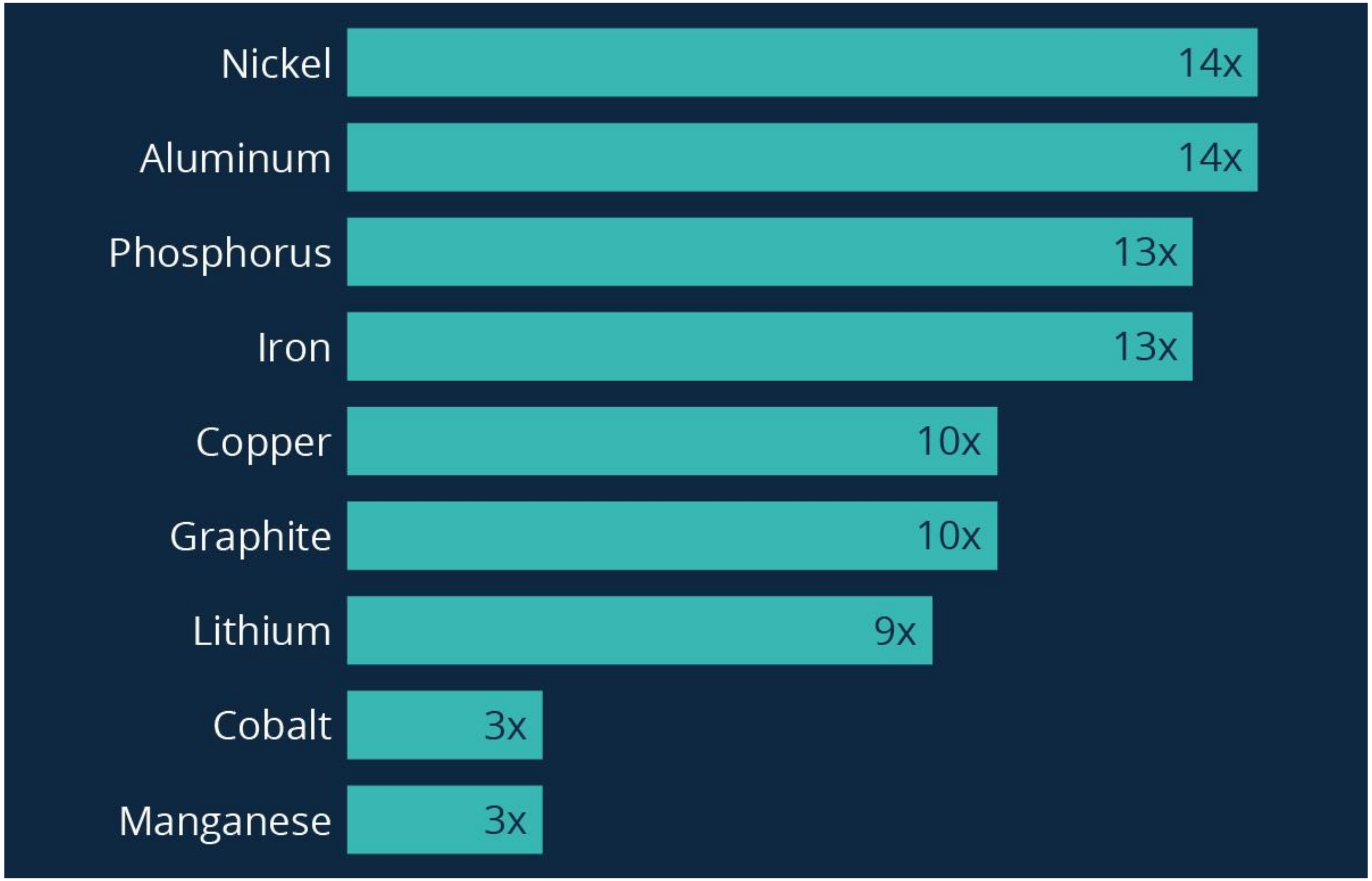


**Demand increase in precious metals and materials between 2019 and 2030.**

Source: Bloomberg/Statista

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Can we solve the problems of Metallurgy?

⇩

Tools available for metallurgy today

# Tools available for metallurgy today

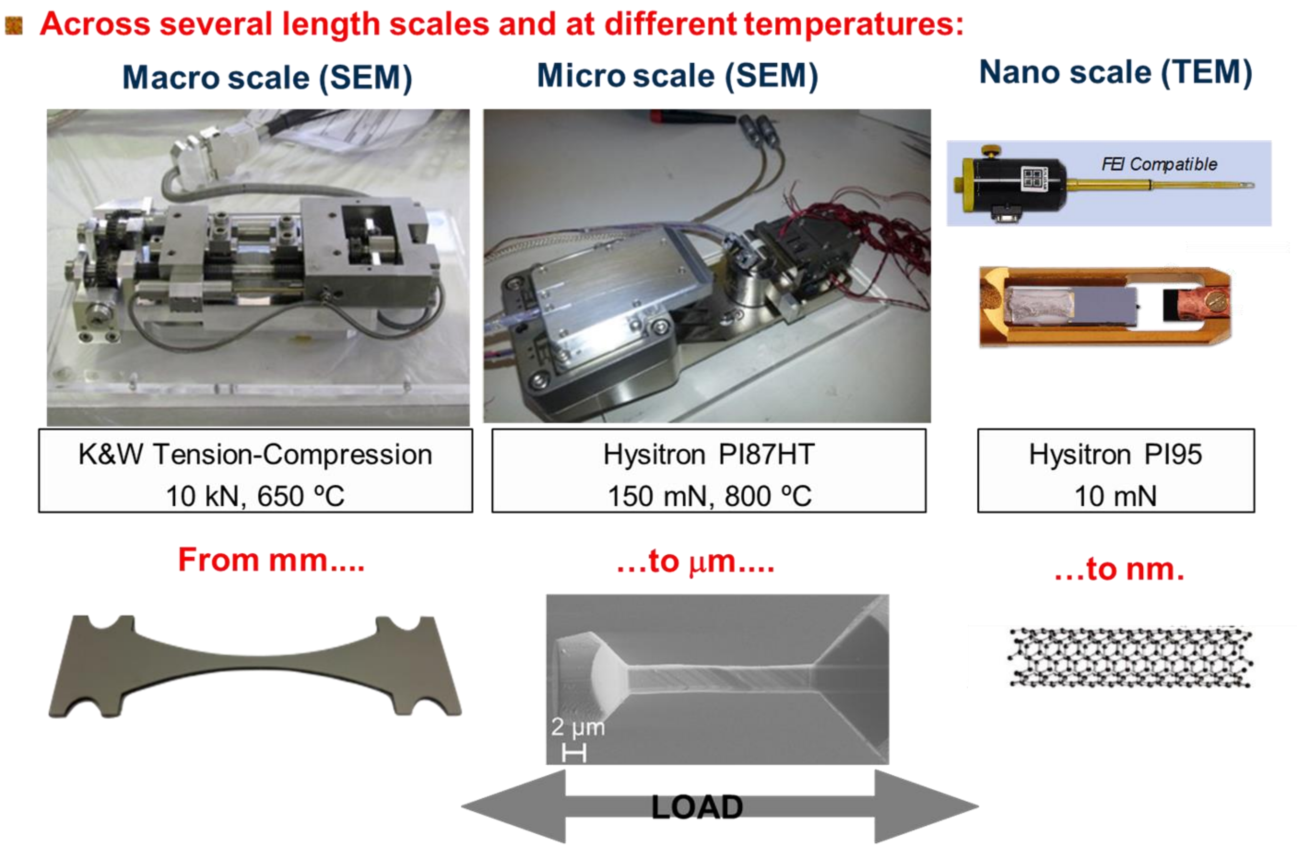
## Advanced Characterization Techniques

# Tools available for metallurgy today

## Advanced Characterization Techniques

SEM
FIB-FEGSEM
STEM
TEM
X-Ray Diffraction
X-Ray Tomography
AFM
Sincrotron
Nanoindentation
Atom Probe Tomography
……………………………….

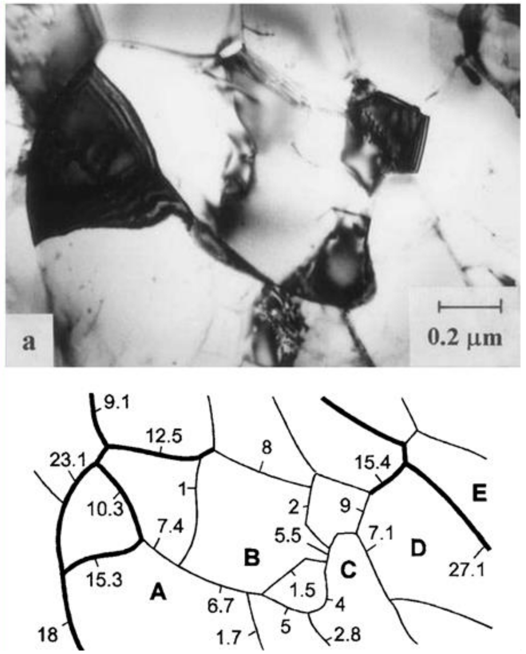
### In situ test techniques



# Tools available for metallurgy today

## Advanced Characterization Techniques

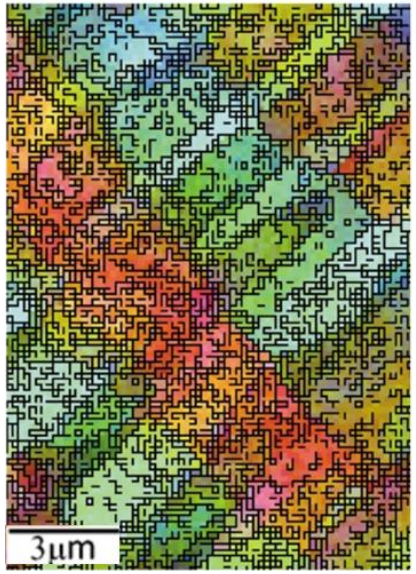
**Rapid microstructural characterization of complex multiphase microstructures (phases and grain boundaries)in metallic materials**




*Grain boundaries in SS*

**1970s – 1980s:**
Manual analysis of TEM data
1 week

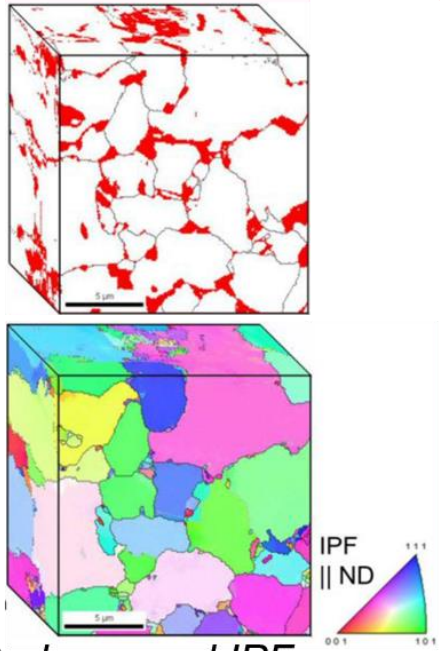
A. Belyakov, T. Sakai. Metall. Mater. Trans. A. 29 (1998) 161.




*Euler map with GBs of deformed and recovered Al alloy*

**Late 1990s – early 2020s:**
EBSD analysis
1 day

F.J. Humphreys. Journal of Materials Science. 36 (2001) 3833




*3D phase and IPF maps of a DP steel*

**Nowadays:**
Fast EBSD analysis 0.5-1 h,
3D EBSD analysis

https://www.dierk-raabe.com/ebsd-and-3d-ebsd/

**Near future**

- Fast CPUs
- Robotization of the preparation process (MPIE)
- AI and ML-supported tools for instant analysis of the EBSD raw data

Ultrafast EBSD analysis (also in 3D)
1 .. 10 min

M. Larmuseau, et. al. Race against the Machine: can deep learning recognize microstructures as well as the trained human eye? Scripta Materialia. 193 (2021) 33-37.

# Tools available for metallurgy today

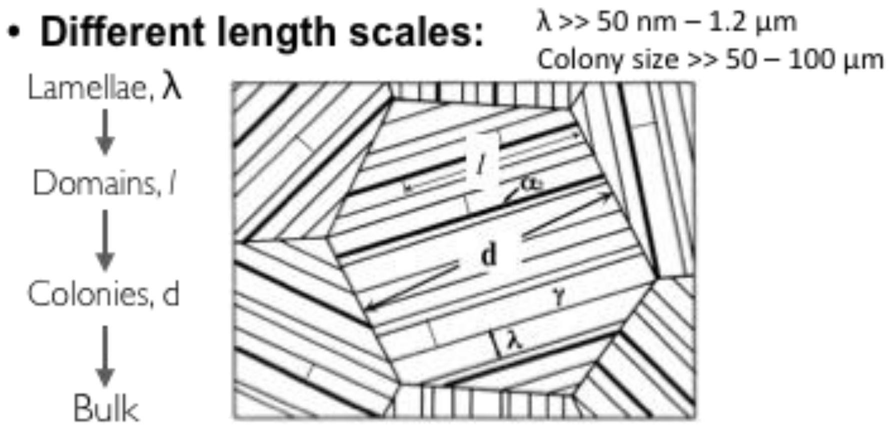
## Advanced Characterization Techniques

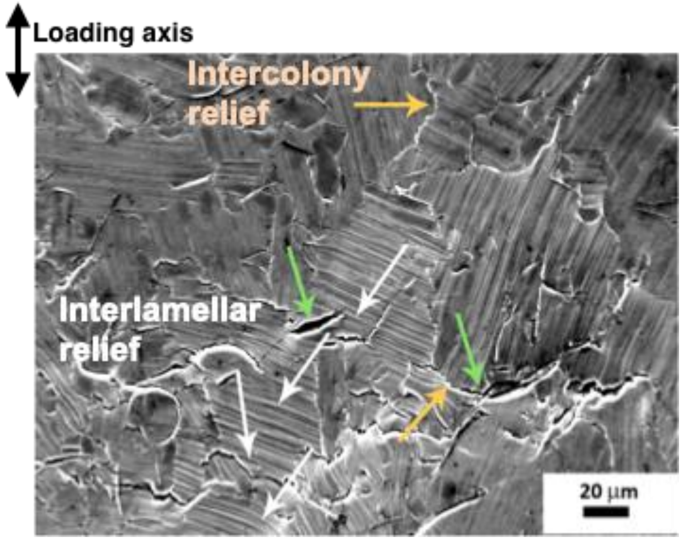
**Case study: Deformation mechanisms**

**2º generation and 3er generation TiAl intermetallics: Ti45Al2Nb2Mn0.8B vs. Ti43.5Al4Nb1Mo0.8B**

- Good high temperature specific strength for aerospace applications.
- Problem : Limited ductility and fatigue strength due to complex deformation of fully-lamellar microstructures

Aim: understand deformation modes of TiAl colonies as a function of loading direction and lamellar width




Palomares-García, A.J., Pérez-Prado, M.T., Molina-Aldareguia, J.M. Effect of lamellar orientation on the strength and operating deformation mechanisms of fully lamellar TiAl alloys determined by micropillar compression (2017) Acta Materialia, 123, pp. 102-114.

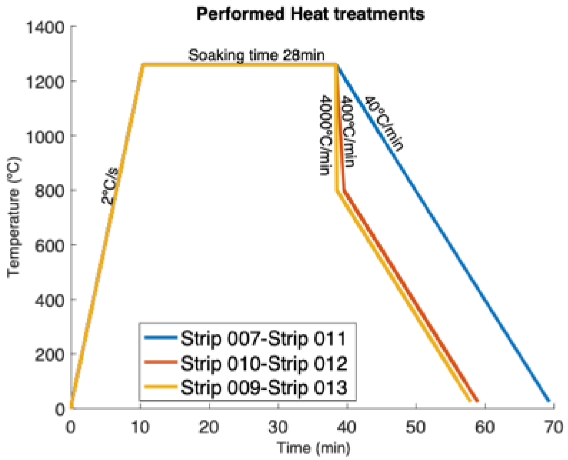
# Tools available for metallurgy today

## Advanced Characterization Techniques

## Deformation mechanisms

**2º generation and 3er generation TiAl intermetallics: Ti45Al2Nb2Mn0.8B vs. Ti43.5Al4Nb1Mo0.8B**

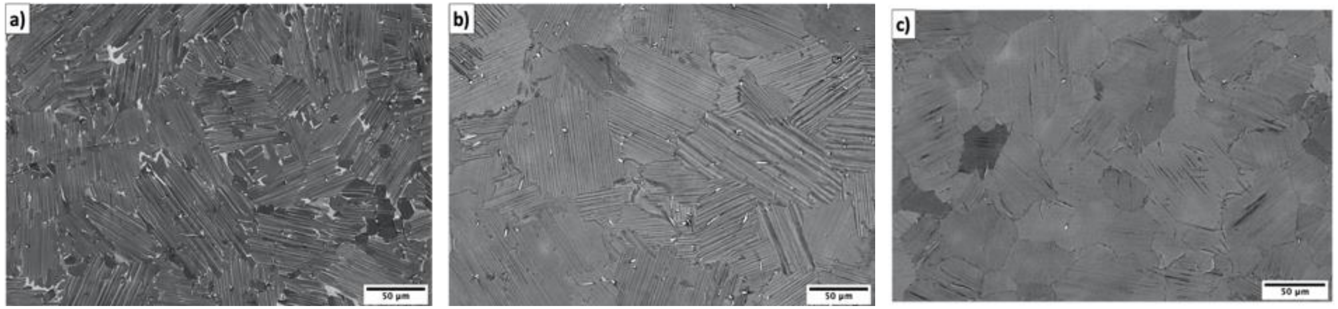
- Lamellar refinement through thermal treatments

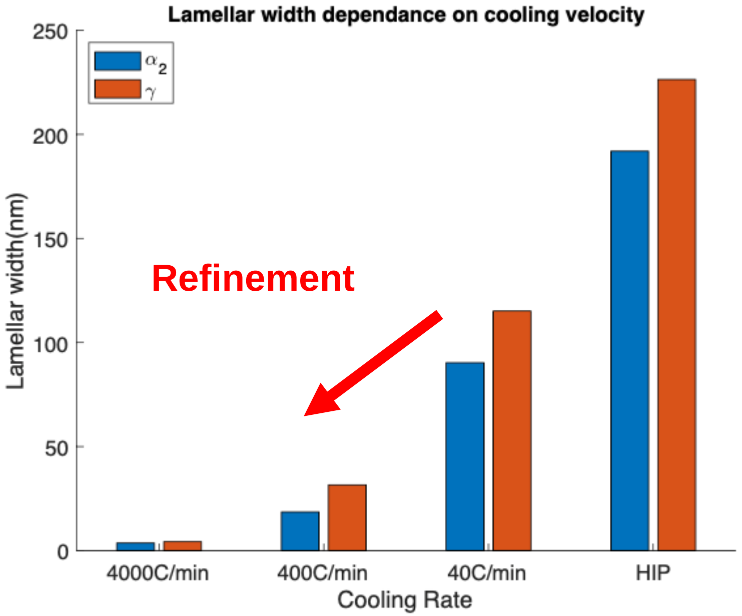



As-received

40ºC/min

400ºC/min

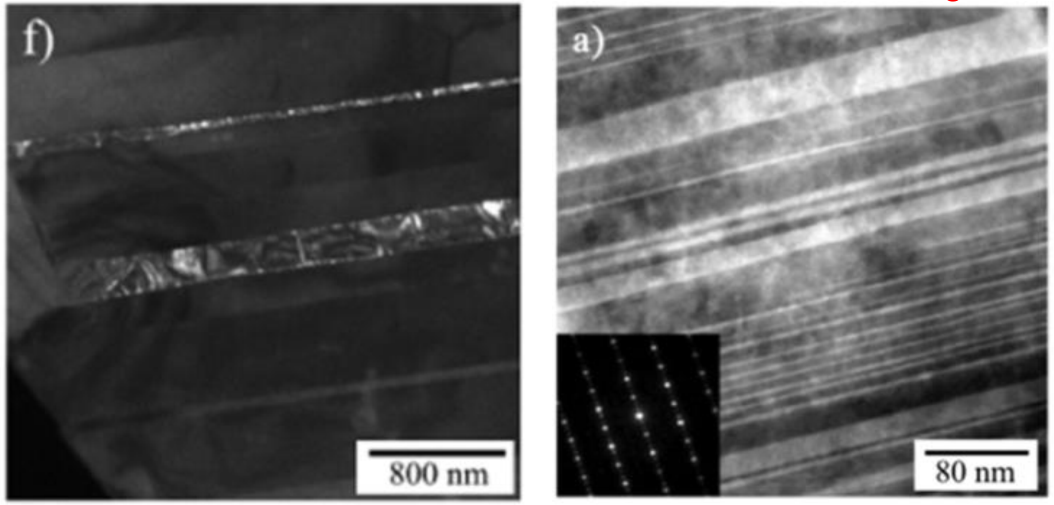



Slow cooling

**TEM**

Fast cooling



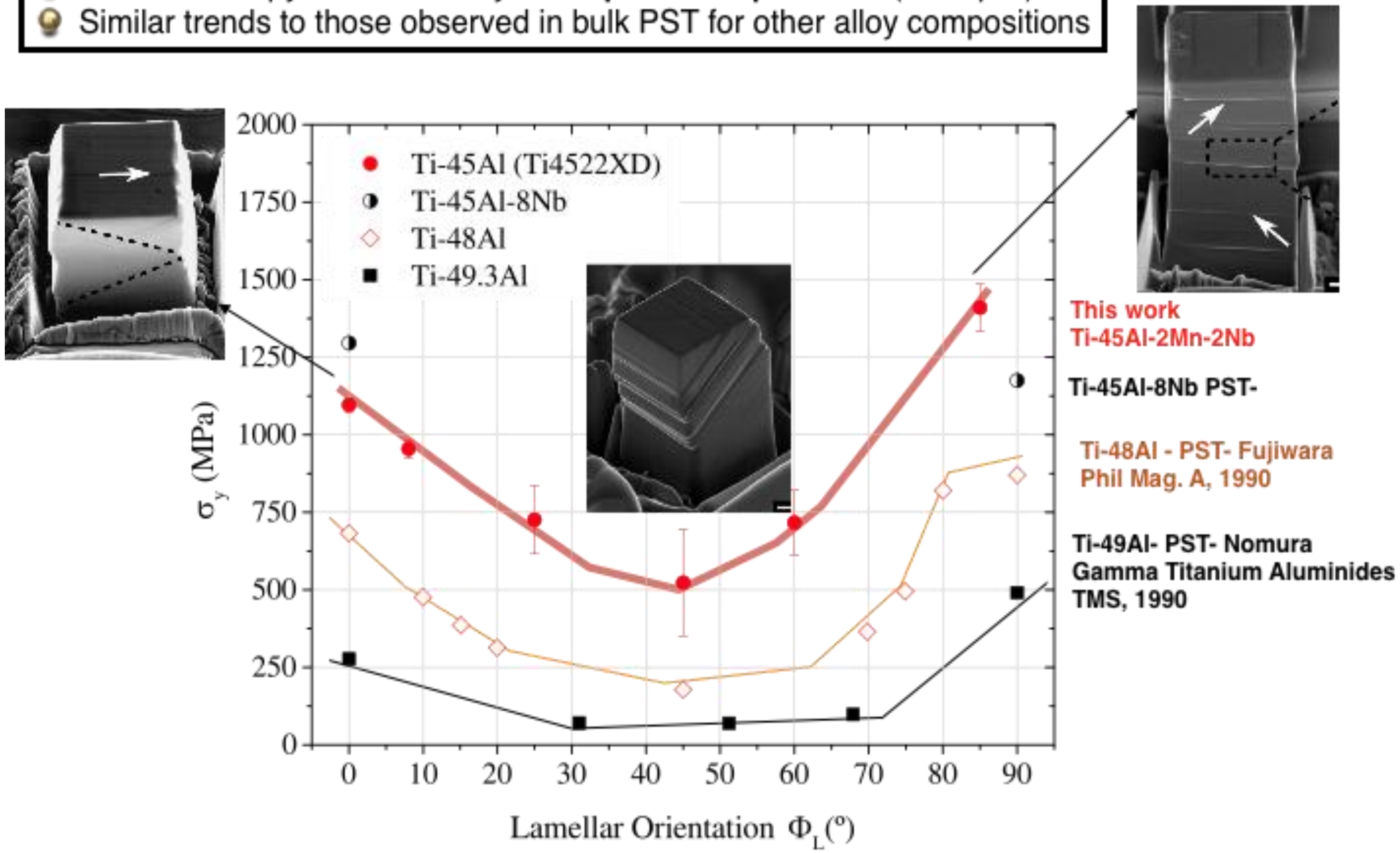
# Tools available for metallurgy today

## Advanced Characterization Techniques

## Deformation mechanisms

### **TiAl intermetallics:** micropillar compression

- Yield anisotropy determined by **micropillar compression** (L = 5 $\mu$m)
- Similar trends to those observed in bulk PST for other alloy compositions




X

Palomares-García, A.J., Pérez-Prado, M.T., Molina-Aldareguia, J.M. Effect of lamellar orientation on the strength and operating deformation mechanisms of fully lamellar TiAl alloys determined by micropillar compression (2017) Acta Materialia, 123, pp. 102-114.

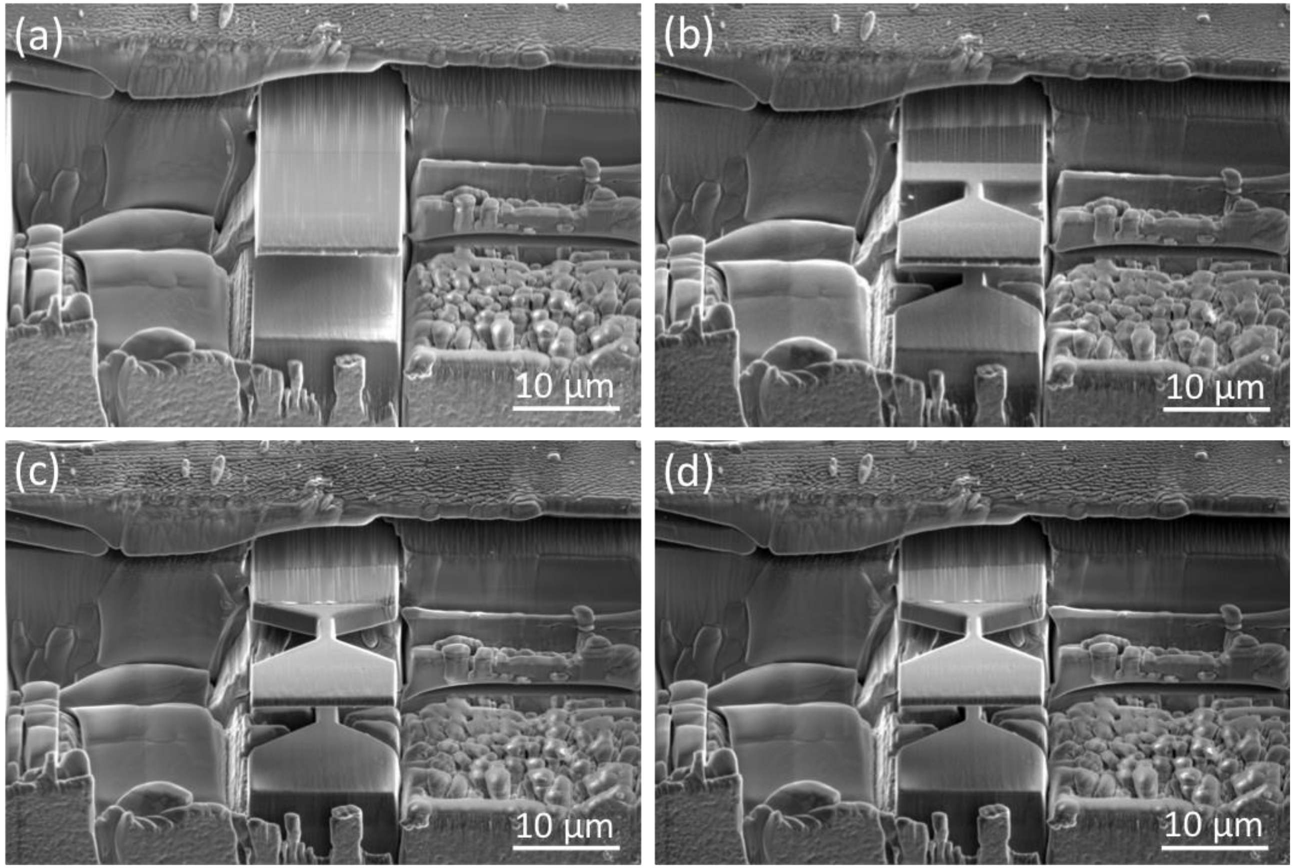
# Tools available for metallurgy today

## Advanced Characterization Techniques

## Deformation mechanisms

**TiAl intermetallics:** microtensile testing

- Microtensile testing: dog-bone micro tensile specimens machined by FIB



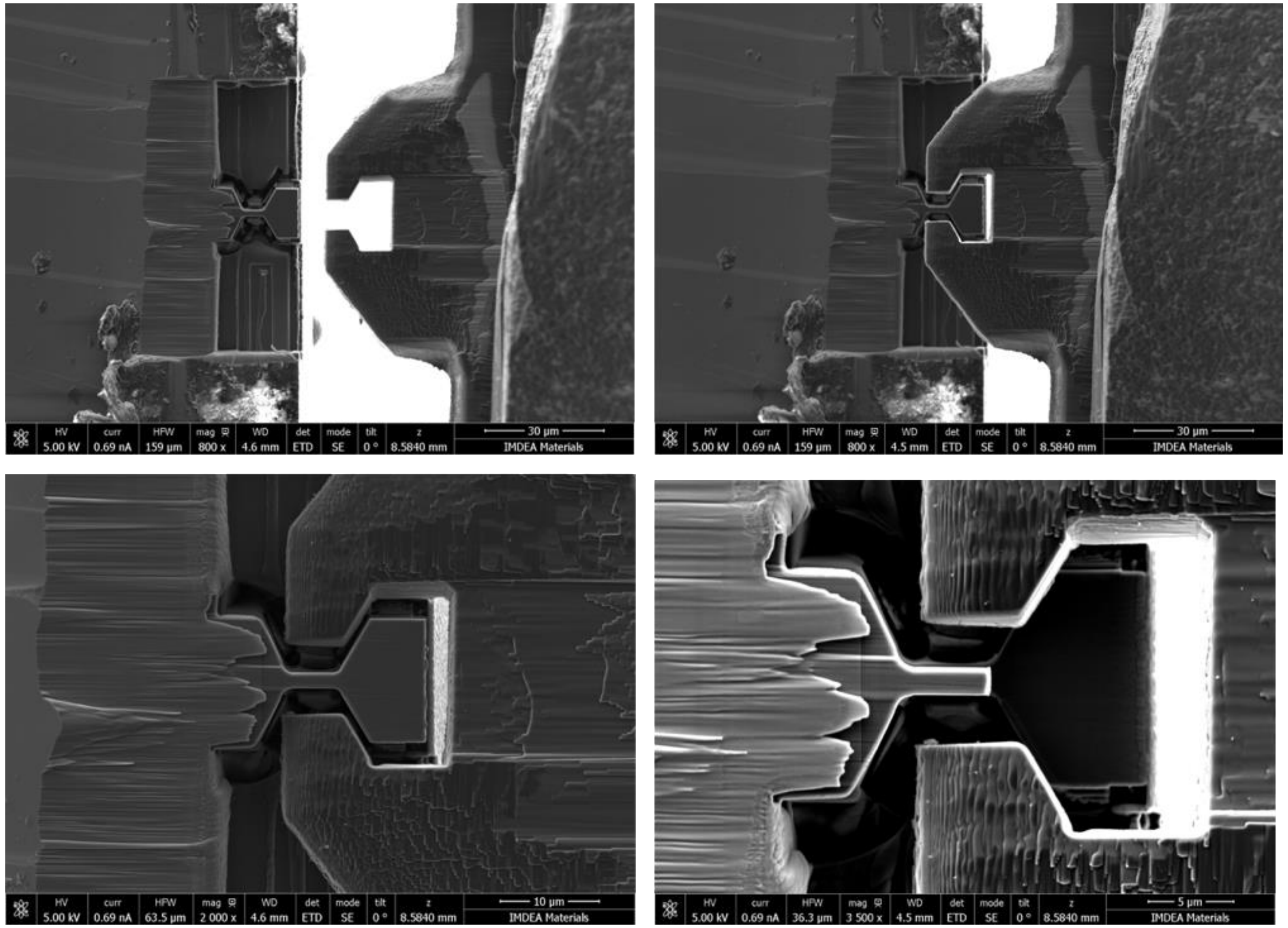

Palomares-García, A.J., Pérez-Prado, M.T., Molina-Aldareguia, J.M. Effect of lamellar orientation on the strength and operating deformation mechanisms of fully lamellar TiAl alloys determined by micropillar compression (2017) Acta Materialia, 123, pp. 102-114.

# Tools available for metallurgy today

## Advanced Characterization Techniques

## Deformation mechanisms

**TiAl intermetallics:** microtensile testing




Palomares-García, A.J., Pérez-Prado, M.T., Molina-Aldareguia, J.M. Effect of lamellar orientation on the strength and operating deformation mechanisms of fully lamellar TiAl alloys determined by micropillar compression (2017) Acta Materialia, 123, pp. 102-114.

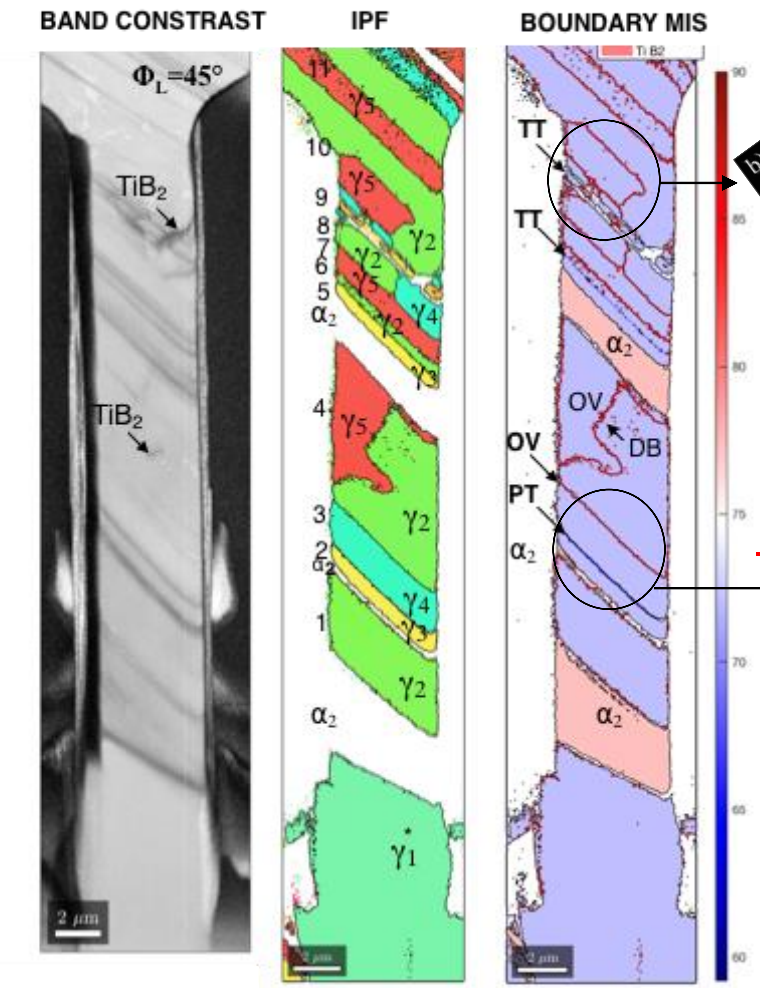
# Tools available for metallurgy today

## Advanced Characterization Techniques

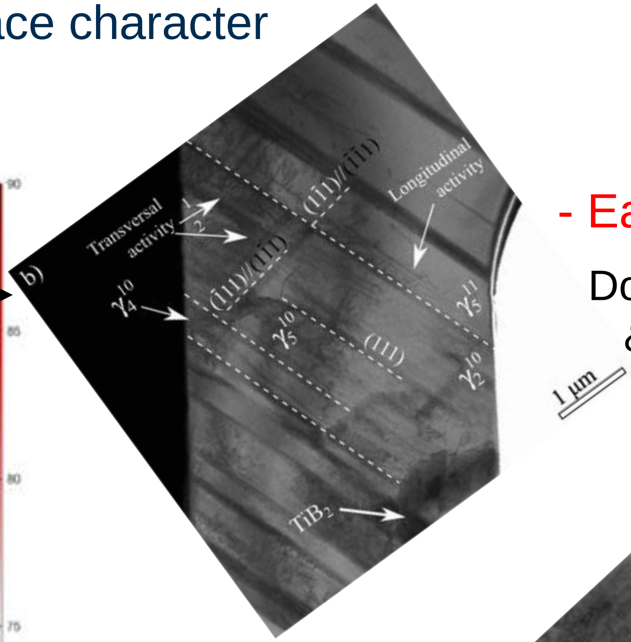
### Deformation mechanisms

- Slip transfer analysis as a function of interface character

**EBSD**



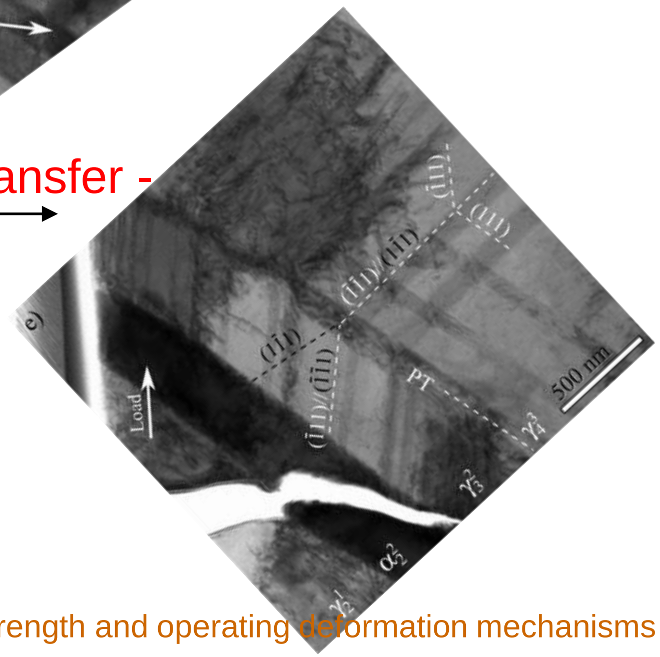

**TEM**




- Easy slip transfer-

Domain boundaries & OV interfaces

- Difficult slip transfer -

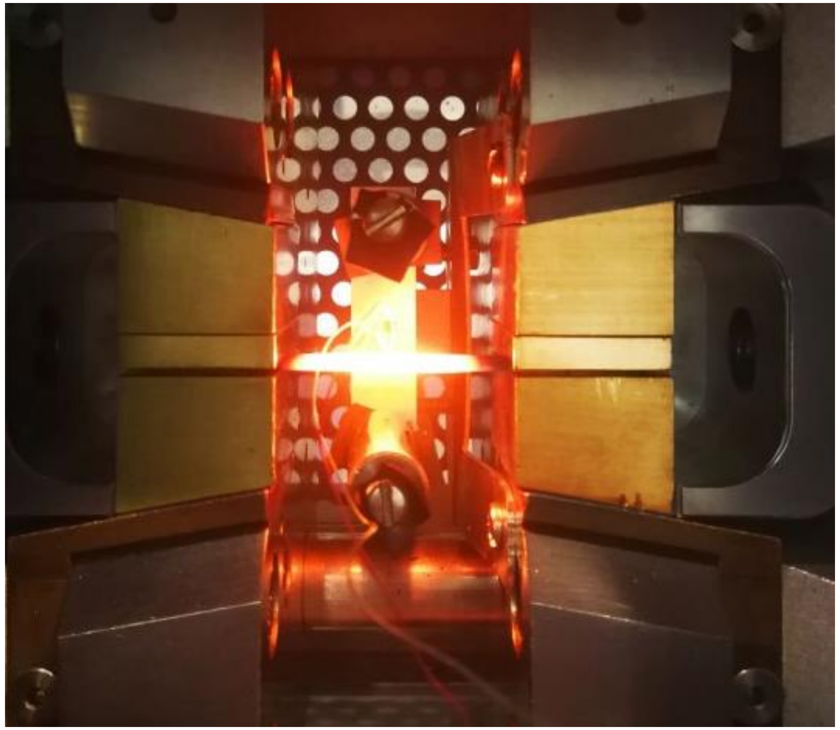


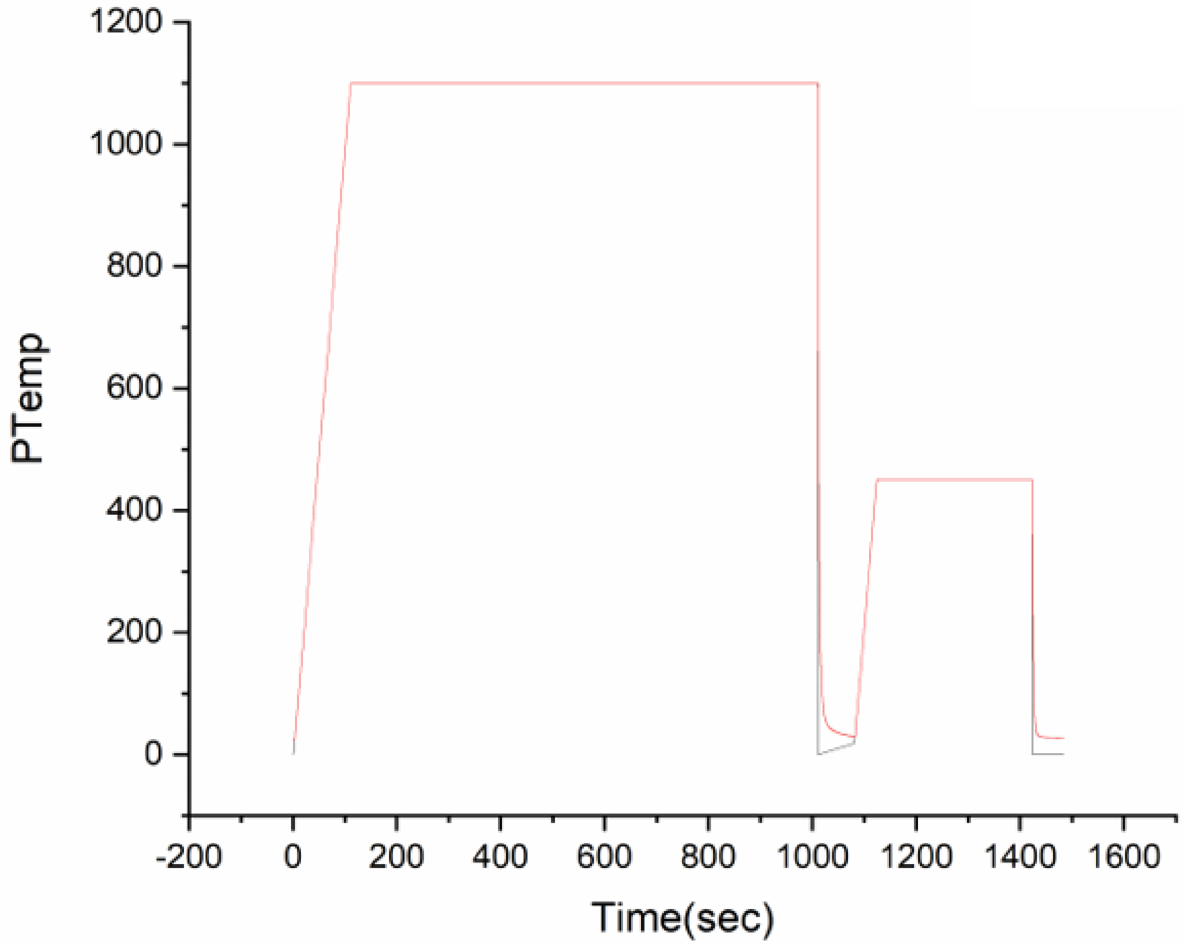

True-twin and pseudo-twin interfaces

Palomares-García, A.J., Pérez-Prado, M.T., Molina-Aldareguia, J.M. Effect of lamellar orientation on the strength and operating deformation mechanisms of fully lamellar TiAl alloys determined by micropillar compression (2017) Acta Materialia, 123, pp. 102-114.

## Advanced Characterization Techniques

### Design of optimal heat treatments using Gleeble system






**Left: a Q&P treatment in a GLEEBLE chamber; Right a typical Q&P thermal cycle applied to stainless steels, where temperatures and times are varied.**

Courtesy Dr. I. Sabirov

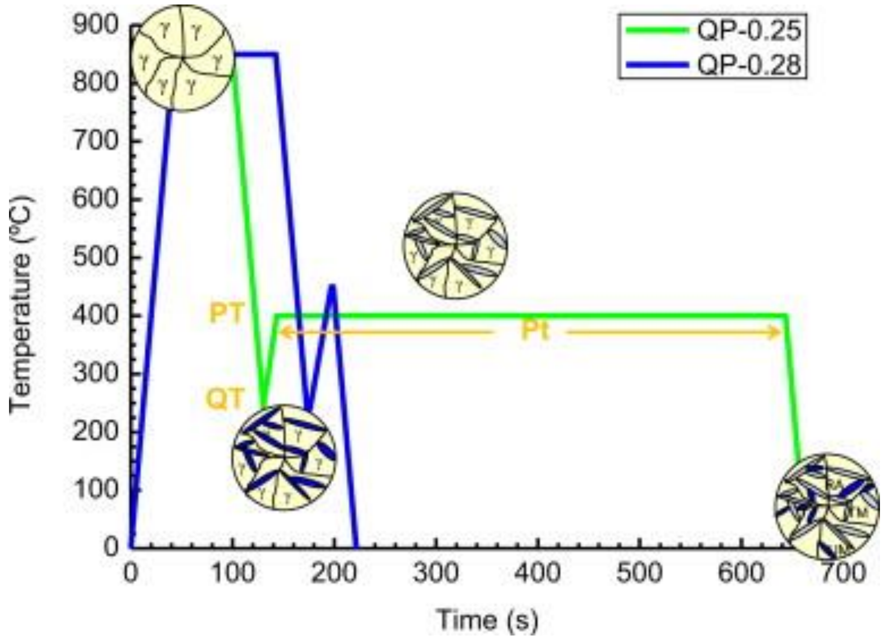
# Tools available for metallurgy today

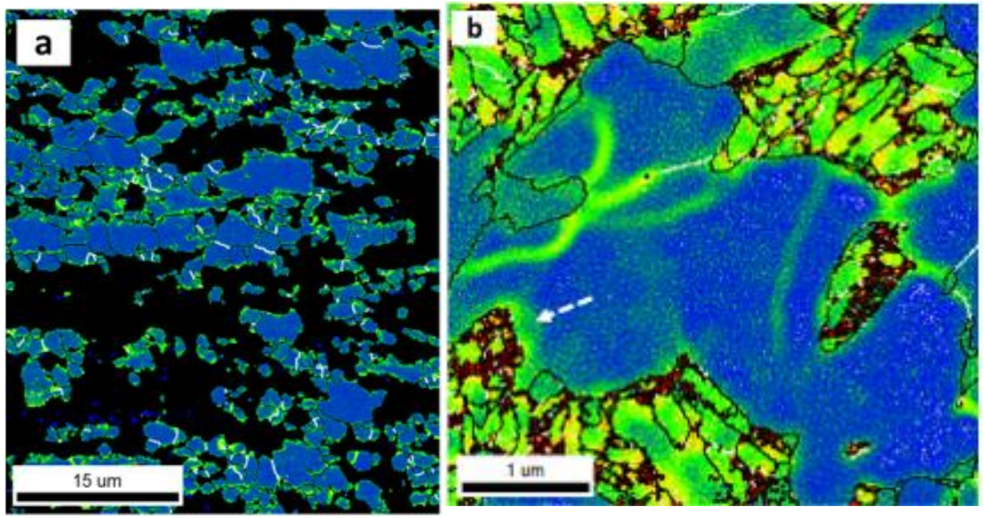
## Advanced Characterization Techniques

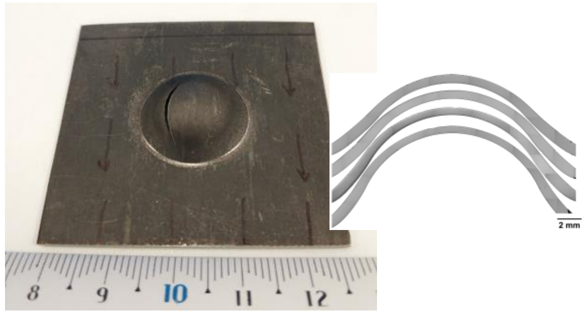
*Processing* → *Microstructure* → *Properties*

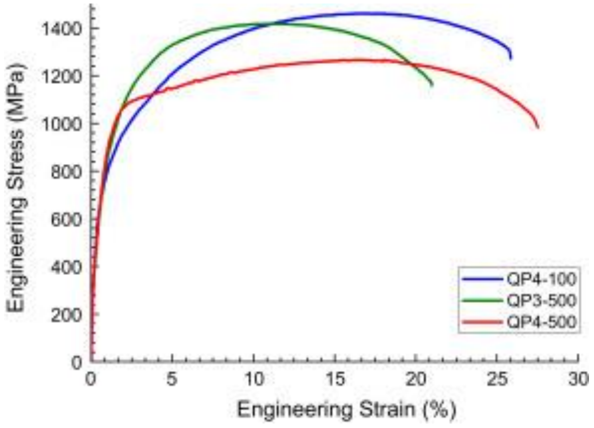
*On macro- and micro-scales*

*On macro-, micro- and nano-scales*






**Microstructural design in advanced metallic materials via thermo-mechanical processing to improve their mechanical and application-related properties.**

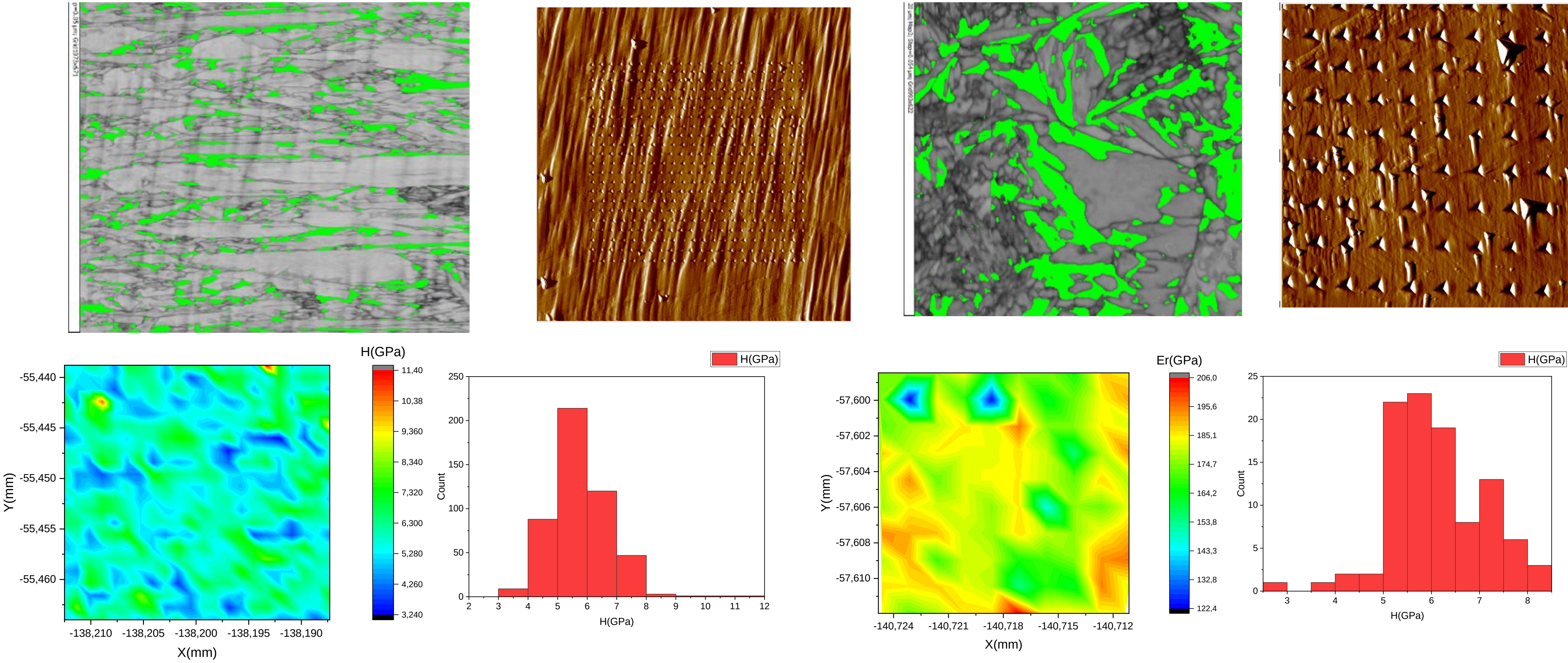
P. Xia, F. Canillas, I. Sabirov. Mater. Sci. Eng. A. 793 (2020) 139829.

M. Valdes-Tabernero, et. al. Mater. Characterization. 155 (2019) 109822.

# Tools available for metallurgy today

## Advanced Characterization Techniques

## Processing–microstructure–properties relationship in Q&P stainless steels



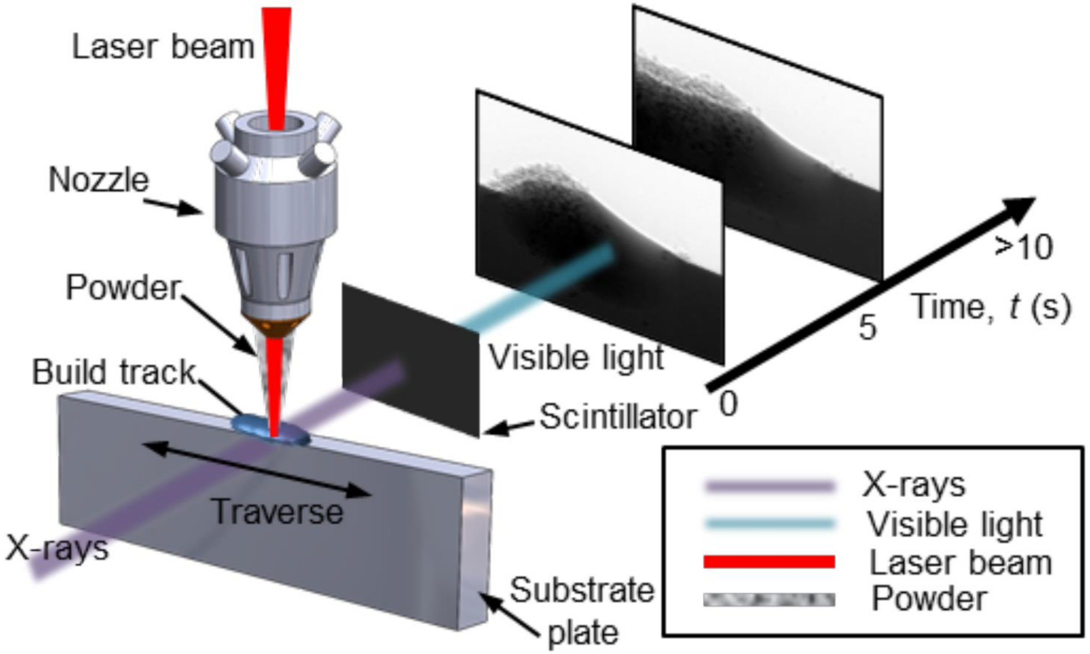

**The effect of chemistry on nanohardness distribution in Q&P treated steels. Left: EBSD phase map, analyzed area, relevant nanohardness distribution map and histogram of nanohardness distribution for a low alloyed steel; Right: for a highly alloyed steel.**

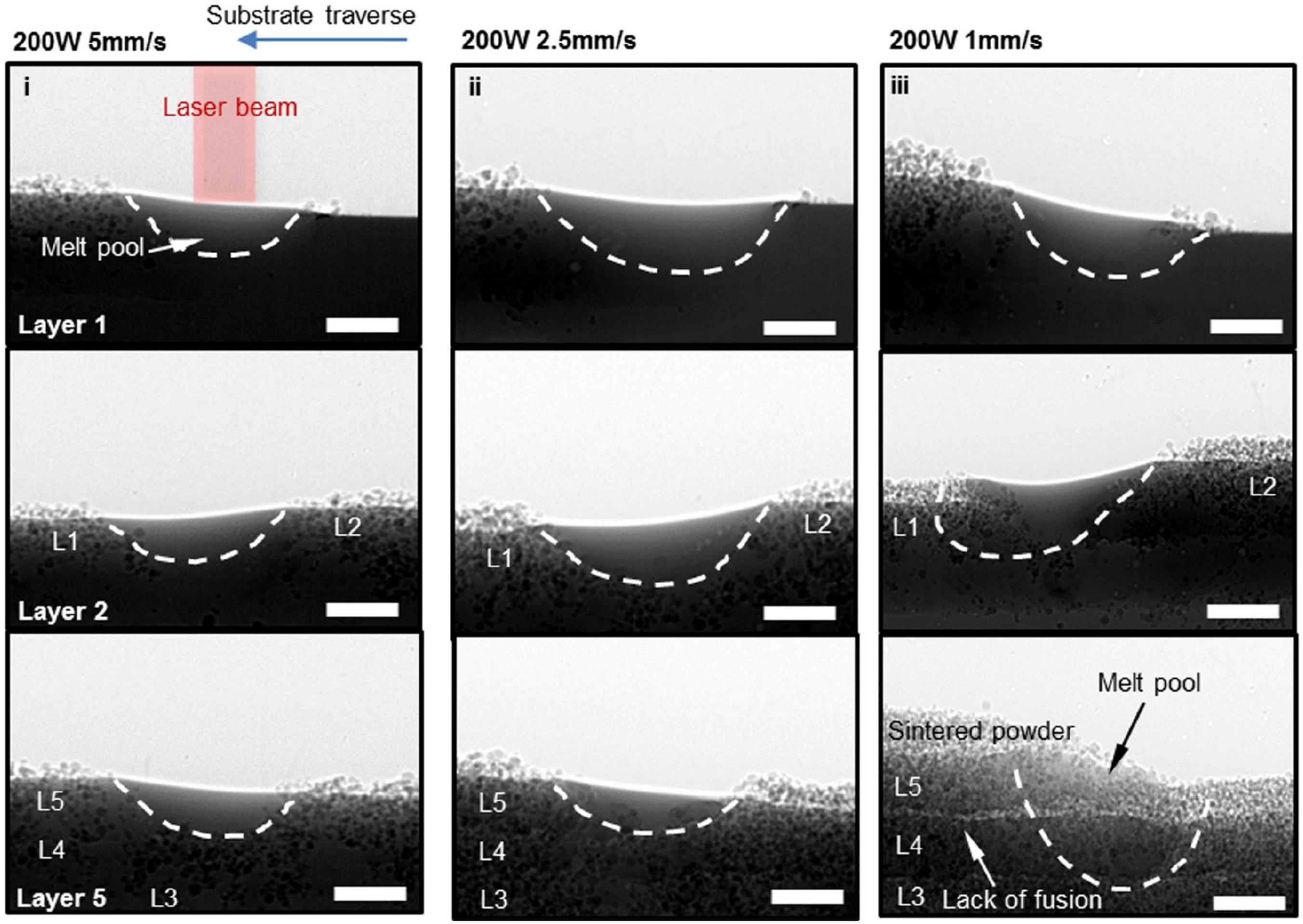
Courtesy Dr. I. Sabirov

# Tools available for metallurgy today

## Advanced Characterization Techniques

# Metals processing: In-situ Direct Energy Deposition of Ti64




**Multi-layer melt track morphologies. Representative radiographs of powder DED AM Ti-6242, showing the variation in melt pool and track morphologies with different substrate traverse speeds and a laser power of 200 W, a powder feedrate of 1 g/min. Scale bar = 500 μm. Note that substrate traverse direction is reversed for layer 2.**

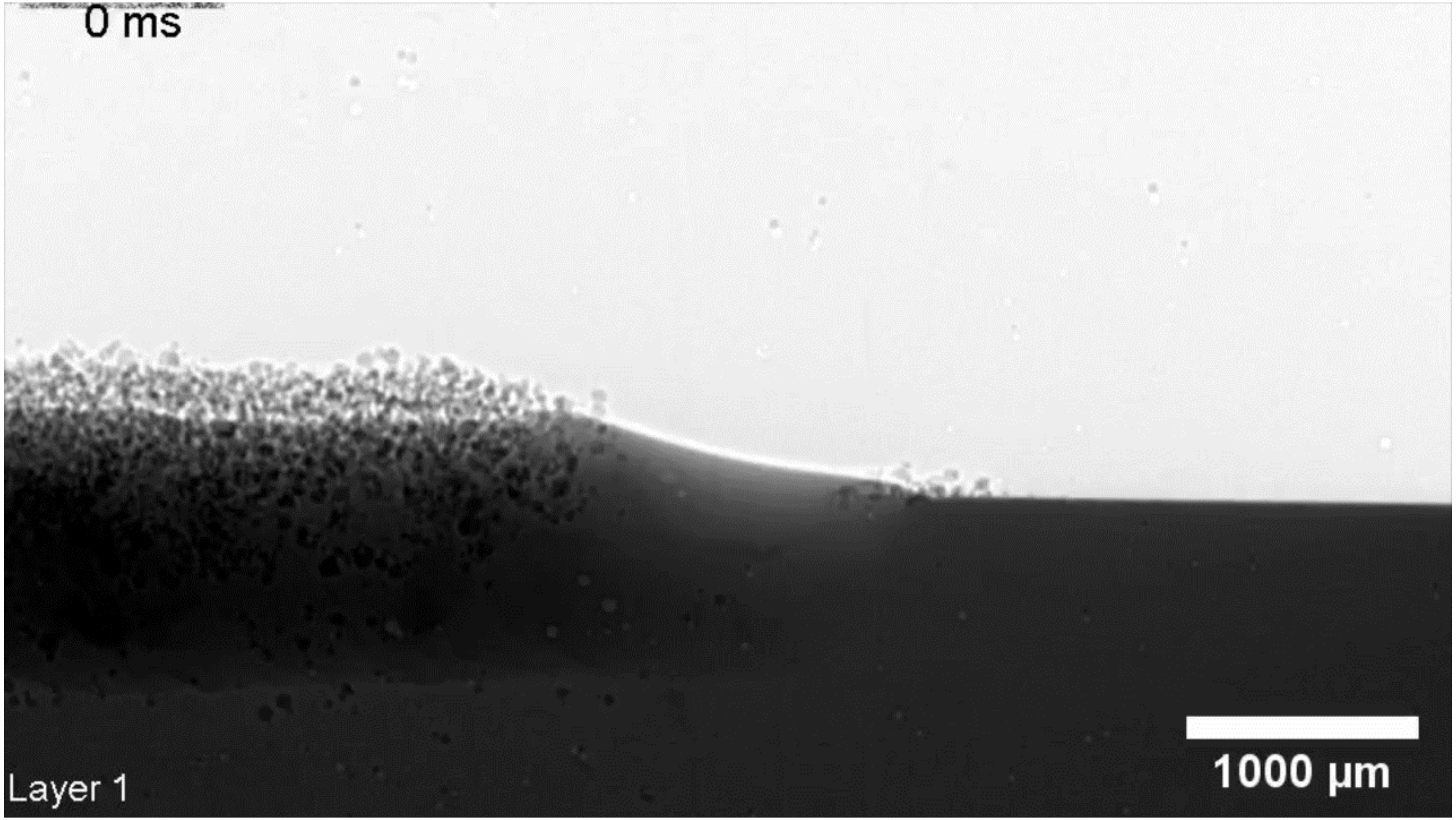
## X-Ray Tomography

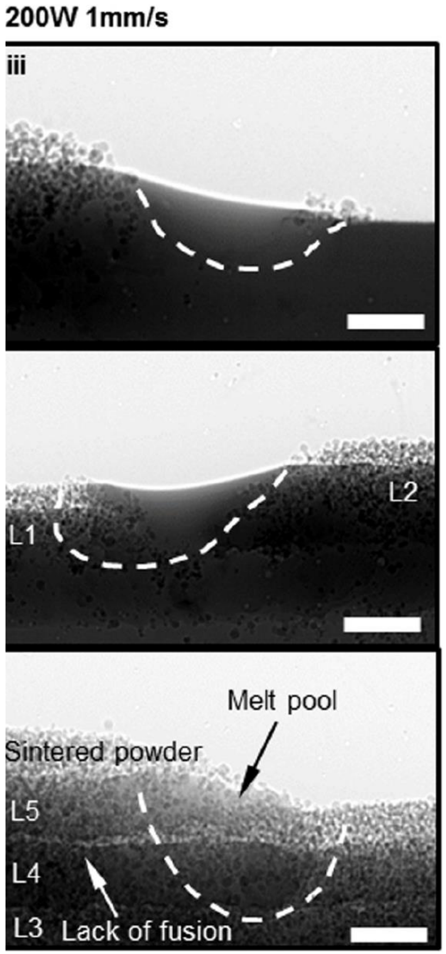
Y. Chen, et al. Additive Manufacturing 41 (2021) 101969

# Tools available for metallurgy today

## Advanced Characterization Techniques

### Metals processing: In-situ Direct Energy Deposition of Ti64



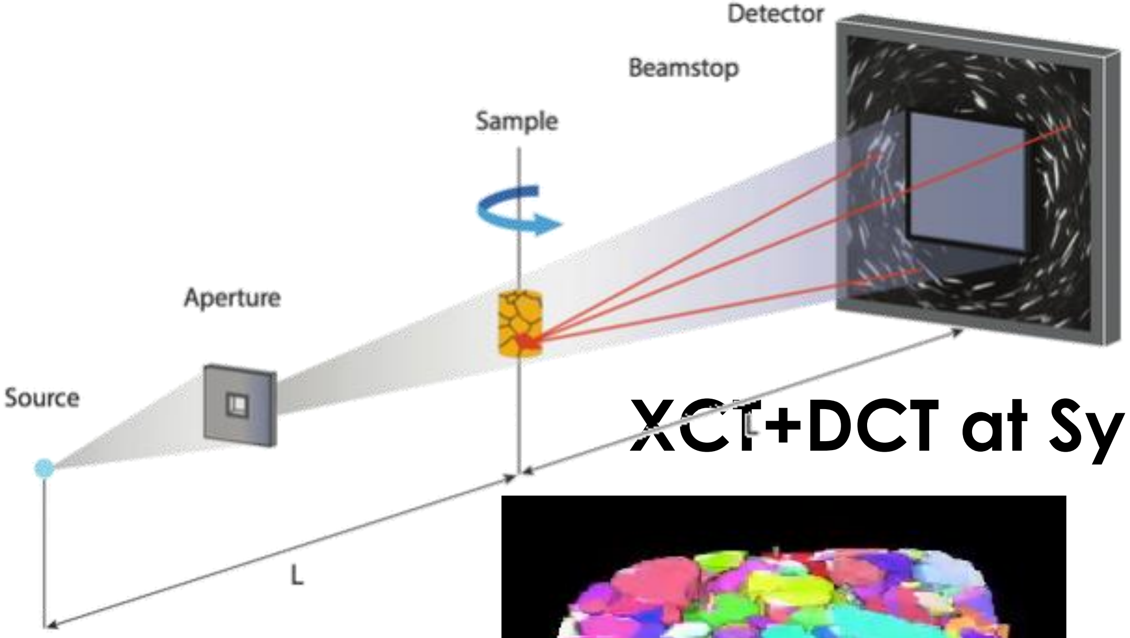




Y. Chen, et al. Additive Manufacturing 41 (2021) 101969

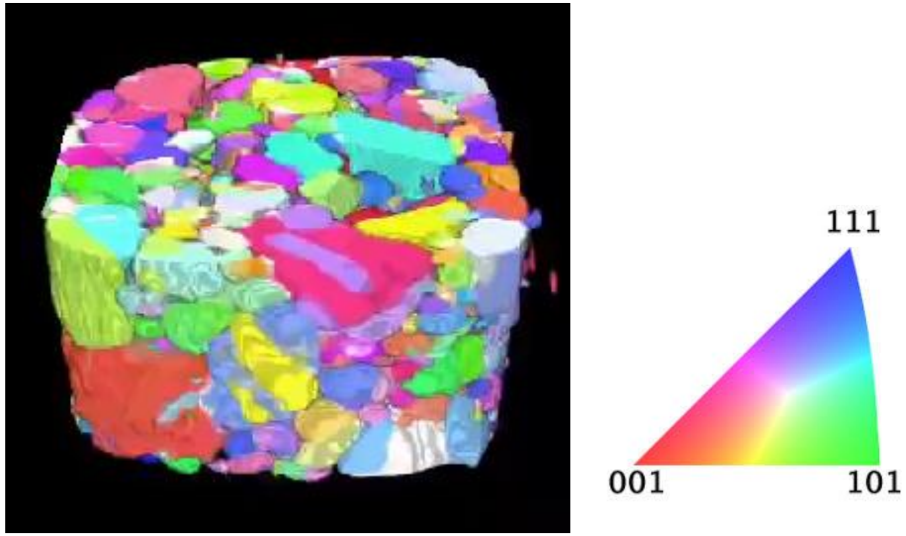
# Tools available for metallurgy today

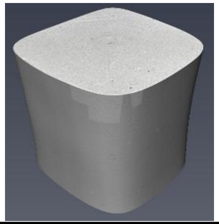
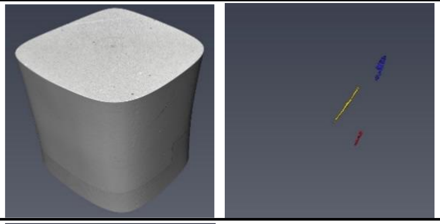
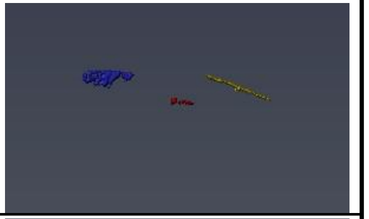
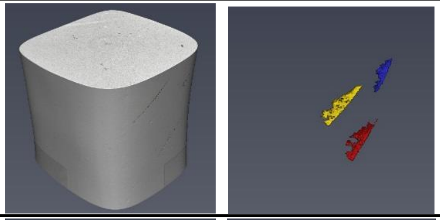
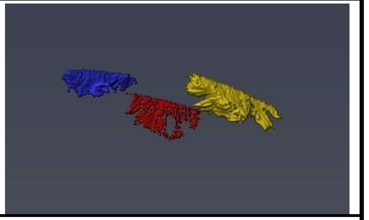
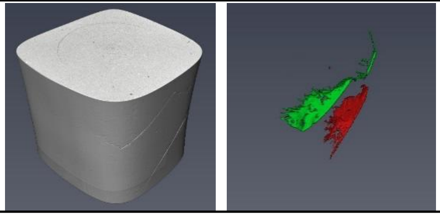
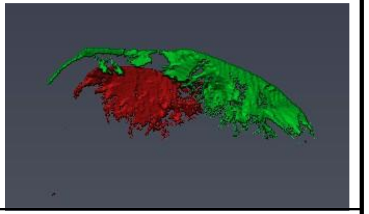
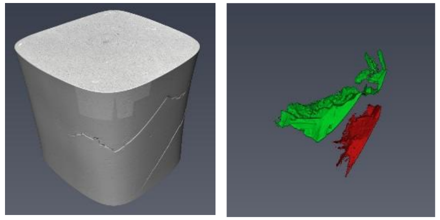
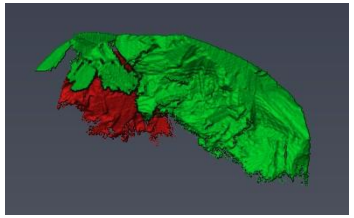
## Advanced Characterization Techniques

### In-situ fatigue studies in Ni Superalloys




**XCT+DCT at Synchrotron**




| CYCLES | PERSPECTIVE | TOP VIEW |
|---|---|---|
| 20 k |  N/A | N/A |
| 40 k |  |  |
| 60 k |  |  |
| 90 k |  |  |
| 100 k |  |  |

Courtesy Dr. F. Sket

# Tools available for metallurgy today

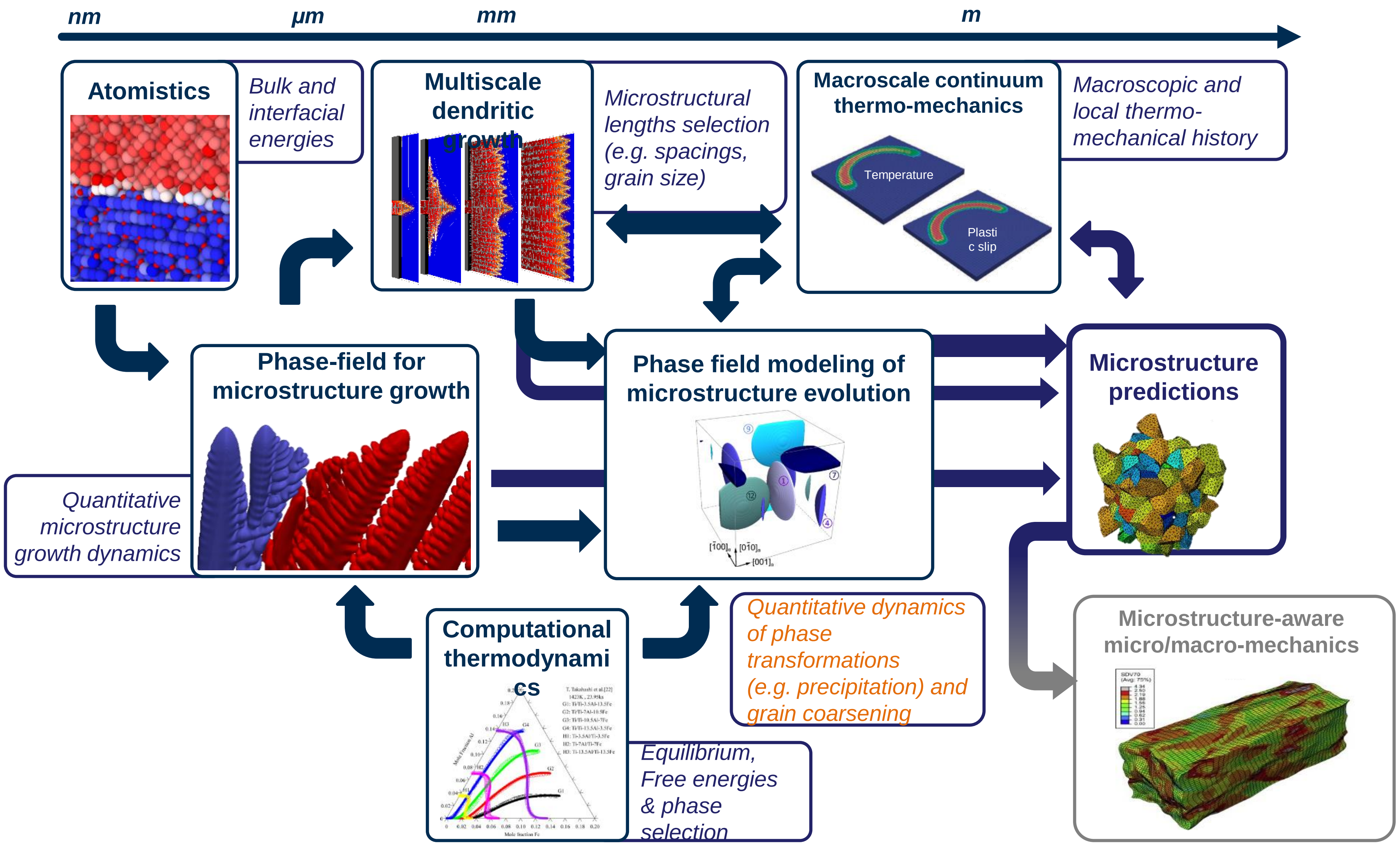
## Advanced Characterization Techniques

## Modelling and simulation

# Tools available for metallurgy today

## Modelling and simulation

## From alloys & processes to microstructures to properties



# Tools available for metallurgy today



## Modelling and simulation

### Virtual testing of SLM Hastelloy-X

Strong influence of processing parameters in response using the same powder

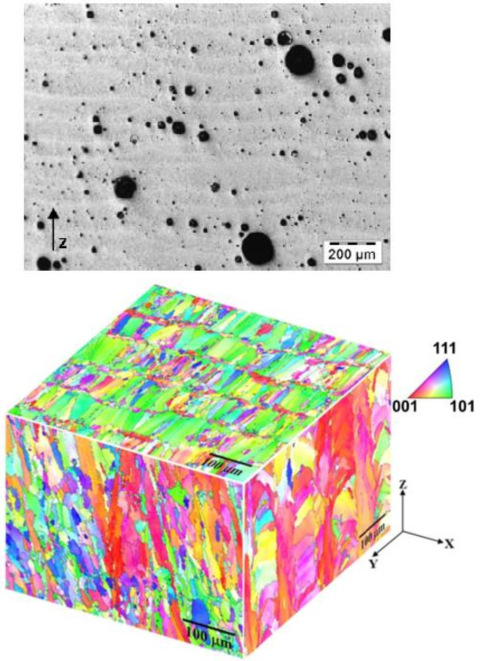
**Process parameters**

- Laser power
- Scan speed
- Hatch distance
- Layer thickness
- Scanning direction
- Energy density

**Building direction and geometry**

- Horizontal and vertical
- Thickness of sample

Processing




**Defects:**

- Surface roughness
- Porosity

**Microstructure**

- Grain size
- Grain aspect ratio
- Grain orientation
- Twinning

If the SLM resulting microstructure is given (experimentally or predicted by virtual testing), is it posible to predict the macroscopic response?

J. Segurado, R. Lebensohn and J.LLorca, Computational Homogenization of Polycrystals. Advances in Applied Mechanics ,51, 1-114, 2018

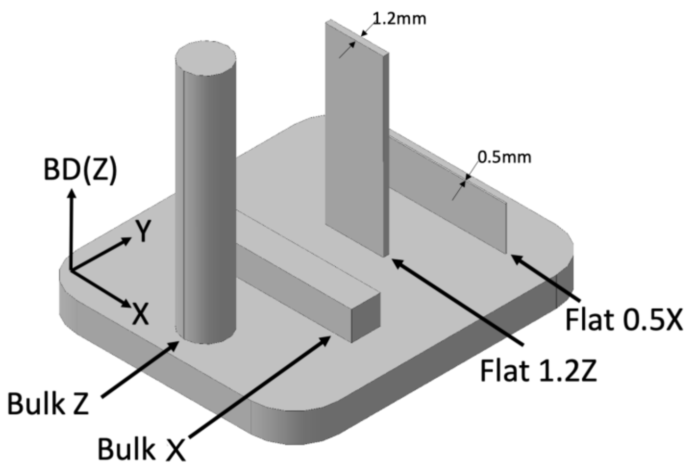
# Tools available for metallurgy today

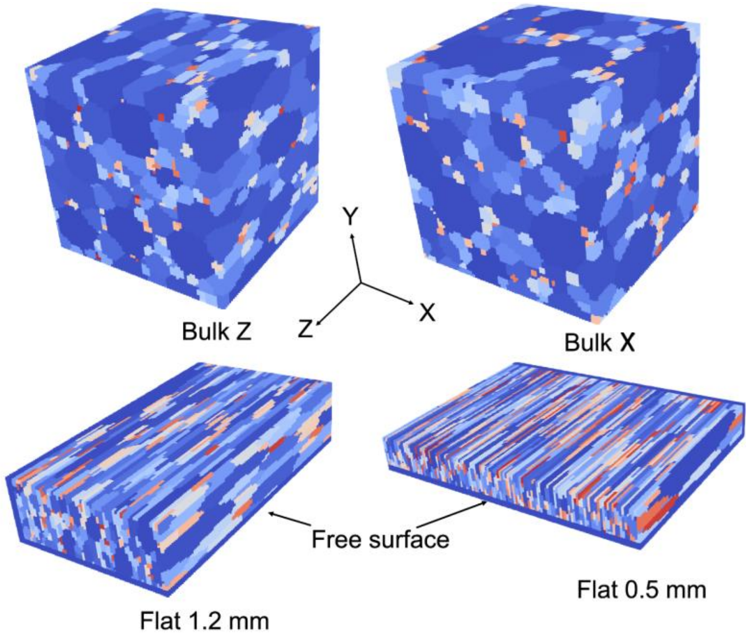
## Modelling and simulation

## Virtual testing of SLM Hastelloy-X: Tensile response

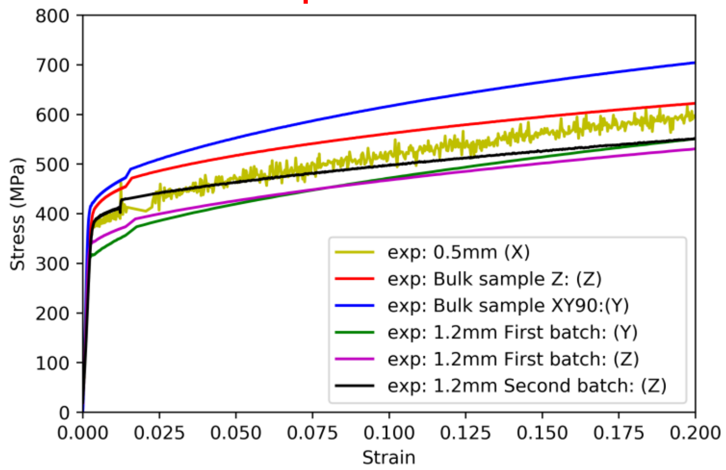
Computational homogenization of polycrystals allowed to determine the macroscopic response for different fabrication directions and speciment thicknesses:

Origin of differences in mechanical response ONLY due to polycrystalline microstructure

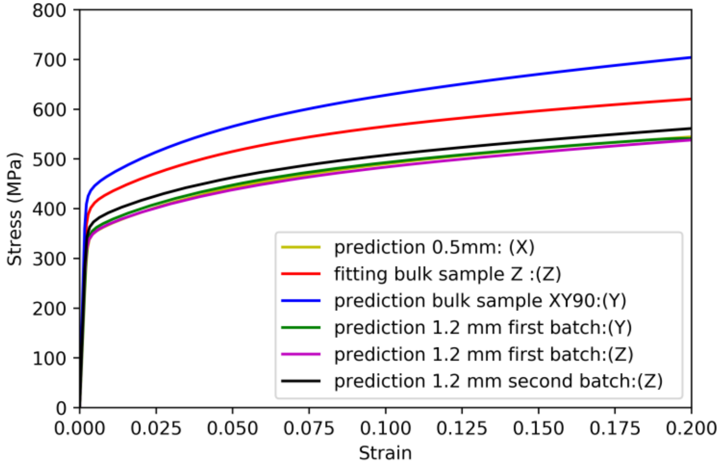



Experiments




Virtual tests



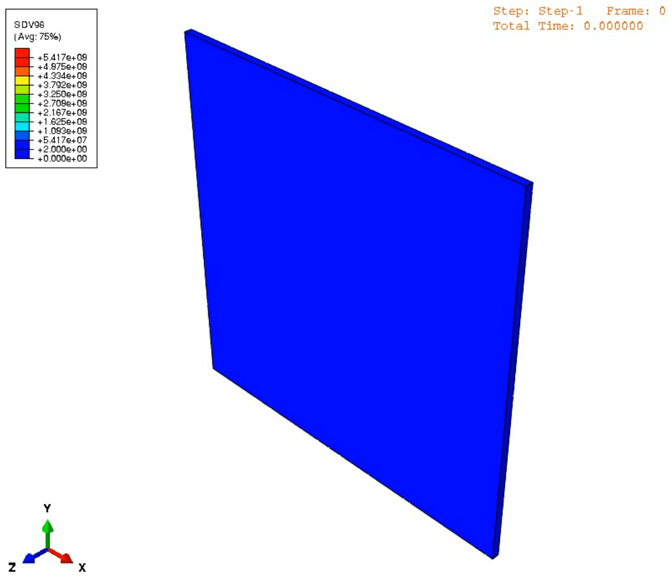

S. Lucarini, M. Upadyhay, J. Segurado, FFT based approaches in micromechanics: fundamentals, methods and applications. Modelling and Simulation in Materials Science and Engineering 30 023002, 2022

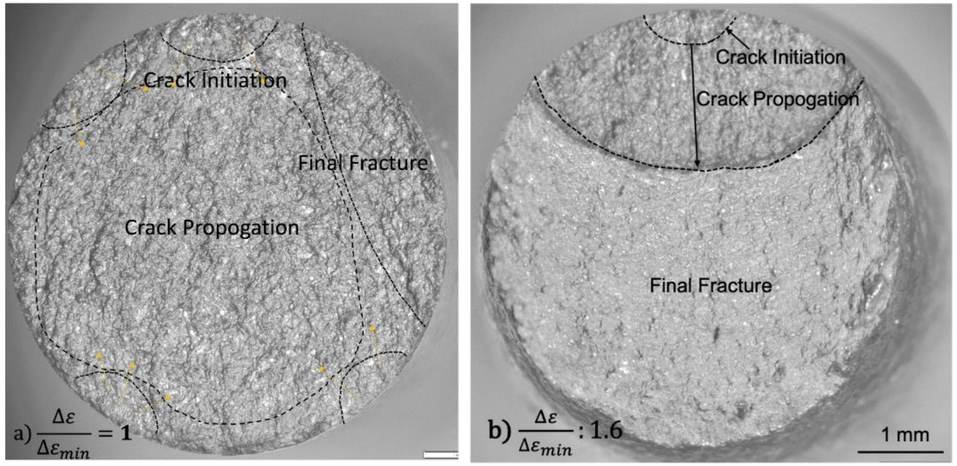
# Tools available for metallurgy today

## Modelling and simulation

## Fatigue life prediction

- In many cases nucleation of cracks take the majority of fatigue life.
- Nucleation is strongly **influenced by microstructure** (pores or cracks or just grains) :
  - Accumulation of plastic slip→slip bands(persistent slip bands)
  - Persistent slip bands → microscopic cracks
- Nucleation can be modeled by studying accumulation of plasticity or some FIP on the hot-spots of the microstructure through micromechanical simulations
- Life can be related with FIP accumulated using simple phenomenological expression



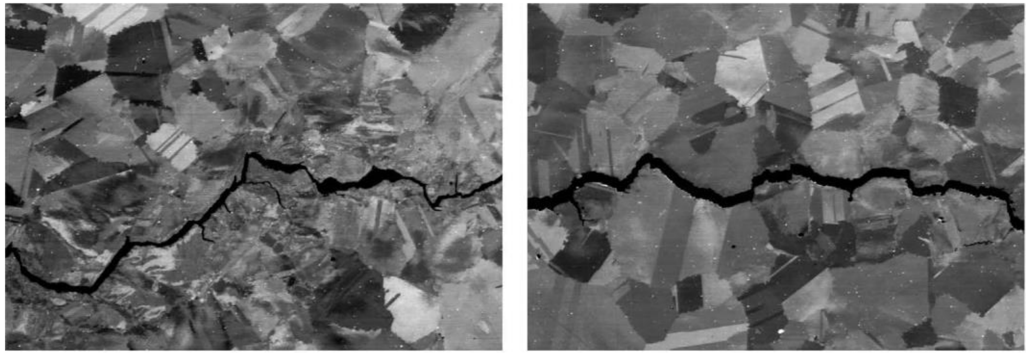

C. M. Pilgar, A. Fernandez, S. Lucarini, J. Segurado, Effect of printing direction and thickness on the mechanical behaviour of SLM fabricated Hastelloy-X, International Journal of Plasticity, 103250, 2022

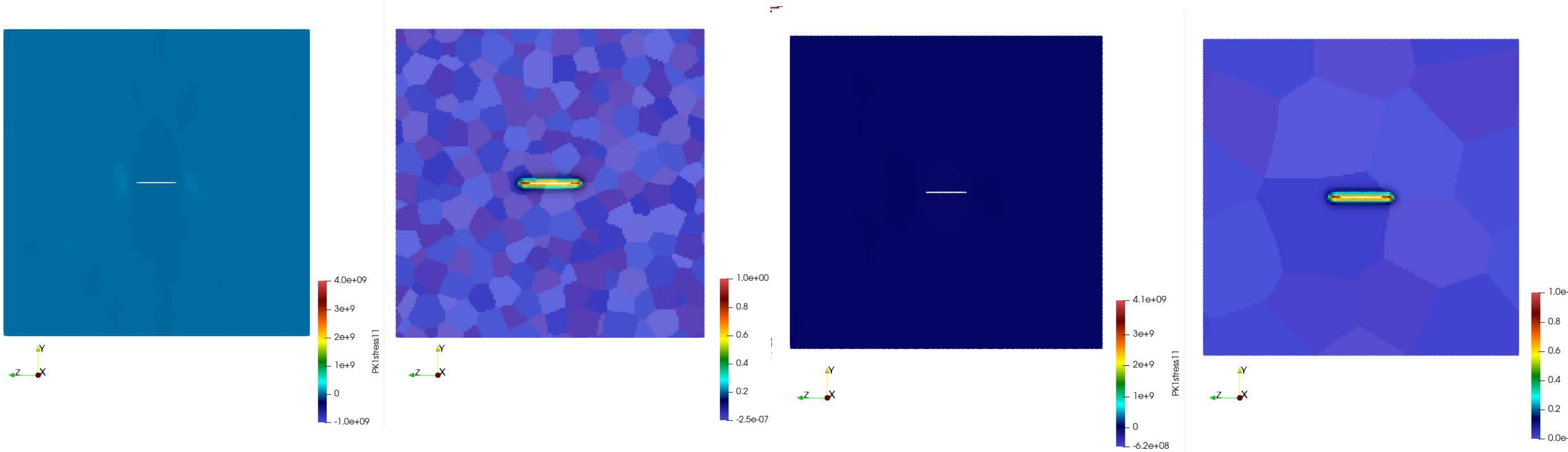
# Tools available for metallurgy today

## Modelling and simulation

## Fracture of polycrstals

**Phase-field fracture** can be combined with **crystal plasticity and FFT-based homogenization** to study the effect of microstrucure in crack propagation of polycrystals





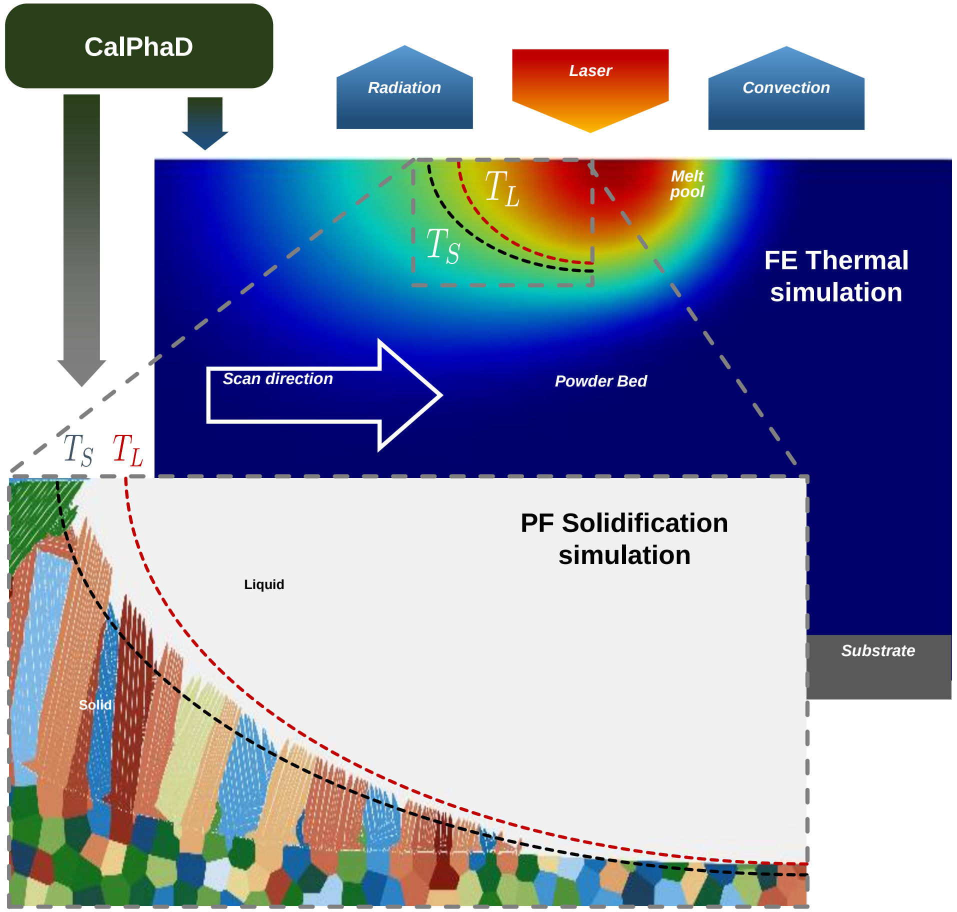

C. M. Pilgar, A. Fernandez, J. Segurado, Microstructure sensitive fatigue life prediction model for SLM fabricated Hastelloy-X, International Journal of Fatigue, 2023

# Tools available for metallurgy today

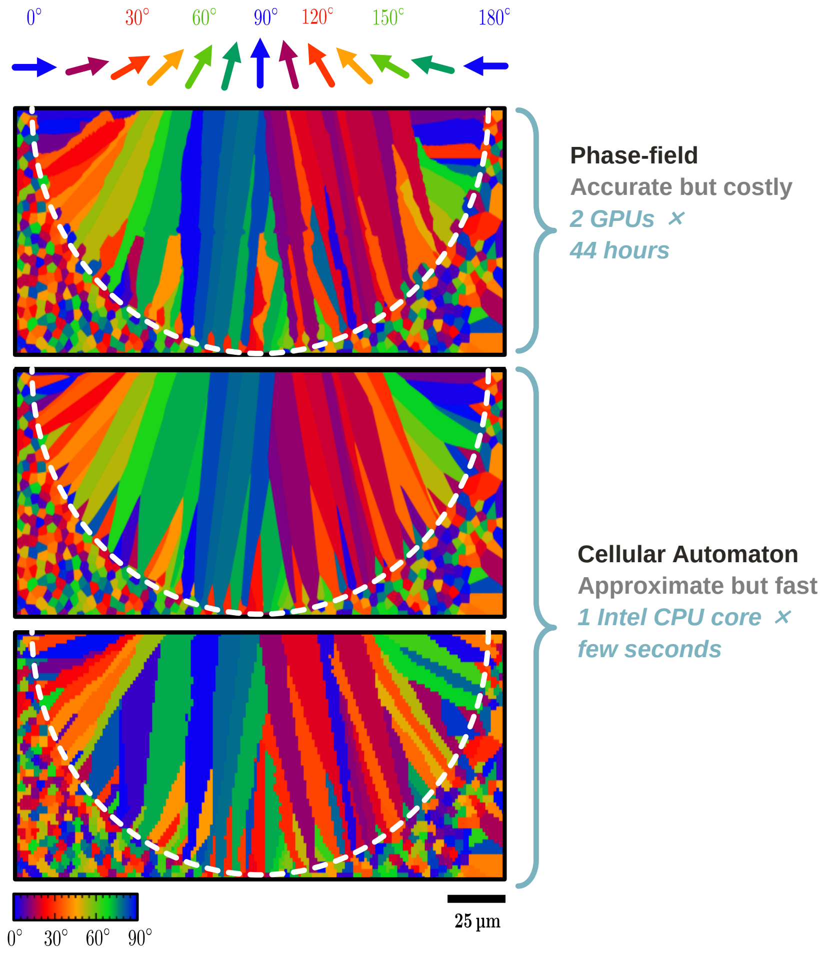
## Modelling and simulation

**Understand, model & predict the emergence & evolution of complex microstructure in advanced materials**

### Multiscale modeling of microstructure formation in additive manufacturing




Elahi et al. Comput. Mater. Sci. 209 (2022) 111383



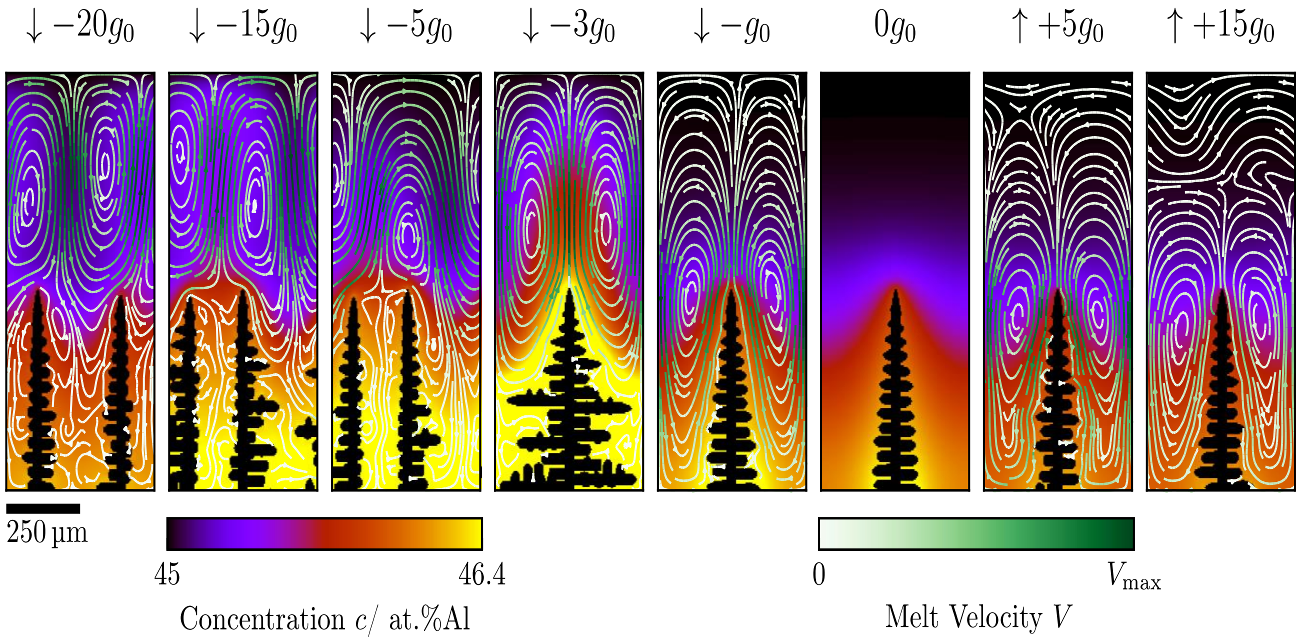

Elahi et al. Comput. Mater. Sci. 216 (2023) 111882

# Tools available for metallurgy today

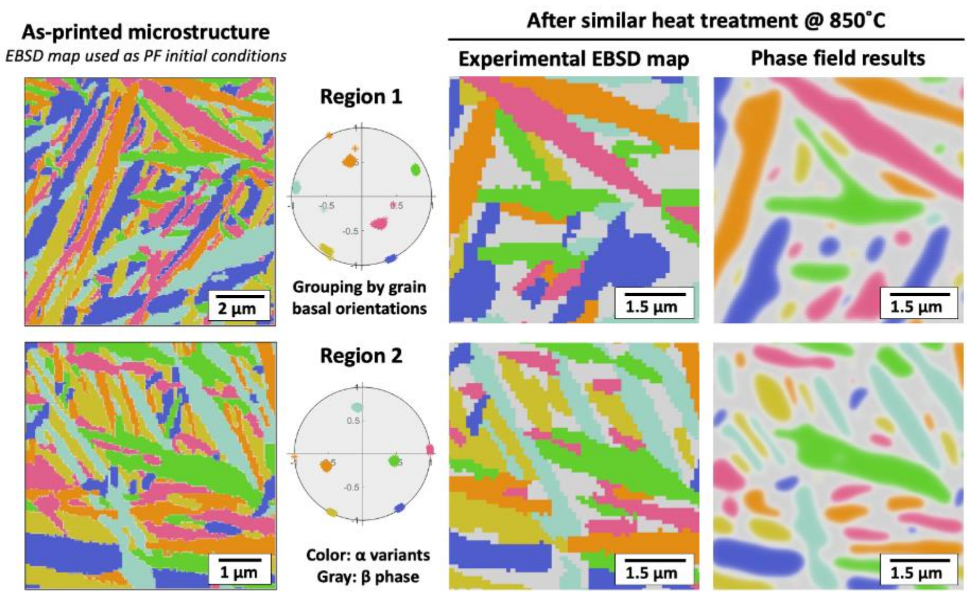
## Modelling and simulation

## Understand, model & predict the emergence & evolution of complex microstructure in advanced materials

### Effect of fluid flow on dendritic growth




### Solid-state microstructure evolution during heat treatment




Isensee & Tourret Acta Materialia 234 (2022) 118035

UNIT OF EXCELLENCE MARÍA DE MAEZTU

# Tools available for metallurgy today

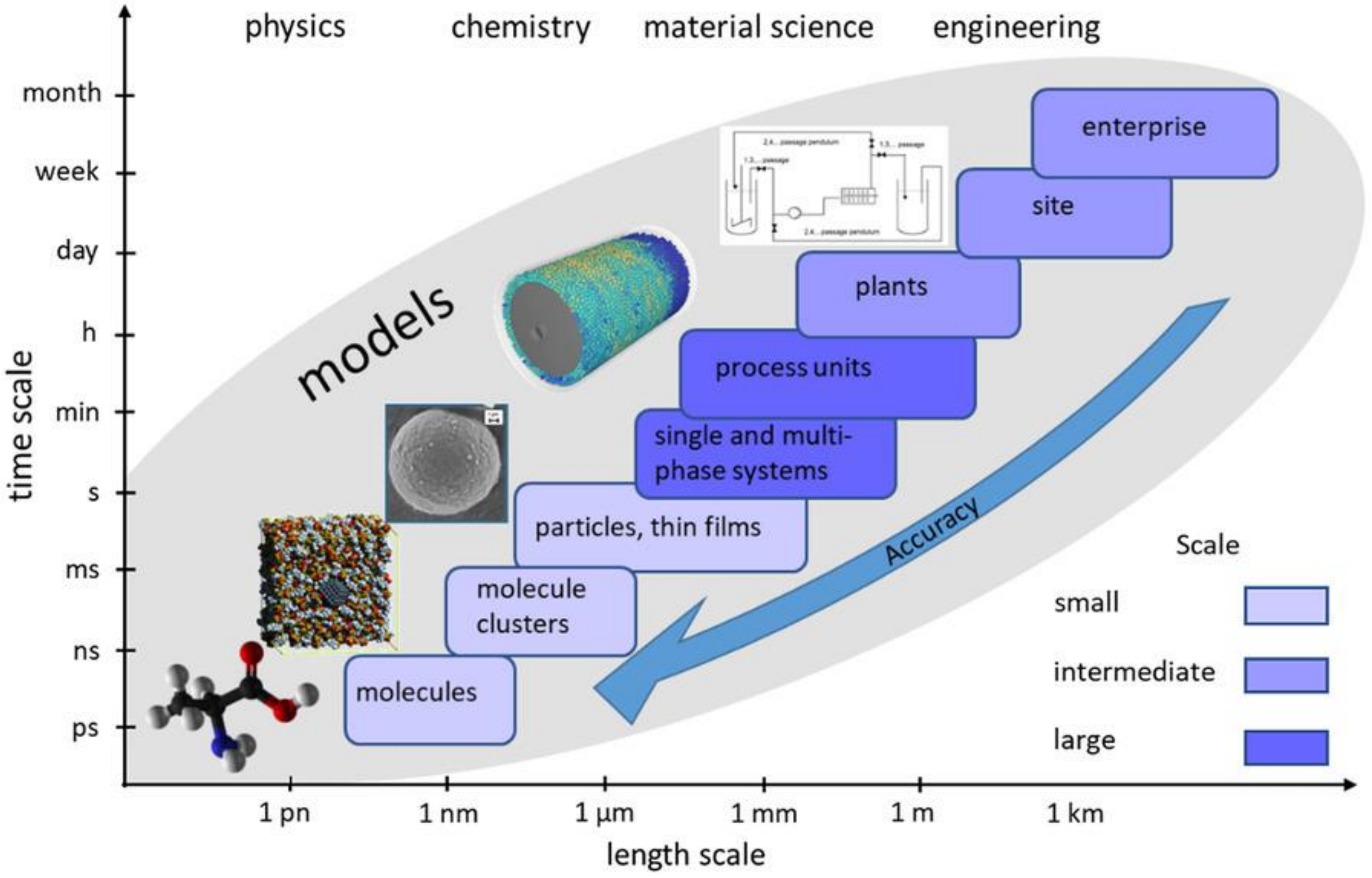
## Advanced Characterization Techniques

## Modelling and simulation

## Artificial inteligence/Machine learning

# Tools available for metallurgy today

## AI-assisted alloy and process design

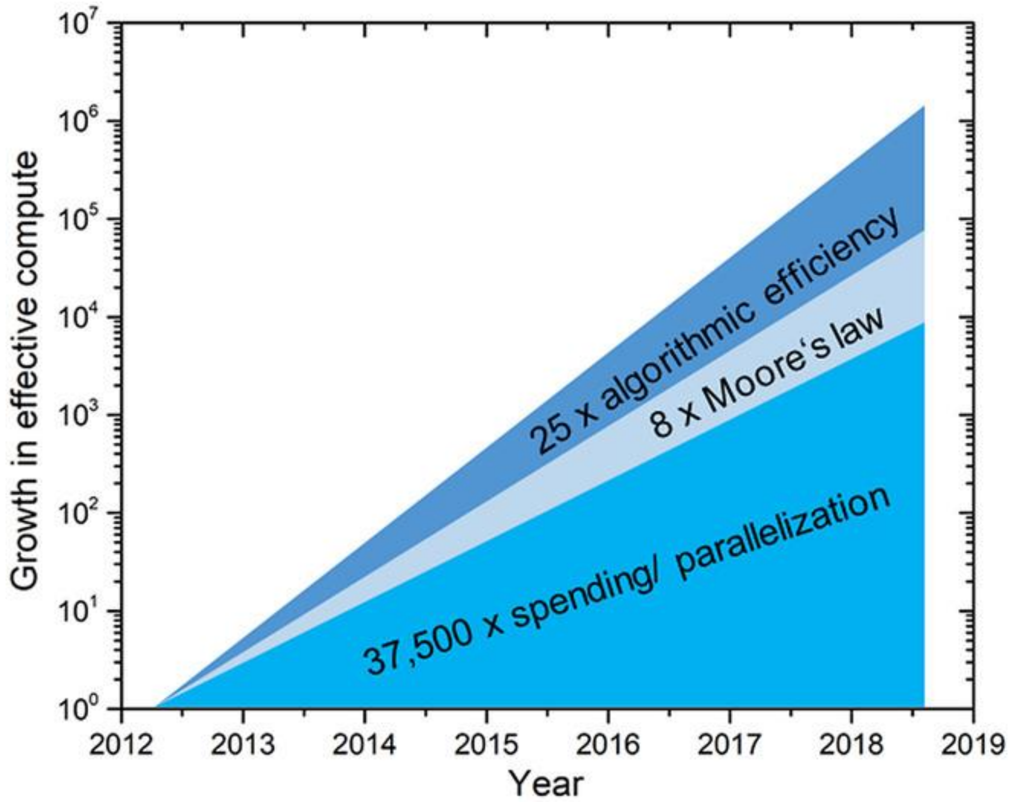



Process engineering operates on various length and timescales which are linked with specific models, simulations, unit operations, process parameters, and conditions.


Thon, C., Finke, B., Kwade, A. and Schilde, C. (2021), Artificial Intelligence in Process Engineering. Adv. Intell. Syst., 3: 2000261.

# Tools available for metallurgy today

## AI-assisted alloy and process design



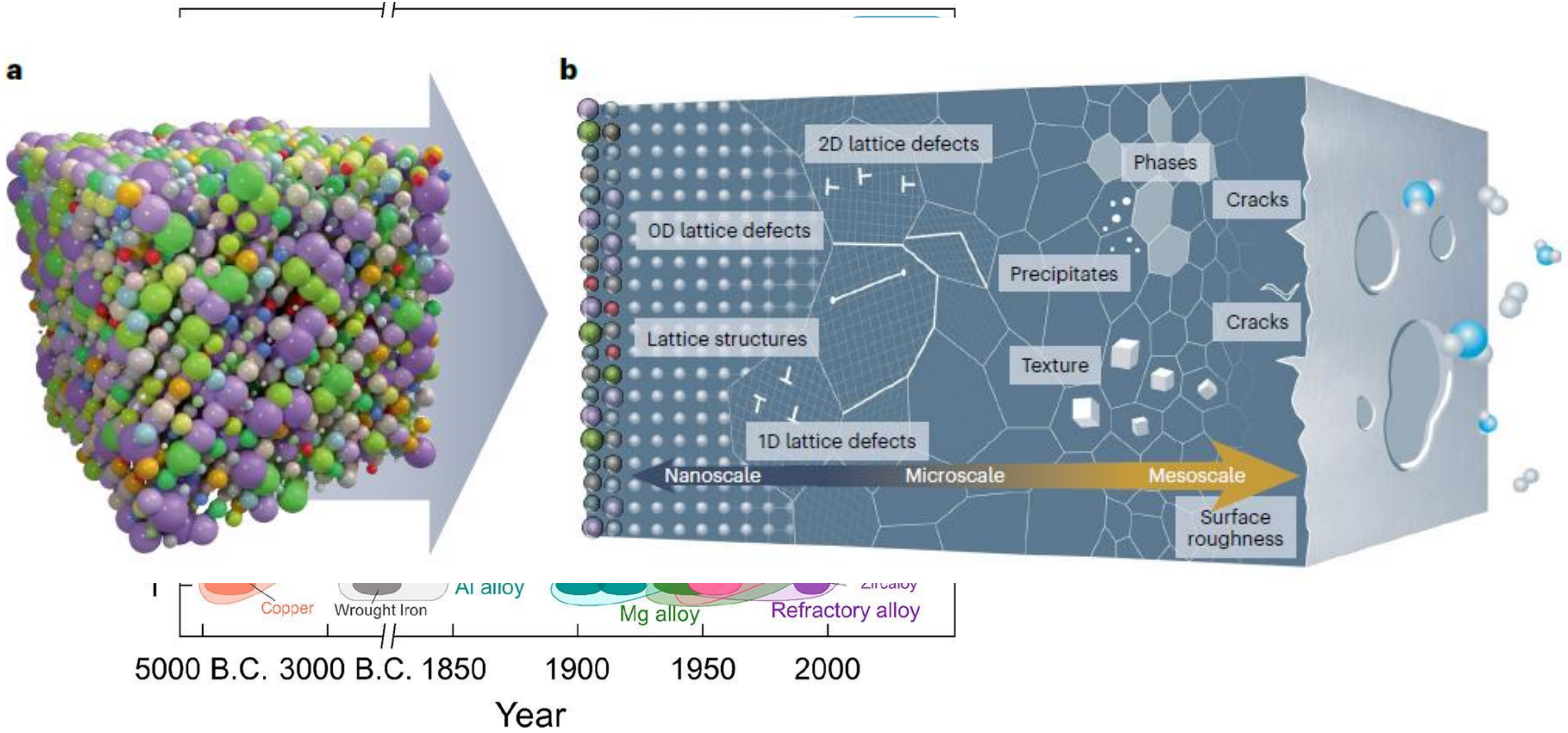

Approximated growth in effective compute between 2012 and 2018 with respective factors.

- Computing efficiency of computers has been continuously increasing, whereas its cost saturated.
- In the near future, the application of AI will enable new levels of process automation and process optimization. The prediction of highly complex production system behaviour will be possible.
- Over all, labor-intensive research procedures currently occupying years could be reduced to weeks or less, cutting costs, reducing resource consumption.


Thon, C., Finke, B., Kwade, A. and Schilde, C. (2021), Artificial Intelligence in Process Engineering. Adv. Intell. Syst., 3: 2000261.

# Tools available for metallurgy today

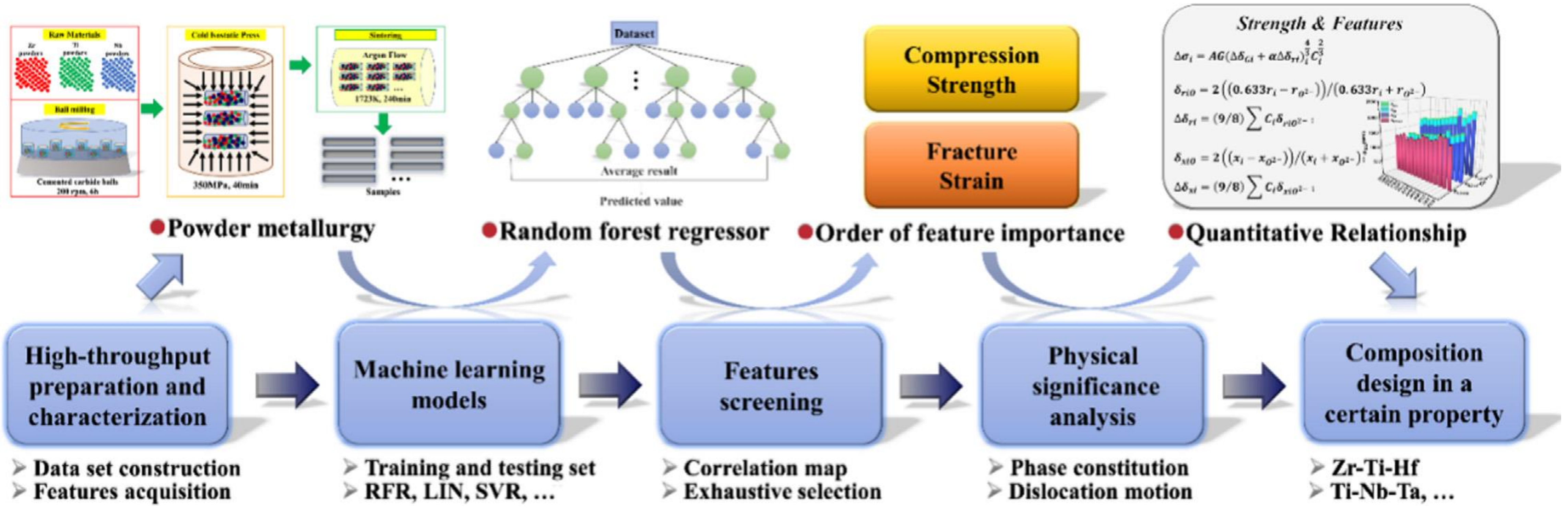
## AI-assisted alloy and process design




Raabe, D., Mianroodi, J.R. & Neugebauer, J. Accelerating the design of compositionally complex materials via physics-informed artificial intelligence. Nat Comput Sci 3, 198–209 (2023).

# Tools available for metallurgy today

## AI-assisted alloy and process design




(i) constructing the database and acquiring the features; (ii) selecting models; (iii) screening features; (iv) establishing a quantitative relationship between the key features and mechanical properties.

Shengping Si et.al. "Study on strengthening effects of Zr-Ti-Nb-O alloys via high throughput powder metallurgy and data-driven machine learning", Materials & Design, 2021, 109777.

# Tools available for metallurgy today

## AI-assisted alloy and process design

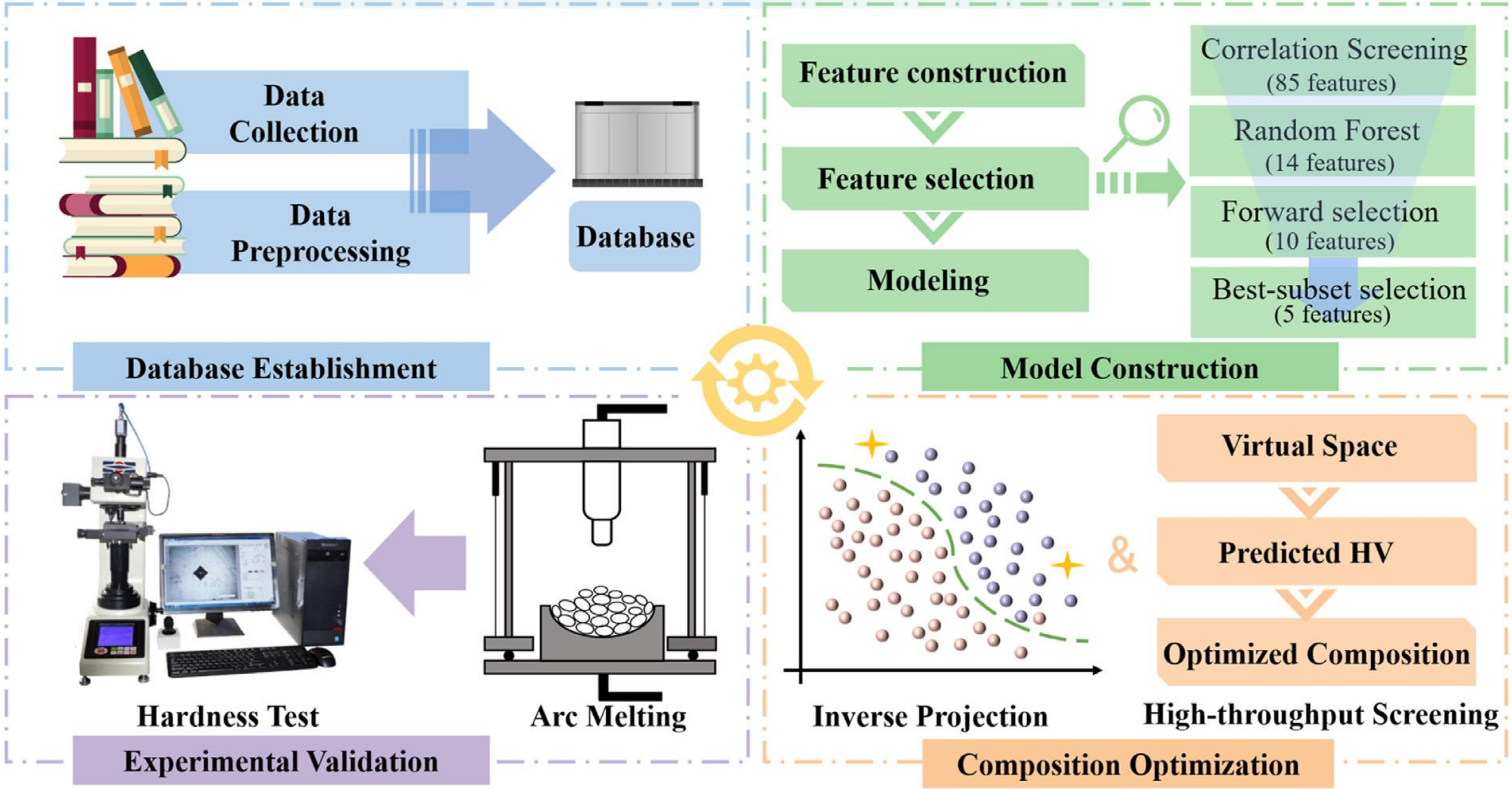


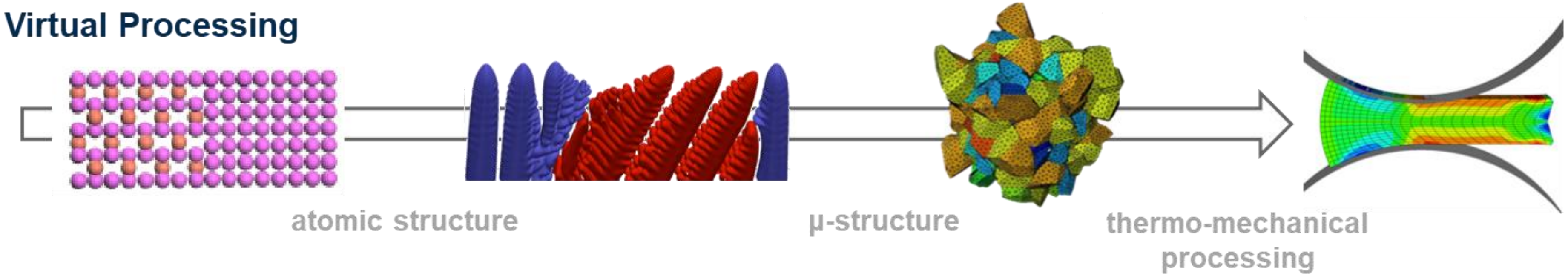

Diagram of machine learning-based alloy design system for the HEAs with desired hardness.

Chen Yang, et.al. "A machine learning-based alloy design system to facilitate the rational design of high entropy alloys with enhanced hardness", Acta Materialia, 2022, 117431

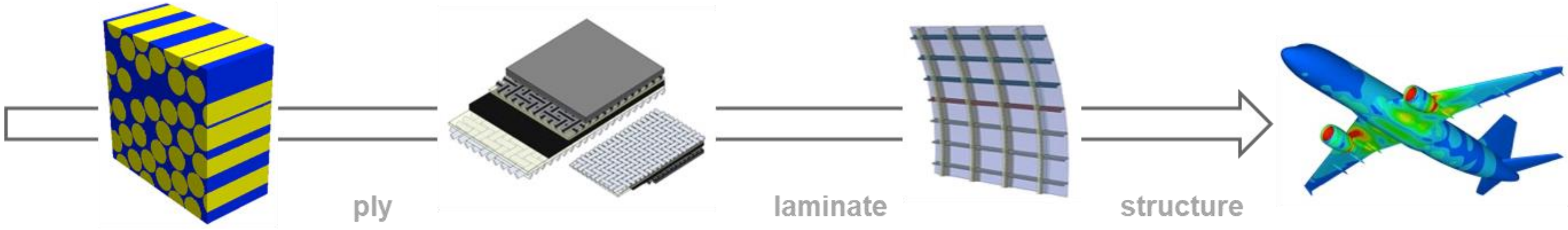
# Tools available for metallurgy today

**Multiscale Materials Modelling: Metals, Composites, Nanomaterials, Advanced Porous Materials,…**

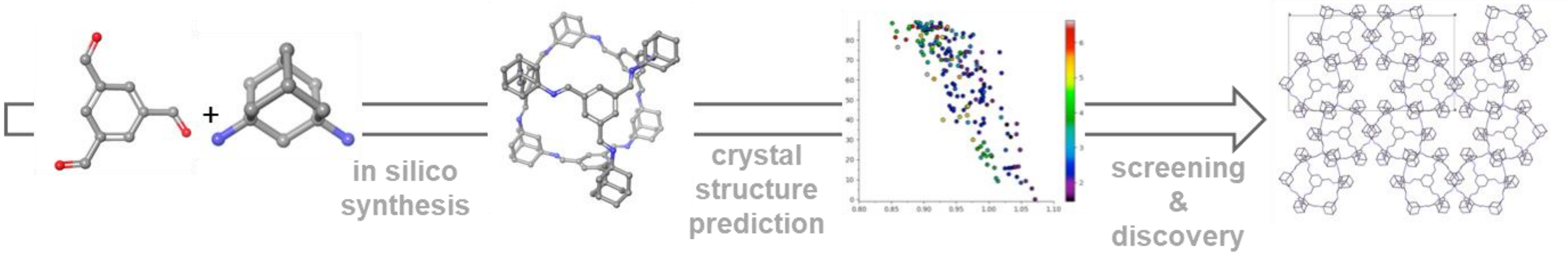
## Virtual Processing




## Virtual Testing




## Computational, data-driven materials discovery



- Metallurgy (what is this?).
- Metallurgy in the past.
- Metallurgy today, through some numbers
- Some of the problems metallurgy faces today as a result of its success
- Tools available for metallurgy today.
- What about the future?.
- Some final remarks.

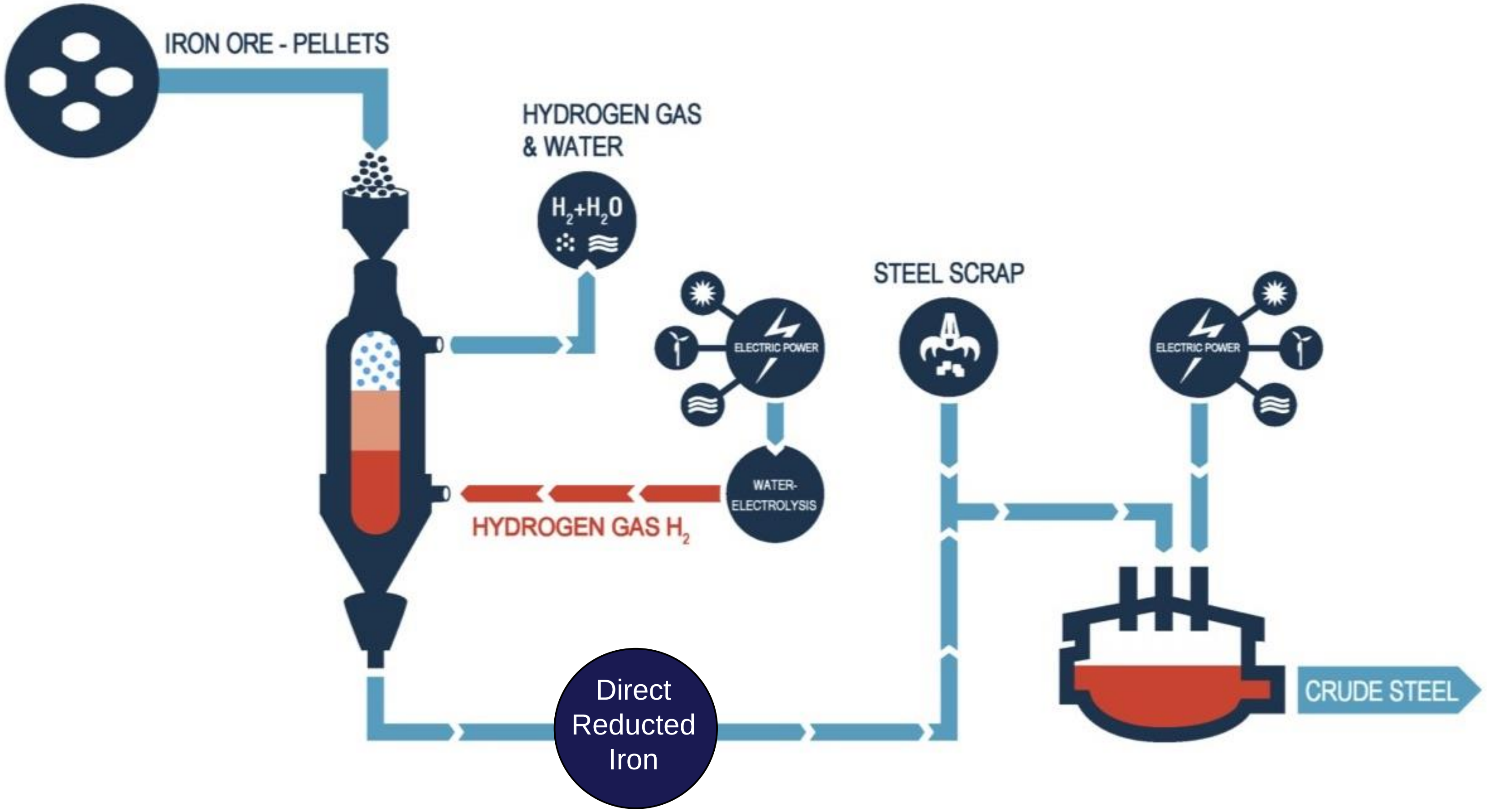
# What about the future?.

“Greener” technologies

# What about the future?.

## We have to move to “greener” technologies

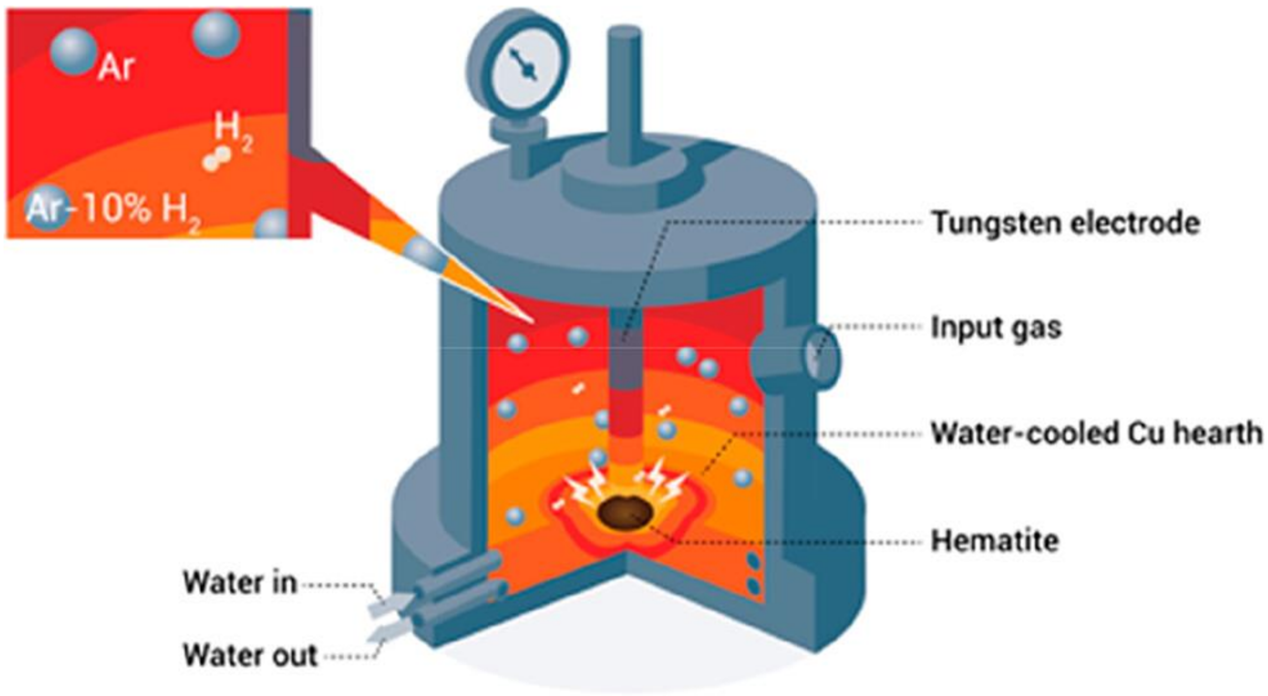
### Hydrogen based Direct Reduction




Source: Steel Institute VDEh

# What about the future?.

## We have to move to “greener” technologies

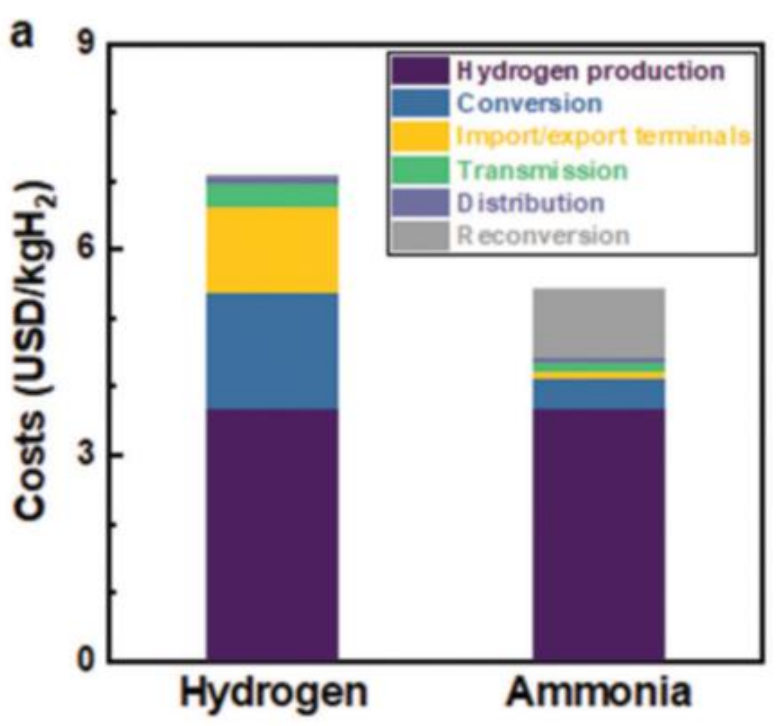


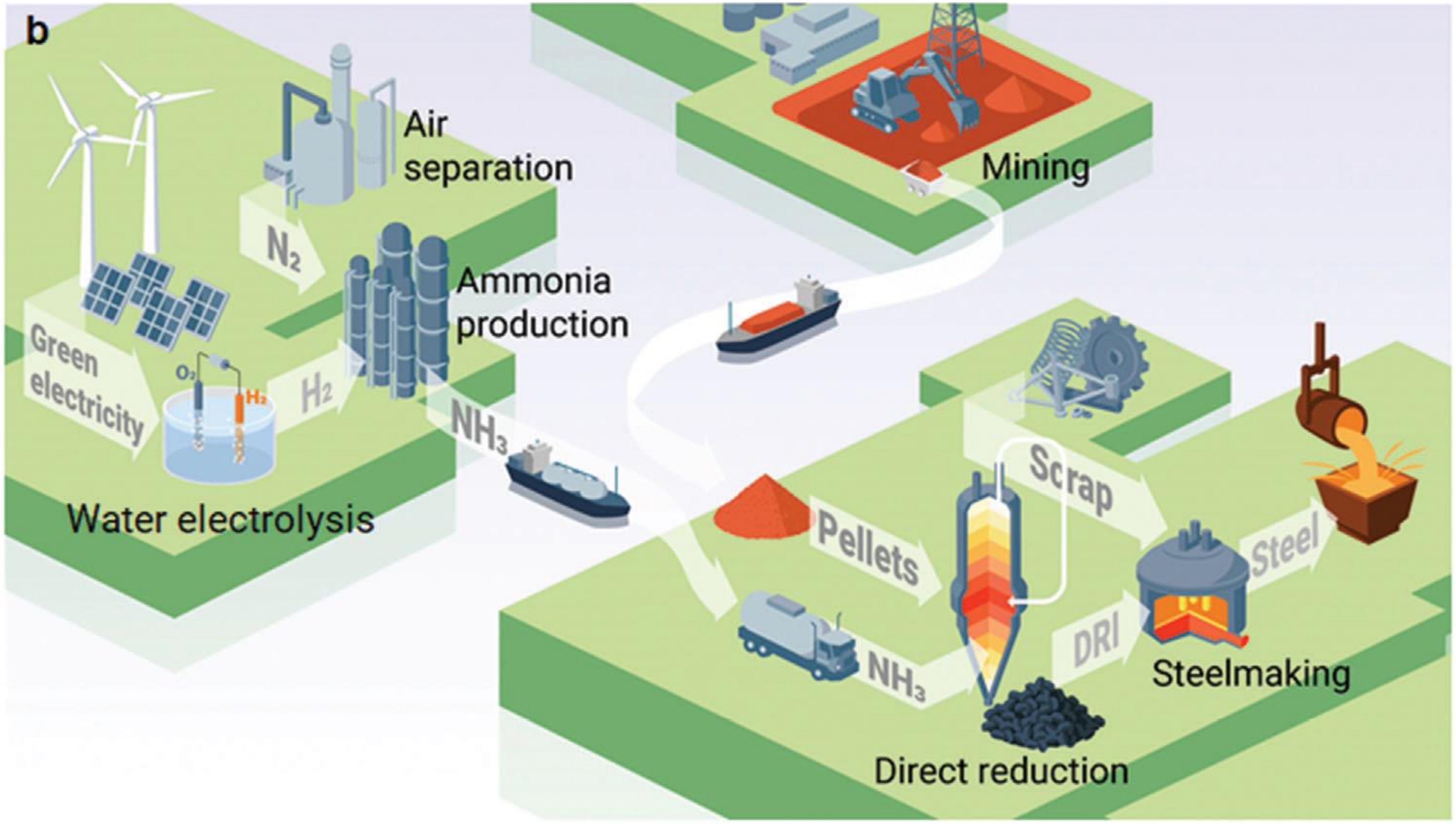

Experimental setup for hydrogen-plasma-based smelting reduction of iron oxides with a process using a 10% H2–90% Ar gas mixture to produce the plasma.

Souza Filho, et.al. “Sustainable Steel through Hydrogen Plasma Reduction of Iron Ore: Process, Kinetics, Microstructure, Chemistry”. Acta Mater. 2021, 213, 116971.

# What about the future?.

## We have to move to “greener” technologies




Ma, Y., et al.Reducing Iron Oxide with Ammonia: A Sustainable Path to Green Steel. Adv. Sci. 2023, 2300111. https://doi.org/10.1002/advs.202300111

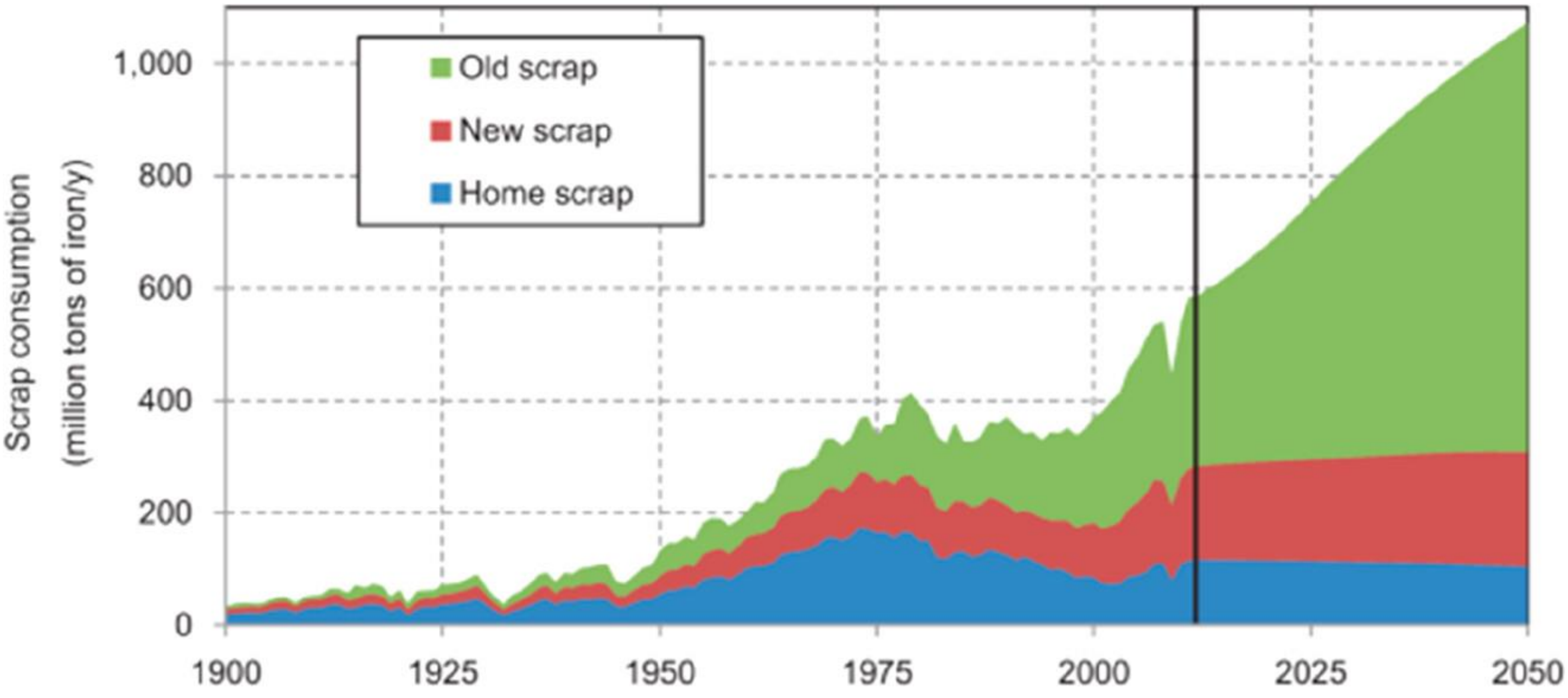
# What about the future?.

“Greener” technologies

Recycling

# What about the future?.

## Recycling

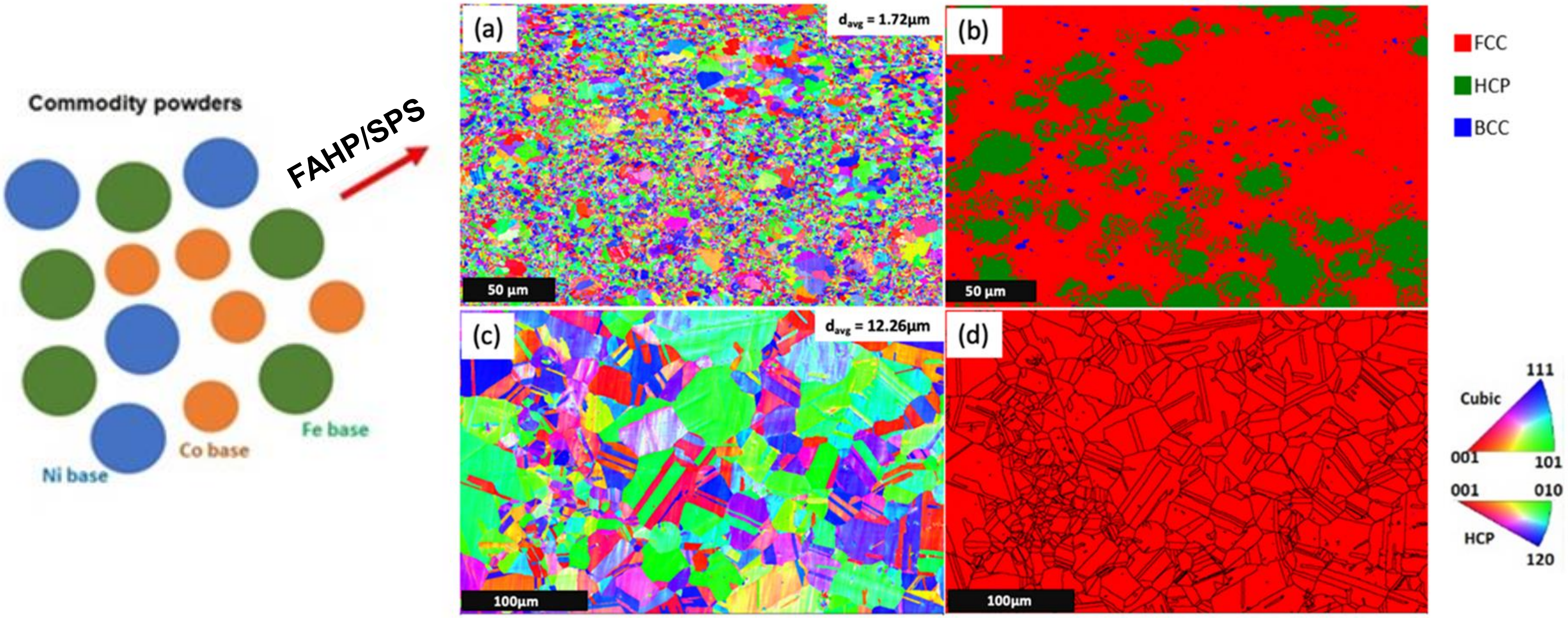



Oda, J.; Akimoto, K.; Tomoda, T. Long-Term Global “Availability of Steel Scrap”. Resour. Conserv. Recycl. 2013, 81, 81−91.

# What about the future?.

## Recycling

### High-Entropy Alloys: recycling philosophy




José M. Torralba, S. Venkatesh Kumarán, Development of competitive high-entropy alloys using commodity powders, Materials Letters, 2021, 130202,.

# What about the future?.

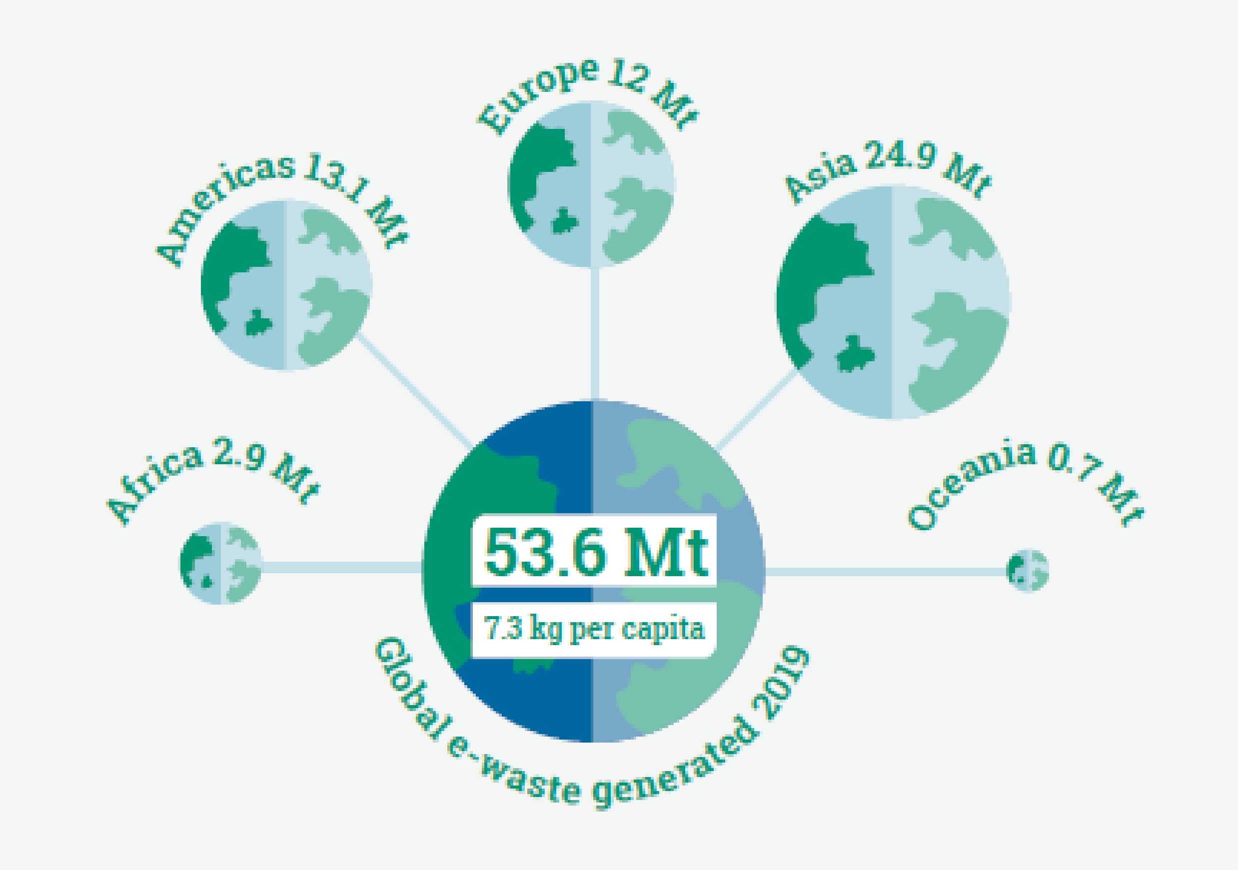
"Greener" technologies

Recycling

Urban mining and e-waste mining

# What about the future?.

## Urban mining and e-waste mining



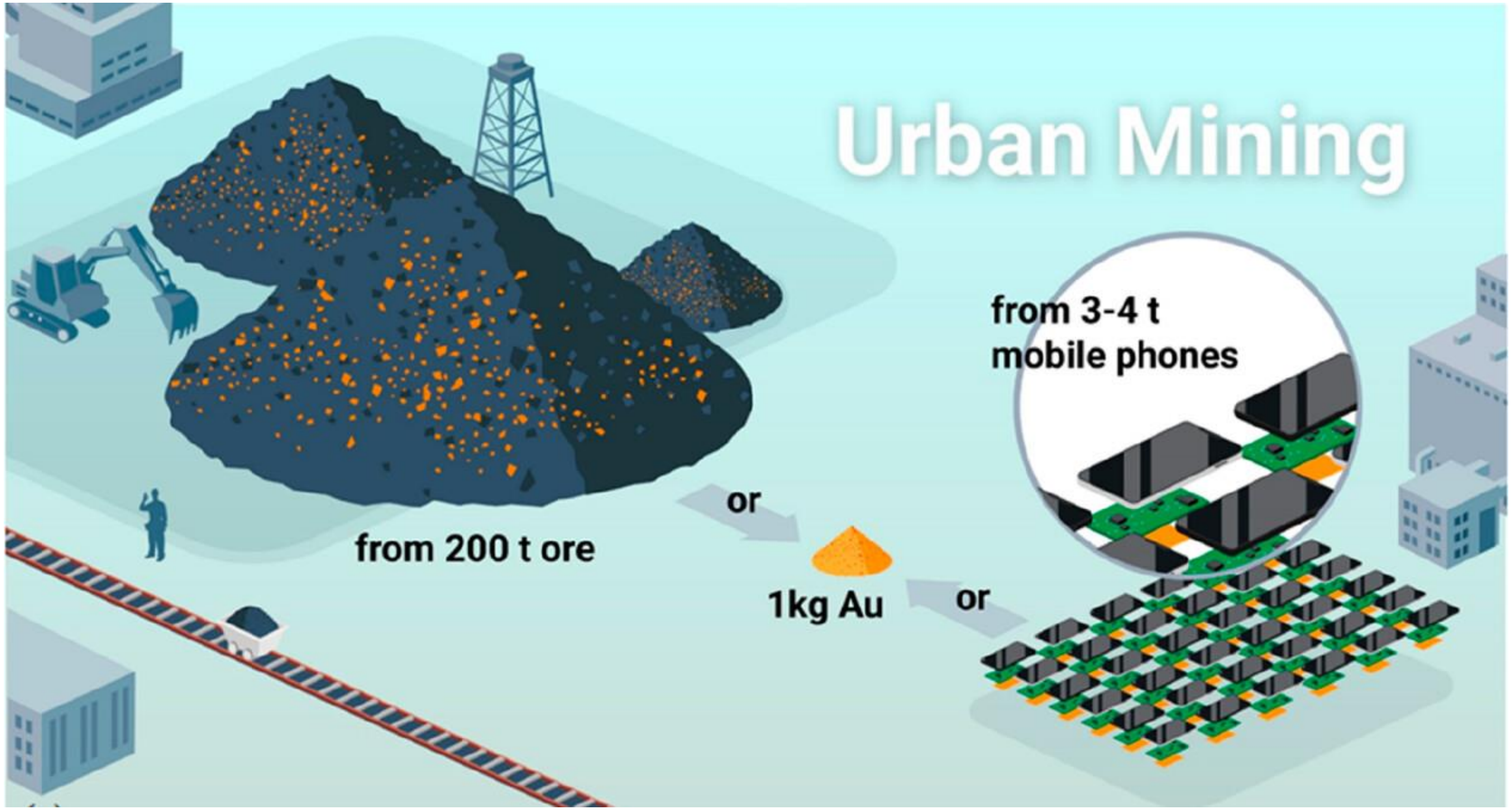

On average, the total weight (excluding photovoltaic panels) of global EEE consumption increases annually by 2.5 million metric tons (Mt).

In 2019, the formal documented collection and recycling was 9.3 Mt, thus 17.4% compared to e-waste generated.

Forti V., Baldé C.P., Kuehr R., Bel G. The Global E-waste Monitor 2020: Quantities, flows and the circular economy potential. United Nations University (UNU)/United Nations Institute for Training and Research (UNITAR) – co-hosted SCYCLE Programme, International Telecommunication Union (ITU) & International Solid Waste Association (ISWA), Bonn/Geneva/Rotterdam.

# What about the future?.

## Urban mining and e-waste mining




Hagelüken, C.; Corti, C. W. Recycling of Gold from Electronics: Cost-Effective Use through "Design for Recycling.". Gold Bull. 2010, 43, 209−220.

Park, Y. J.; Fray, D. J. Recovery of High Purity Precious Metals from Printed Circuit Boards. J. Hazard. Mater. 2009, 164, 1152−1158.

# What about the future?.

“Greener” technologies

Recycling

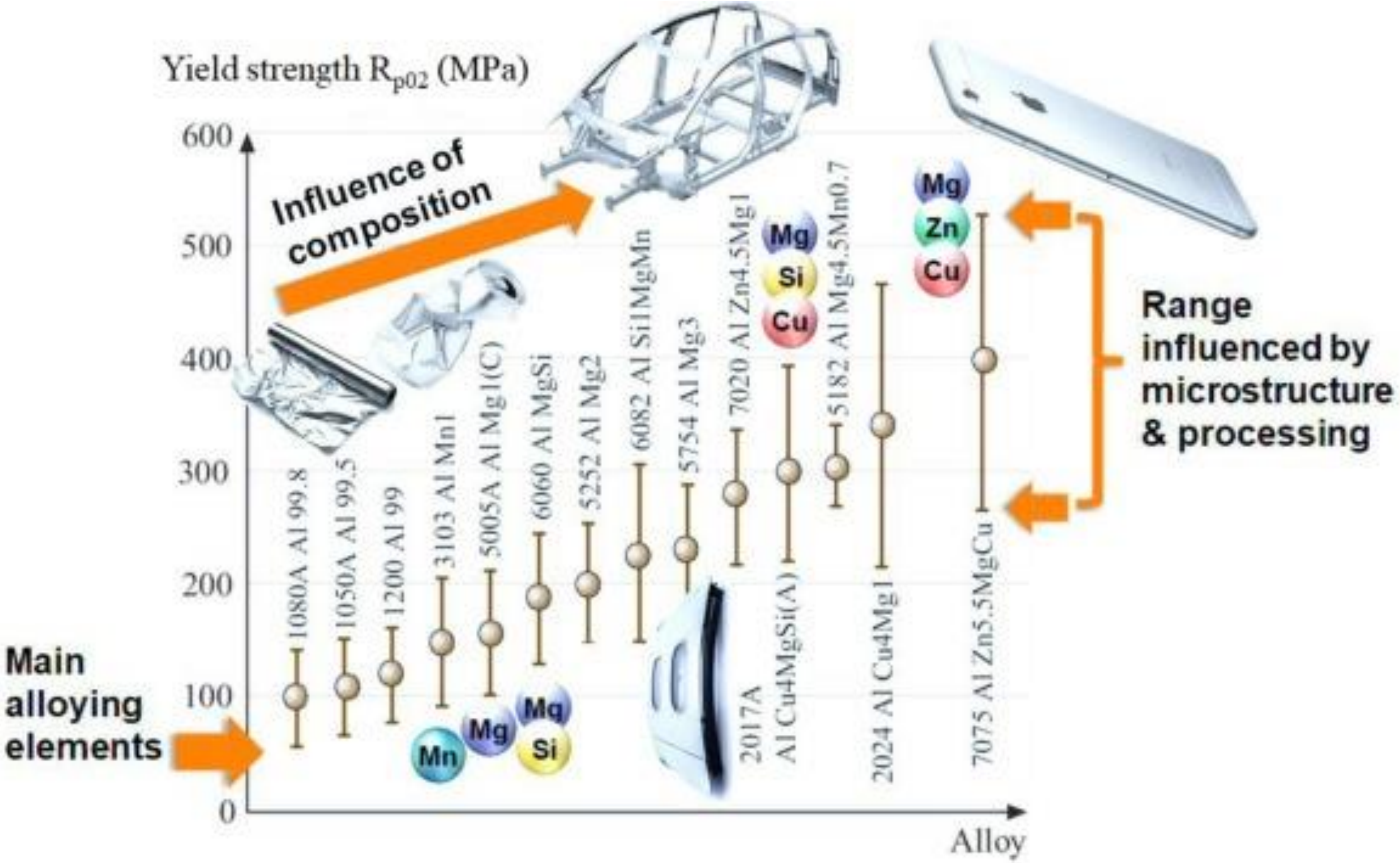
Urban mining and e-waste mining

Sustainable alloy concept

# What about the future?.

## Sustainable alloy concept

### Microstructure-Oriented versus Composition-Oriented Alloy Design

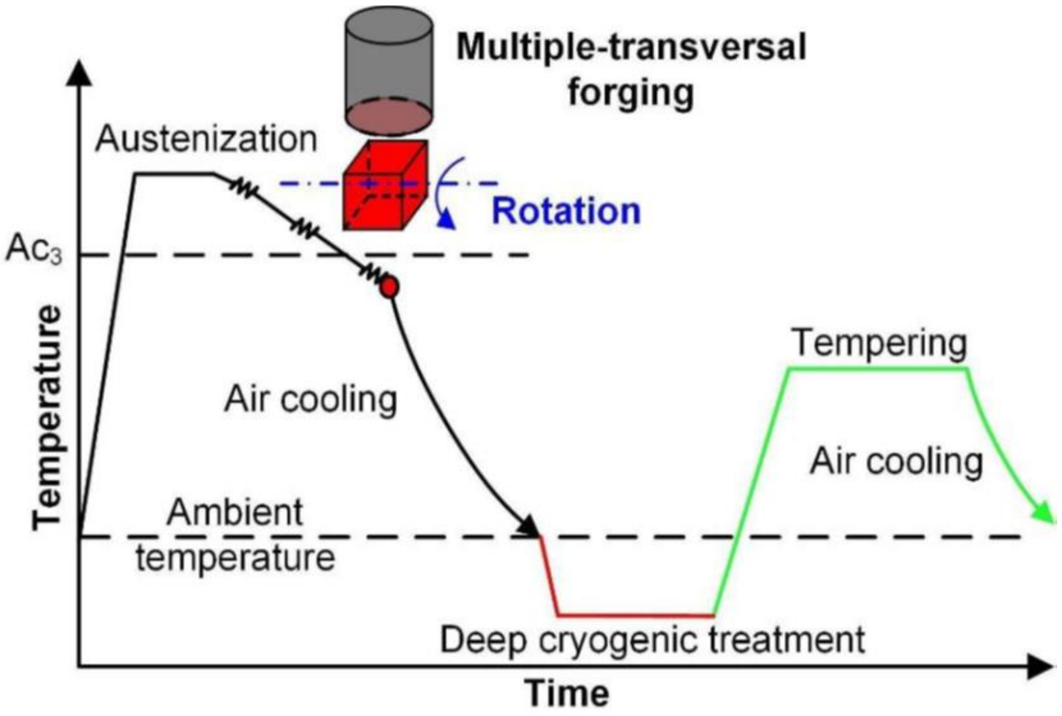


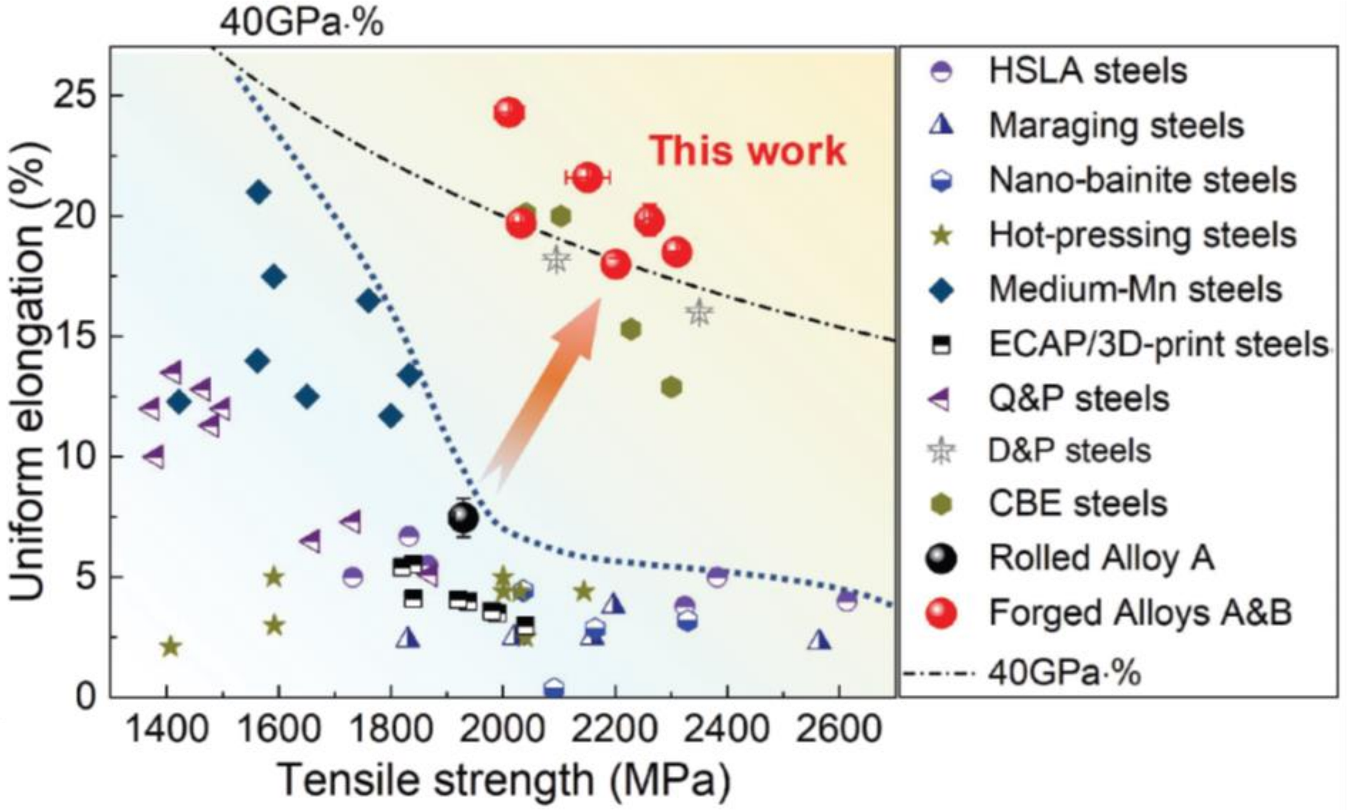

Kammer C. Aluminum and Aluminum Alloys. In: Warlimont H, Martienssen W, editors. Springer Handb. Mater. Data. Springer Handbooks, Springer, Cham; 2018.

# What about the future?.

## Sustainable alloy concept

Fe-7.4Mn-0.34C-1Si-0.2V wt %





Li Y, Yuan G, Li L, Kang J, Yan F, Du P, Raabe D, Wang G. Ductile 2-GPa steels with hierarchical substructure. Science. 2023 Jan 13;379(6628):168-173.

# What about the future?.

“Greener” technologies

Recycling

Urban mining and e-waste mining

Sustainable alloy concept

Sustainable technologies

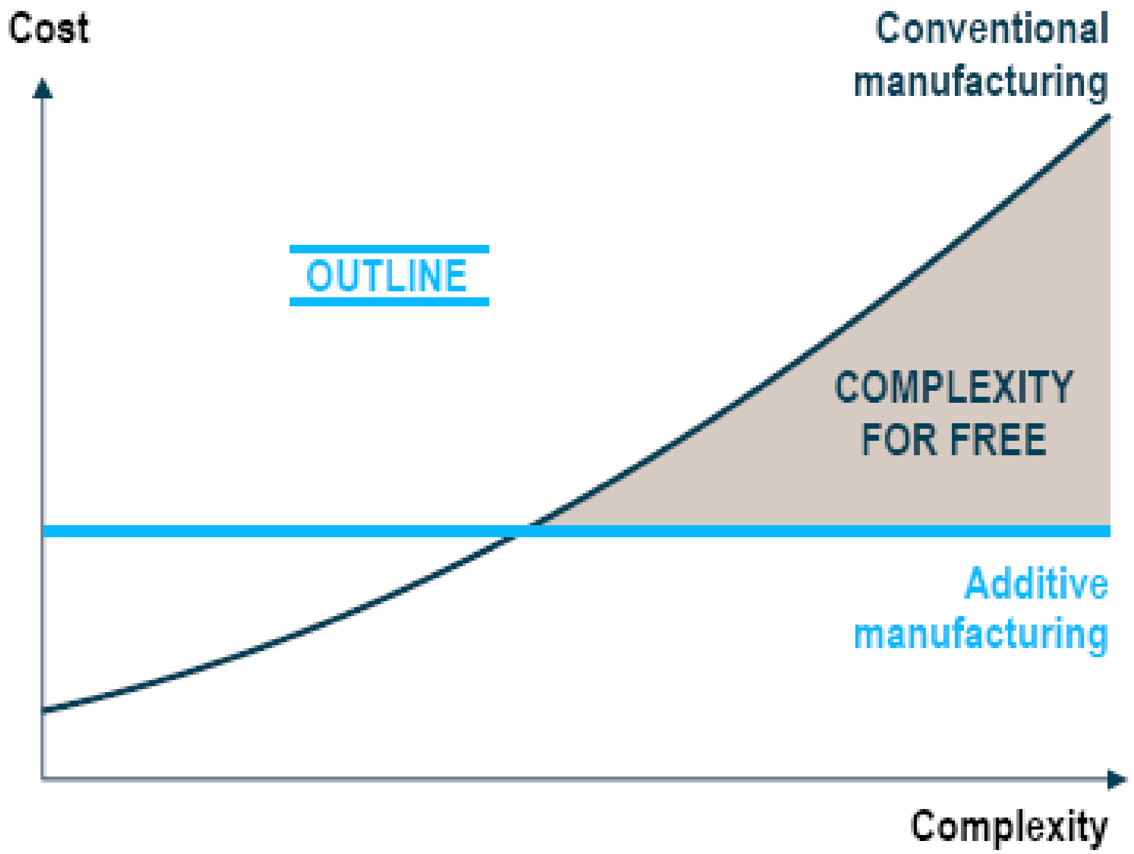
# What about the future?.

## Sustainable technologies

## 3D printing

## Complexity for free

**AM enables new geometric shapes…**

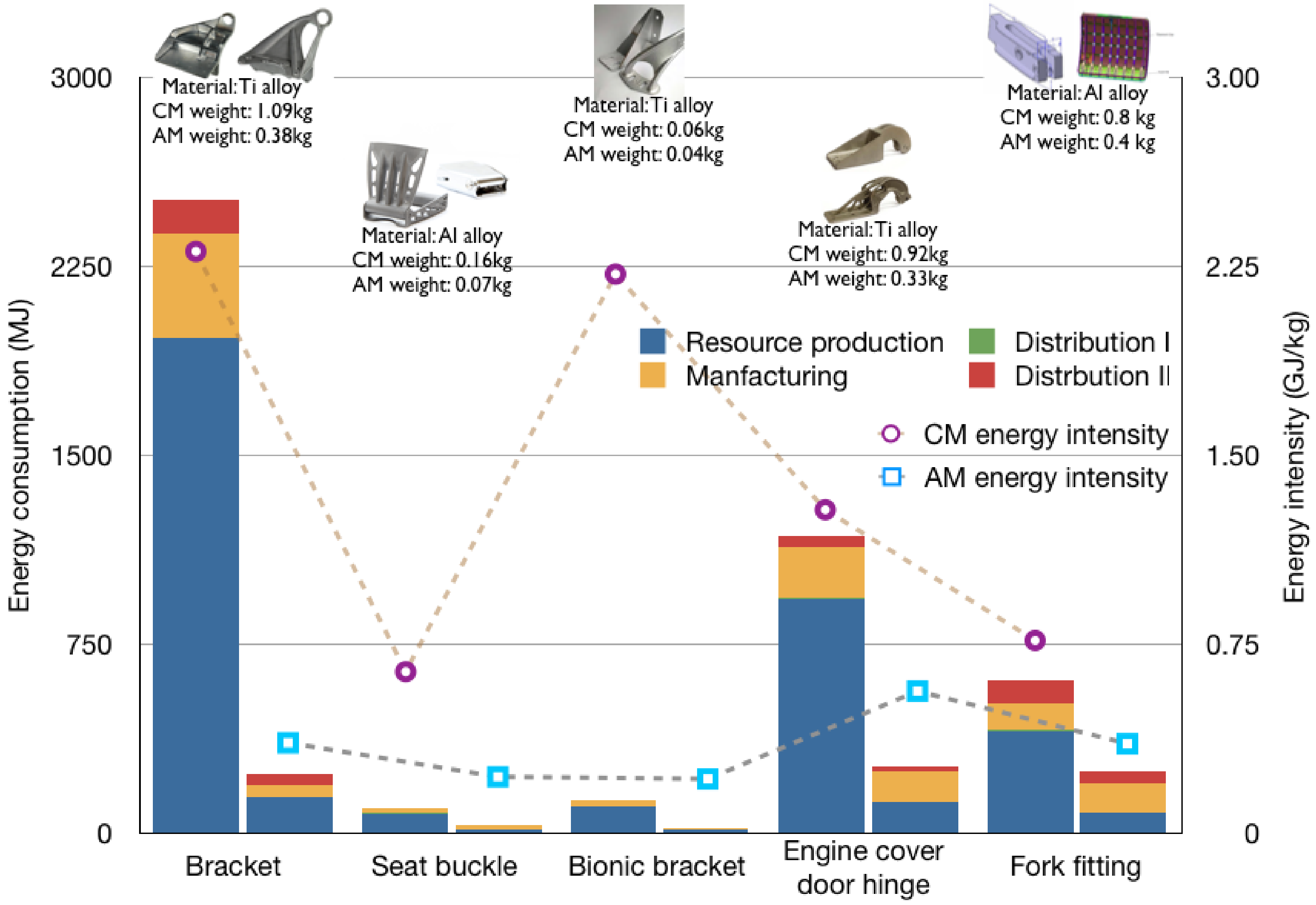



**… at NO ADDITIONAL COST**

# What about the future?.

## Sustainable technologies

## 3D printing




**Cradle to gate primary energy results for case study components**

Runze Huang et al. Energy and emissions saving potential of additive manufacturing: the case of lightweight aircraft components, Journal of Cleaner Production, Volume 135, 2016, (1559-1570)

# What about the future?.

## Sustainable technologies

## 3D printing

**Weight reduction**

- ✓ Less material.
- ✓ Reduced waste.
- ✓ Less energy consumption during transport.

### TRADITIONAL DESIGN

Source: SAVING project

> A conventional steel buckle weights 155 g[1)]

> Weight should be reduced on a like-for-like basis within the SAVING project

> Project partners are Plunkett Associates, Crucible Industrial Design, EOS, 3T PRD, Simpleware, Delcam, University of Exeter

### AM OPTIMIZED DESIGN

Source: SAVING project

> Titanium buckle designed with AM weighs 70 g – reduction of 55%

> For an Airbus 380 with all economy seating (853 seats), this would mean a reduction of 72.5 kg

> Over the airplane's lifetime, 3.3 million liters of fuel or approx. EUR 2 m could be saved, assuming a saving of 45,000 liters per kg and airplane lifetime

# What about the future?.

## Sustainable technologies

## 3D printing

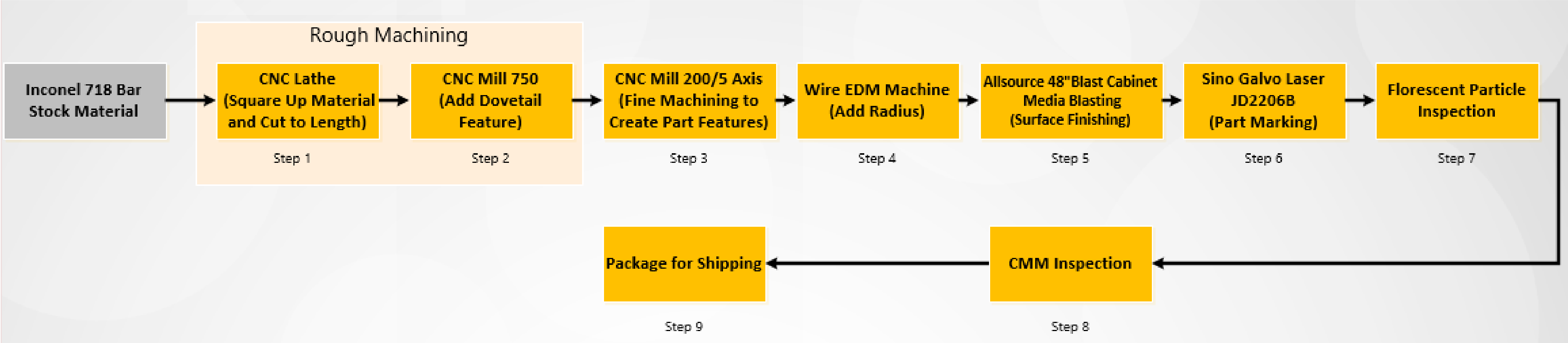
Life Cycle Assessment (LCA) Report: Comparative LCA of a Low-Pressure Turbine (LPT) Bracket by Two Manufacturing Methods
Golisano Institute for Sustainability Rochester Institute of Technology (March 28, 2023)

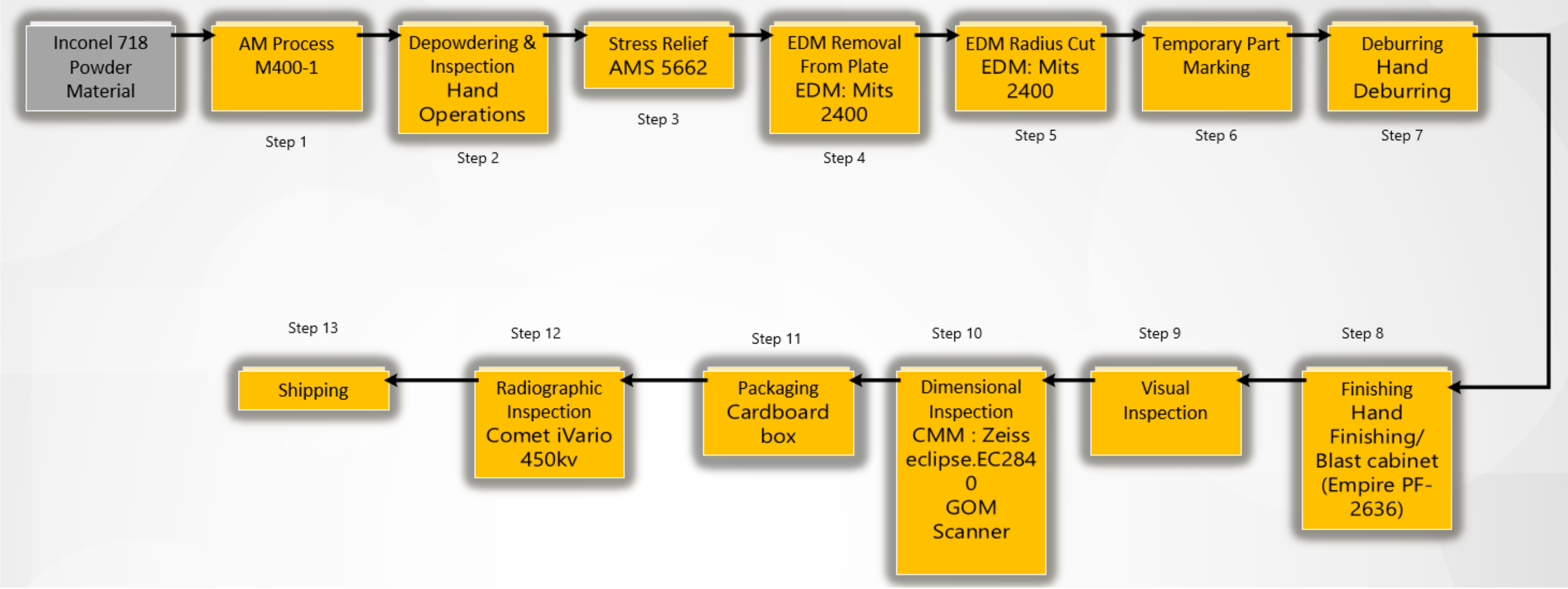
Traditional version (left) and AM-designed bracket (right).

# What about the future?.

## Sustainable technologies

## 3D printing



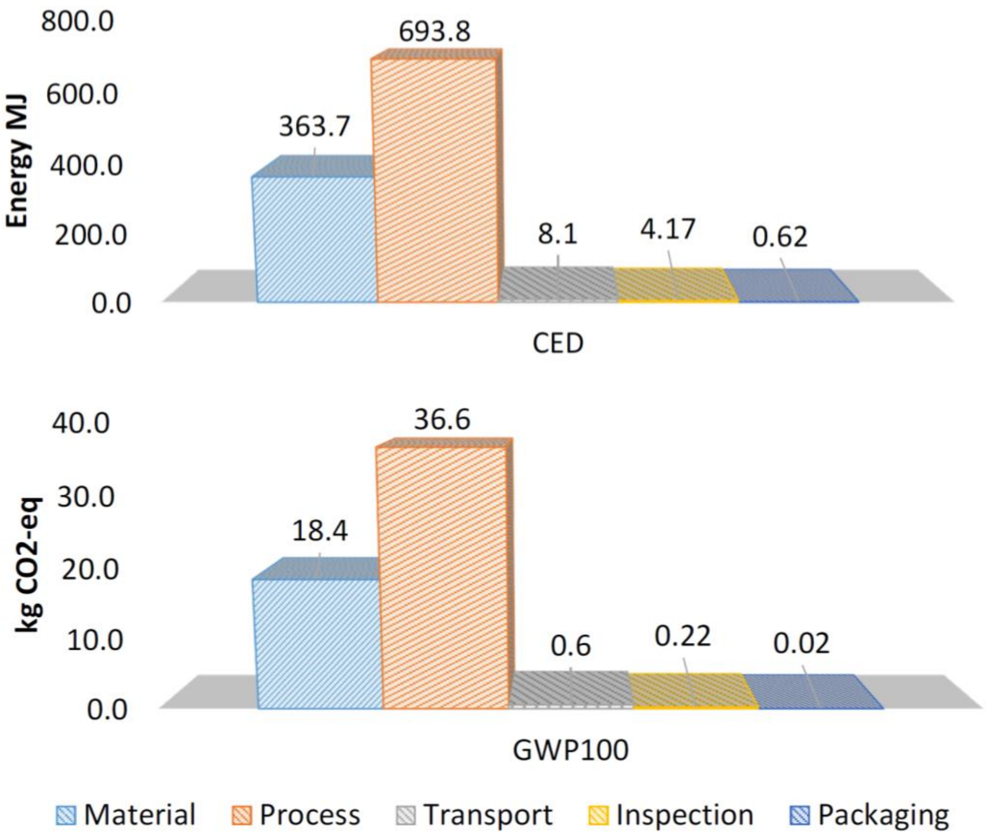

Life Cycle Assessment (LCA) Report: Comparative LCA of a Low-Pressure Turbine (LPT) Bracket by Two Manufacturing Methods
Golisano Institute for Sustainability Rochester Institute of Technology (March 28, 2023)

# What about the future?.

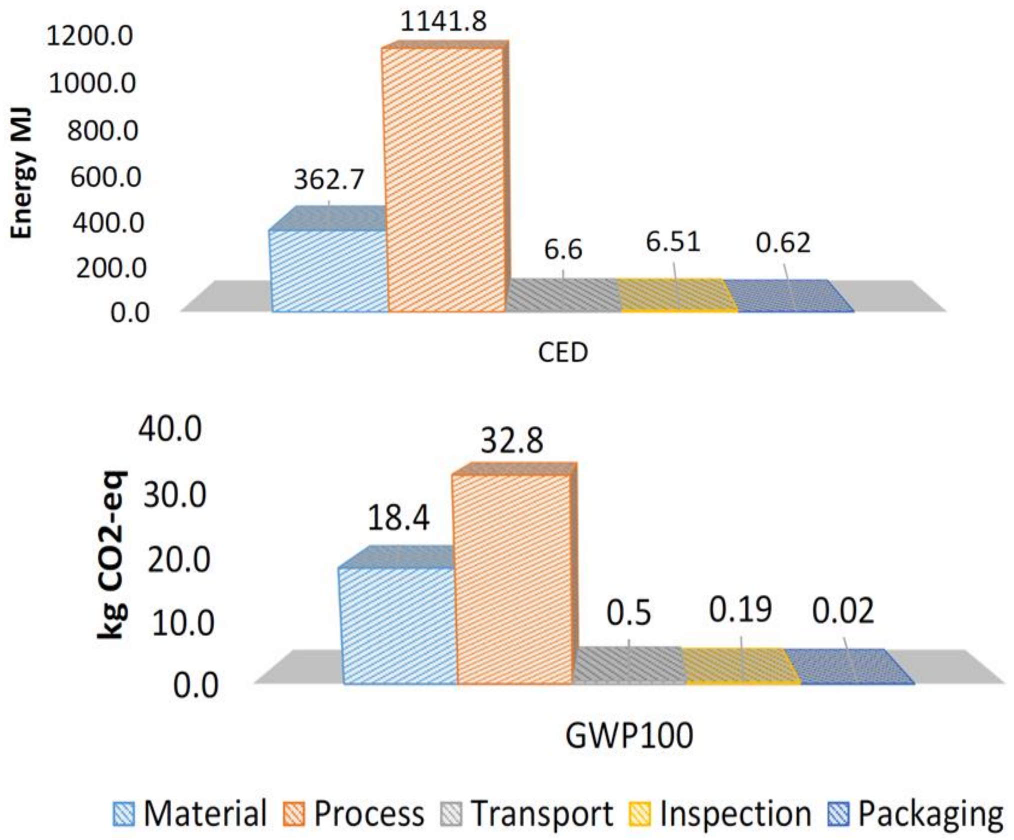
## Sustainable technologies

## 3D printing

### Energy and emissions impact




**Additive manufacturing**




**Traditional manufacturing**

Life Cycle Assessment (LCA) Report: Comparative LCA of a Low-Pressure Turbine (LPT) Bracket by Two Manufacturing Methods
Golisano Institute for Sustainability Rochester Institute of Technology (March 28, 2023)

# What about the future?.

## Sustainable technologies

## 3D printing

### Conclusions of the CA Report:

Analysis of an AM-made bracket's use phase relied on a model of a long-haul Boeing-767 flight from London to Boston. We discovered through this simulation that a lighter weight version of the conventional LPT bracket would, over the course of the aircraft's lifetime, significantly lower its overall fuel consumption. The reduction in fuel use over that period would offset about 20,225 kg CO2-eq through the lightweighted design.

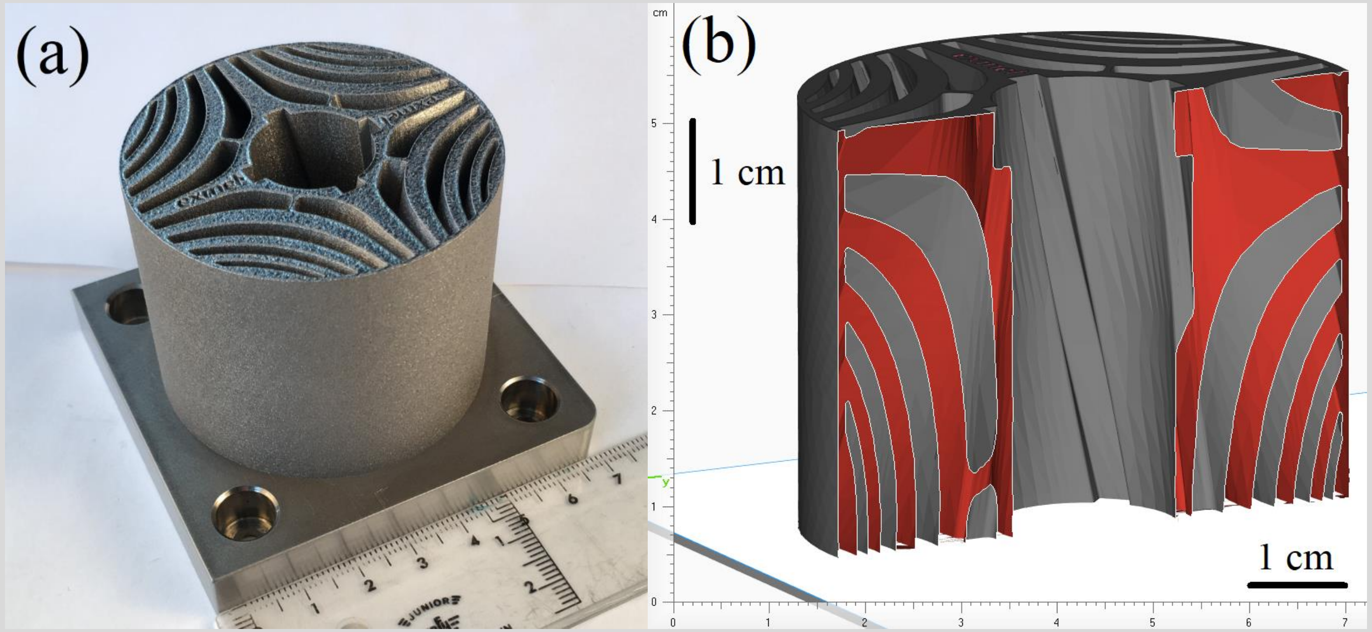
This investigation found that the sustainability benefits of a lighter airplane that could be attributed to 24 LPT brackets—each weighing 51.6 percent less than the conventional versions—were more than enough to counterbalance those of the parts' cradle-to-gate life cycle. And AM presents a unique pathway for reducing the mass of products, which will lower costs, emissions, and other impacts purely through the use of less material.

Life Cycle Assessment (LCA) Report: Comparative LCA of a Low-Pressure Turbine (LPT) Bracket by Two Manufacturing Methods.  Golisano Institute for Sustainability Rochester Institute of Technology (March 28, 2023)

# What about the future?.

## Sustainable technologies

## 3D printing of efficient e-motors




Materials & Design 215 (2022) 110483

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ELSEVIER

Selective laser melting of a Fe-Si-Cr-B-C-based complex-shaped amorphous soft-magnetic electric motor rotor with record dimensions

Lena Thorsson [a], Mattias Unosson [a], María Teresa Pérez-Prado [b], Xueze Jin [b], Paola Tiberto [c], Gabriele Barrera [c], Bastian Adam [d], Nico Neuber [d], Amirhossein Ghavimi [d], Maximilian Frey [d], Ralf Busch [d], Isabella Gallino [d,*]

[a] Exmet AB, c/o Swerim, PO Box 7047, S-164 07 Kista, Sweden
[b] IMDEA Materials Institute, Calle Eric Kandel 2, 28906 Getafe, Madrid, Spain
[c] INRIM, strade delle Cacce 5, Torino, Italy
[d] Saarland University, Chair of Metallic Materials, Campus C6.3, 66123 Saarbrücken, Germany

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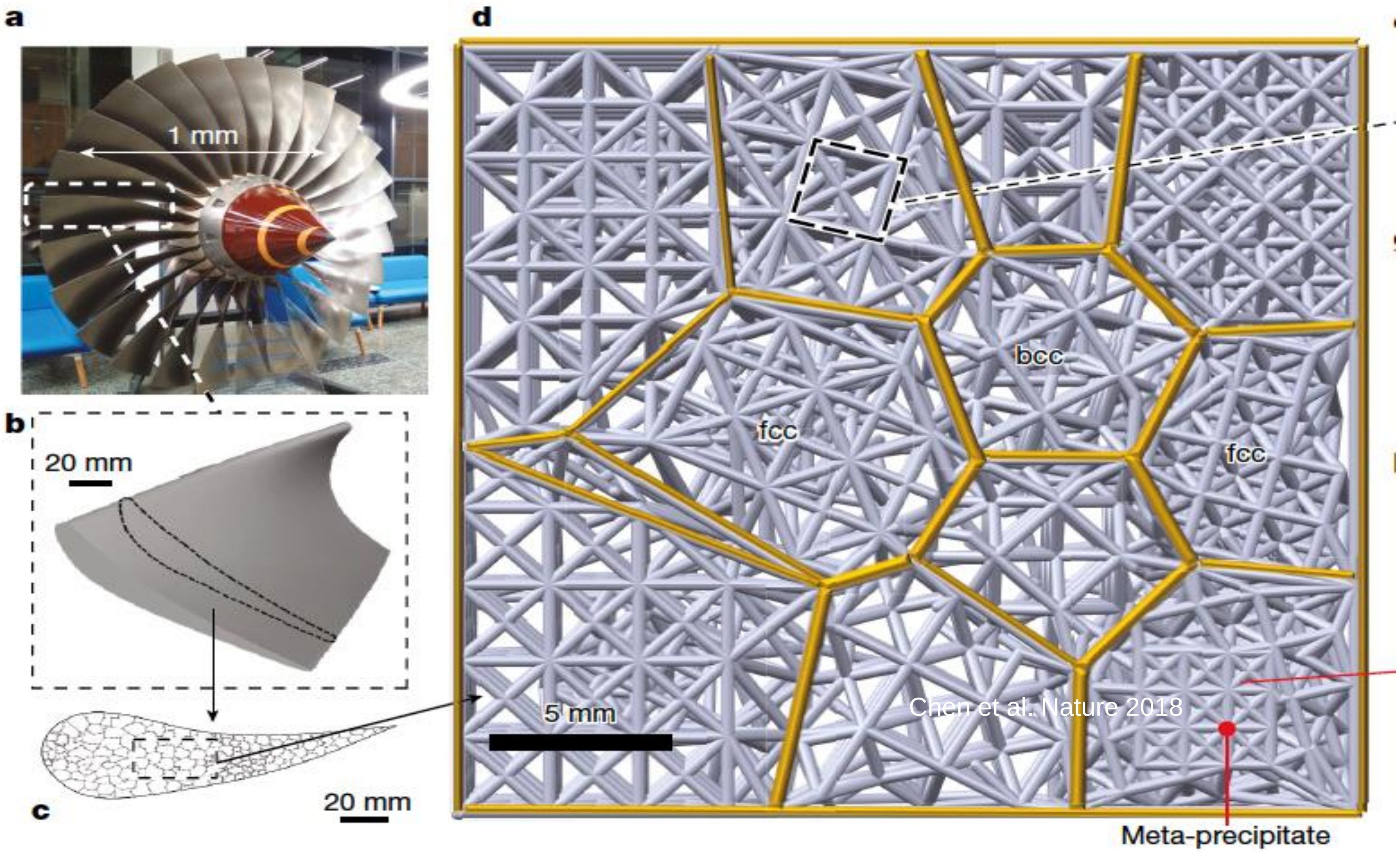
# What about the future?.

## Sustainable technologies

### 3D Printing of ultralight structures




Chen et al. Nature 2018

# What about the future?.

## Sustainable technologies

## 3D printing in aerospace

ITP Aero desingn and manufacture a main structure of a new airplane engine UltraFan® through SLM
19/10/2021

# What about the future?.

## Sustainable technologies

## 3D printing in architecture

# What about the future?.

“Greener” technologies

Recycling

Urban mining and e-waste mining

Sustainable alloy concept

Sustainable technologies

**Sustainable Metallurgy**

- Metallurgy (what is this?).
- Metallurgy in the past.
- Metallurgy today, through some numbers
- Some of the problems metallurgy faces today as a result of its success
- Tools available for metallurgy today.
- What about the future?.
- Some final remarks.

# Some final remarks:

- Metallurgy has been a substantial part of mankind's development. Without Metallurgy, there would never have been the technological breakthroughs that have led to our current development as a society.

- Metallurgy, as an industry, is responsible for producing the largest volume of raw materials necessary for the functioning of our society, in particular through the production of steel.

- And this need for raw materials (their acquisition and transformation), necessary in the main economic sectors, puts in the hands of the metallurgical industry the need to solve two major problems:
  - The need to reduce the consumption of critical materials.
  - The need to reduce greenhouse gas emissions.

- But Metallurgy today has the resources to look to the future and solve these problems with solvency:
  - Advanced characterization tools.
  - Modelling.
  - Artificial intelligence, machine learning

# Some final remarks:

**Establishing the paths that will allow us to move towards concepts of sustainable metallurgy.**

institute IMDEA materials
UNIT OF EXCELLENCE MARÍA DE MAEZTU
uc3m

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Prof. Javier Segurado (IMDEA Materials Institute-Technical University of Madrid)
Dr. Federico Sket (IMDEA Materials Institute)
Dr. Paula Alvaredo (UC3M)
Prof. Mónica Campos (UC3M)
Prof. Dirk Raabe (Max-Planck-Institut für Eisenforschung)


sustainable powder technologies

GTP Grupo de Tecnología de Polvos

# Thank you!

torralba@ing.uc3m.es