4th Generation Synchrotrons Revolutionise Materials Research

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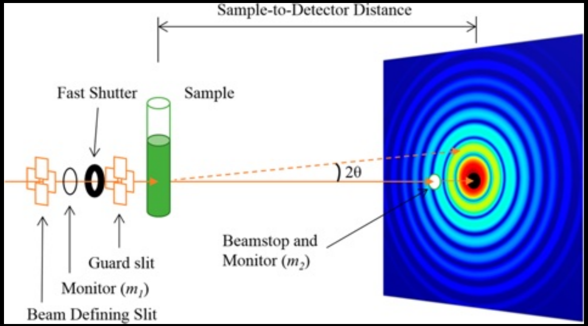
CSO & co-founder, Momentum Transfer

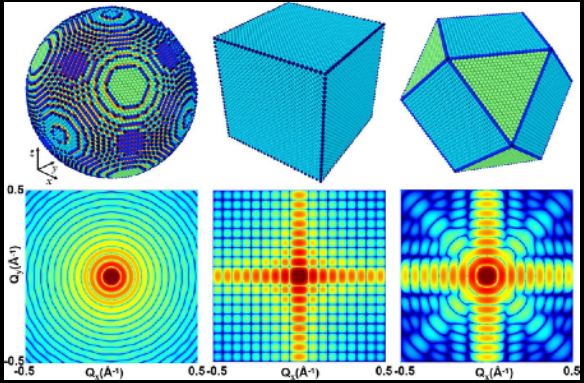
Small Angle X-ray Scattering (SAXS), X-ray Powder Diffraction (XRD), and Pair Distribution Function (PDF) Analysis provide crucial insights into material structures across various scales, from atomic arrangements to nanoscale features, enabling researchers to develop and optimise materials for diverse applications.

Small Angle X-ray Scattering (SAXS)

Small Angle Scattering is a powerful technique for investigating nanoscale structural features in materials, typically ranging from 1 nm to 400 nm. In metals, SAS is invaluable for examining larger-scale structures such as pores, voids, precipitates, and second-phase particles that significantly influence mechanical properties. By analyzing X-ray or neutron scattering at small angles, SAS provides critical information about the size, shape, and distribution of these inhomogeneities within the material.

This insight is crucial for understanding phenomena like strengthening mechanisms, corrosion resistance, and overall material performance in metals.





Li et al., Chemical Reviews 2016 116 (18), 11128-11180, DOI: 10.1021/acs.chemrev.5b00690

Small Angle X-ray Scattering (SAXS)

Size Range

SAS examines structures from 1 nm to 400 nm

Key Features

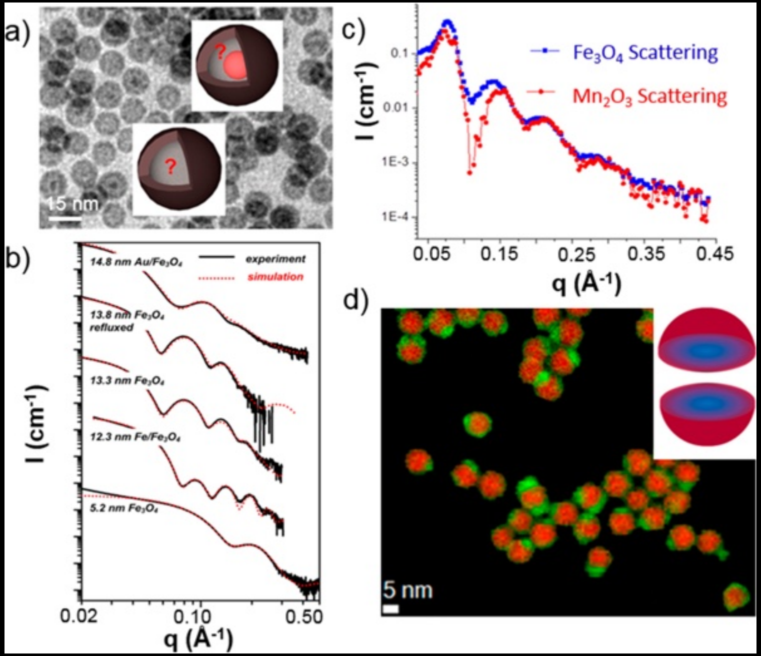
Detects pores, voids, precipitates, and second-phase particles

Applications

Analyzes strengthening mechanisms and corrosion resistance

Importance

Provides insights into material performance and properties



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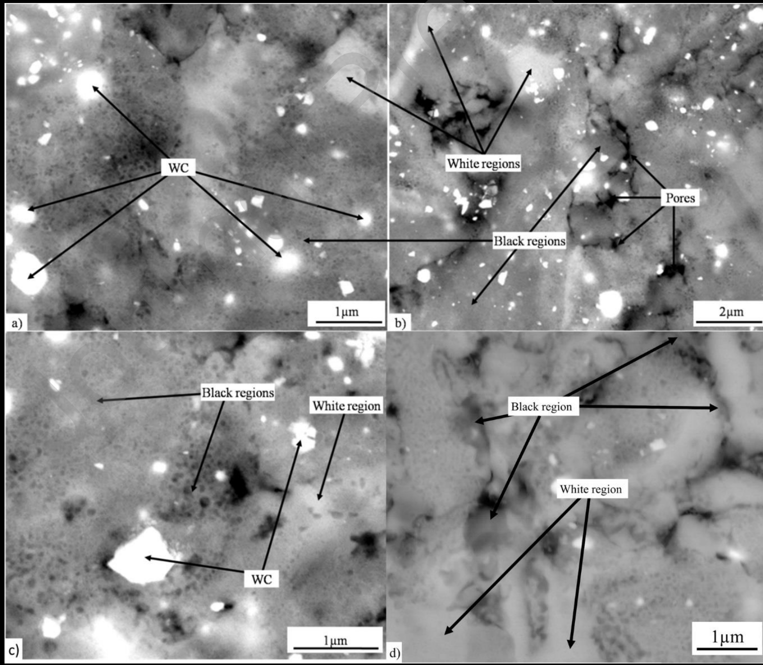


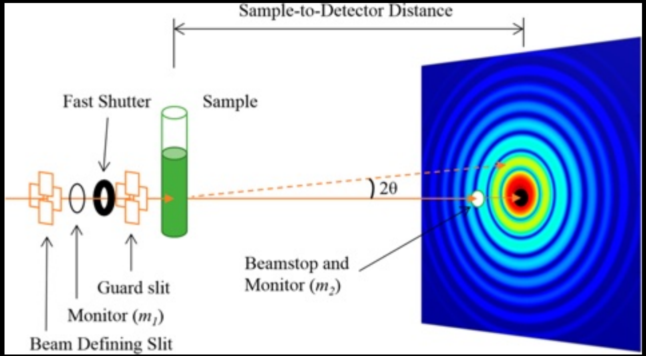
Fig.

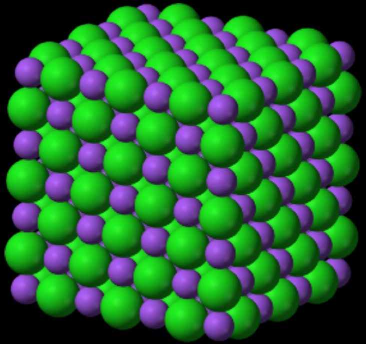
Parakh et al. Journal of Alloys and Compounds, Volume 863, 2021, 158056

X-ray Powder Diffraction (XRD)

X-ray Powder Diffraction is a fundamental technique for determining the crystalline structure of materials. When X-rays are directed at a powdered metal sample, they are diffracted by the regular arrangement of atoms in the crystal lattice. By measuring the angles and intensities of these diffracted beams, XRD reveals information about lattice parameters, identifies different crystalline phases, and determines the crystallographic orientation of grains within the metal.

This technique is essential for phase identification in metal alloys and for understanding how the crystalline structure affects properties such as strength, ductility, and electrical conductivity.





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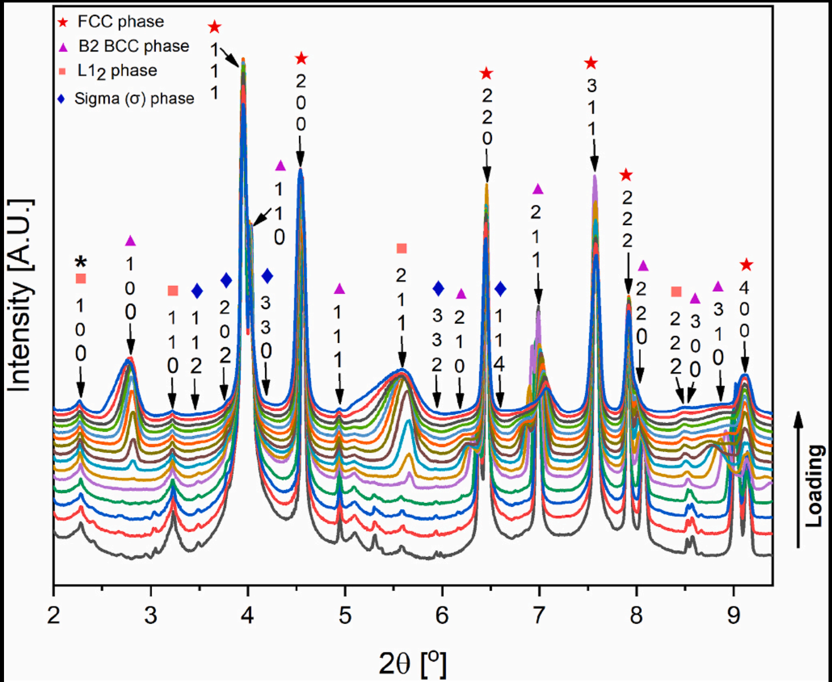
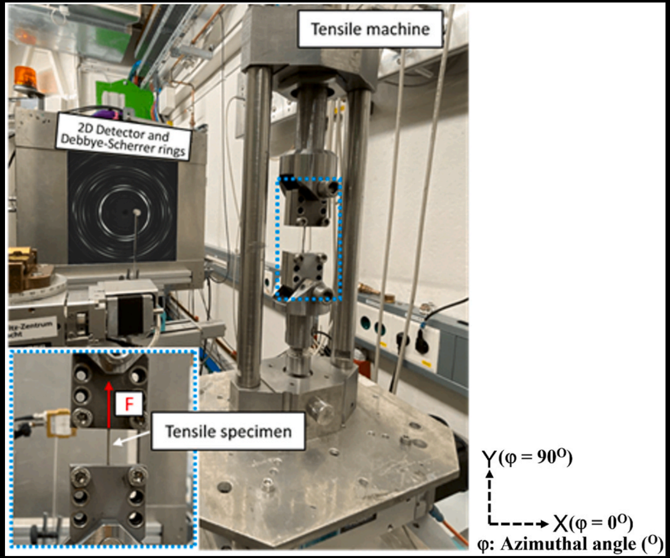




Z. Dai et al., Materials Science & Engineering R 143 (2021) 100590

Pair Distribution Function (PDF) Analysis

Pair Distribution Function analysis provides insights into the local atomic arrangements within a material, regardless of whether it is crystalline or amorphous. PDF analysis measures the probability of finding pairs of atoms at various distances, revealing detailed information about bond lengths and coordination numbers. This technique is particularly useful for studying materials lacking long-range order, such as amorphous metals or nanocrystalline materials, where traditional diffraction methods may not provide sufficient information about the local structure.

PDF analysis can uncover subtle structural features like local distortions, clustering, or the presence of short-range order that significantly impact material properties.

Crystalline Materials

PDF analysis complements traditional diffraction methods by providing detailed local structure information

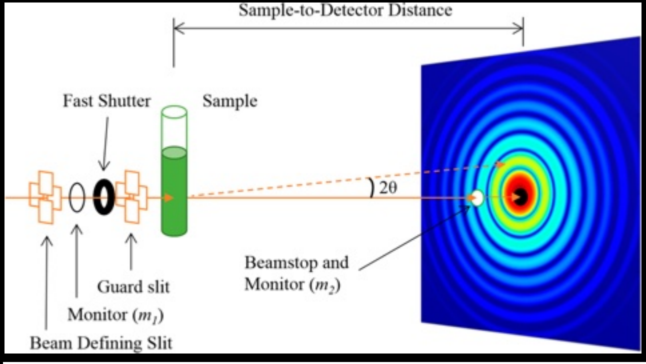
Amorphous Materials

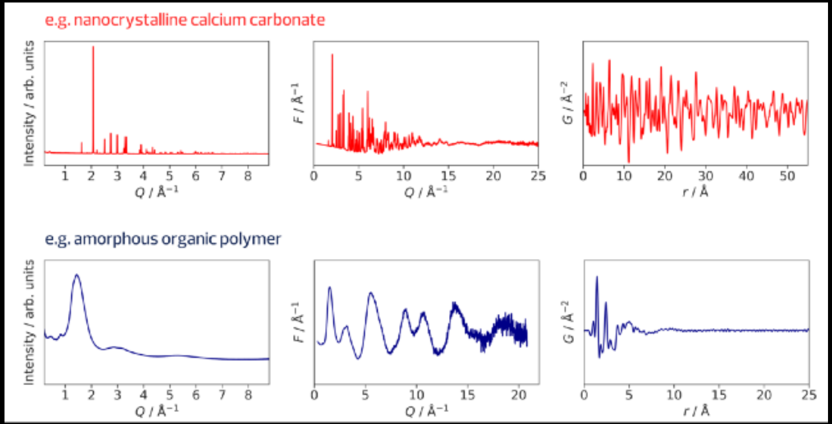
Reveals short-range order and local atomic arrangements in materials lacking long-range crystalline order

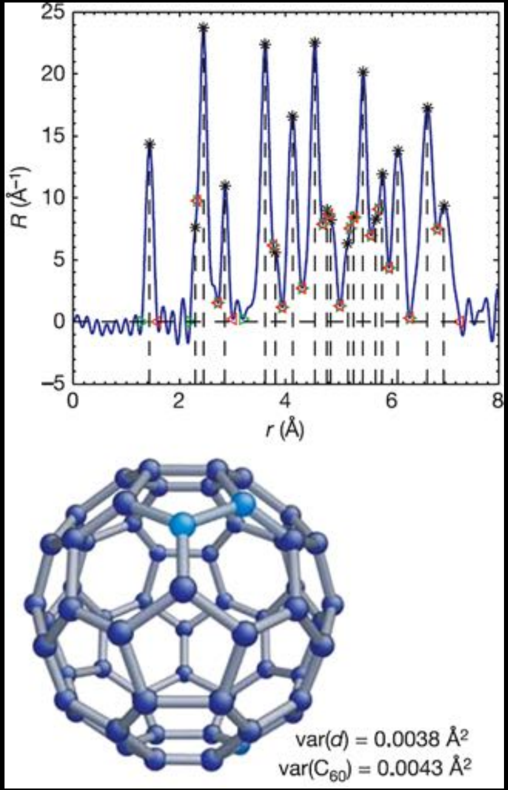
Nanocrystalline Materials

Uncovers structural features and distortions at the nanoscale, crucial for understanding material properties

Pair Distribution Function (PDF) Analysis







Terban et al. ,Chem. Rev. 2022, 122, 1208–1272, DOI:10.1021/acs.chemrev.1c00237

Complementarity of Scattering Methods

The combination of SAS, XRD, and PDF analysis offers a comprehensive understanding of metal microstructures across different length scales and structural complexities. SAS examines nanoscale features like precipitates and voids that affect properties such as toughness and yield strength. XRD provides information on the average long-range crystalline order, phase composition, and crystallographic texture, critical for understanding deformation behaviour and phase stability. PDF Analysis delves into local atomic arrangements and short-range order, shedding light on phenomena like atomic-scale distortions, solute clustering, and local compositional variations.

1 → 2 → 3 → 4

1. Atomic Scale

PDF Analysis reveals local atomic arrangements and short-range order

2. Nanoscale

SAS examines features like precipitates and voids

3. Crystal Structure

XRD provides information on long-range crystalline order and phase composition

4. Macroscale Properties

Combined insights inform understanding of overall material properties and behaviour

High Entropy Alloys (HEAs)

High entropy alloys (HEAs) are an innovative class of materials consisting of five or more elements mixed in near-equiatomic proportions. Unlike traditional alloys, HEAs are stabilised by high configurational entropy, often forming simple solid-solution phases. Current research focuses on understanding their microstructure, mechanical properties, and phase stability, particularly their ability to maintain strength and ductility at elevated temperatures. HEAs are renowned for their excellent mechanical properties, including high strength, hardness, and wear resistance, as well as good ductility and toughness.

High Strength

Excellent mechanical properties for structural applications

Thermal Stability

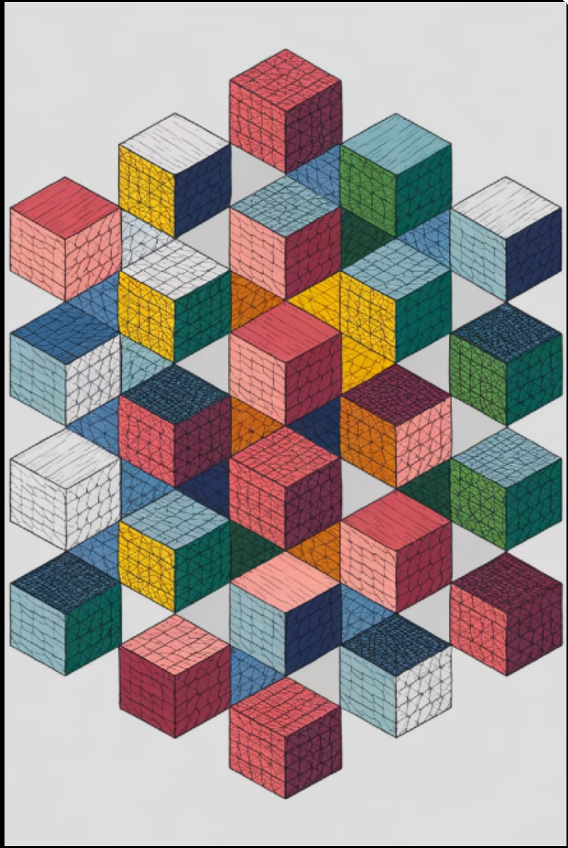
Resistance to softening at elevated temperatures

Corrosion Resistance

Superior resistance in harsh environments

Unique Properties

Intriguing magnetic and electrical characteristics



Momentum Transfer

HEA Research Focus

1

Microstructure

Understanding phase stability and atomic arrangements.

2

Mechanical Properties

Investigating strength and ductility at elevated temperatures.

3

Applications

Exploring potential uses in aerospace and power generation.

Reduced-Activation Ferritic-Martensitic (RAFM) Steels

1. **Development**

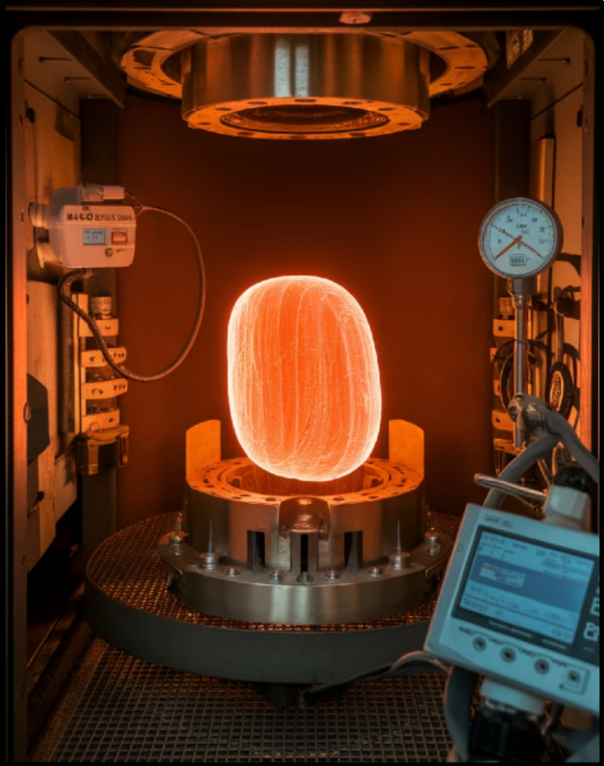
   Designed for nuclear fusion reactors and high-temperature environments.

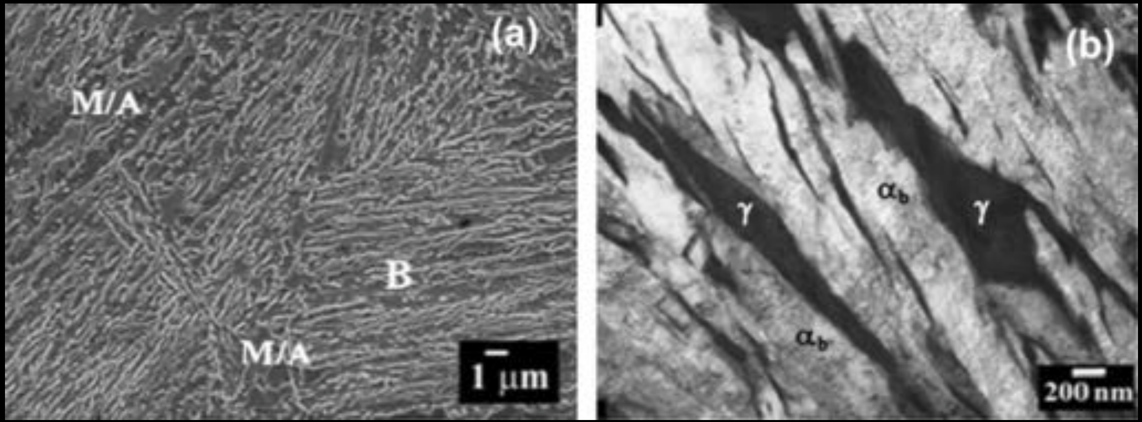
2. **Alloying**

   Zirconium, nitrogen, and titanium promote stable nanoprecipitates.

3. **Properties**

   Improved creep resistance and impact toughness at high temperatures.





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SAXS

Size distribution different phases & nano pores

XRD

Size & strain analysis and phase quantification

PDF

Local order of amorphous and nano-crystalline phases

Z. Dai et al., Materials Science & Engineering R 143 (2021) 100590

CO_2 Emission Mitigation in Steel Industry

Industry Challenge

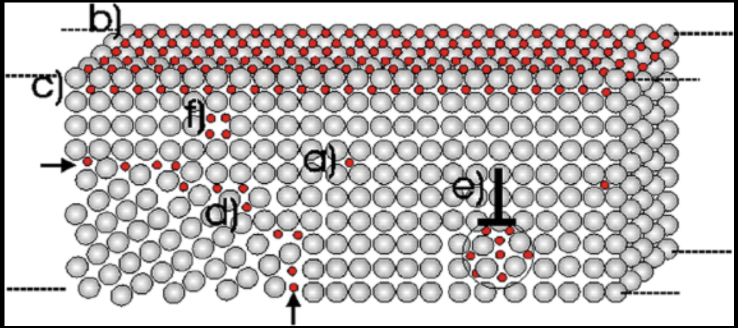
Steel production is a significant CO_2 emitter.

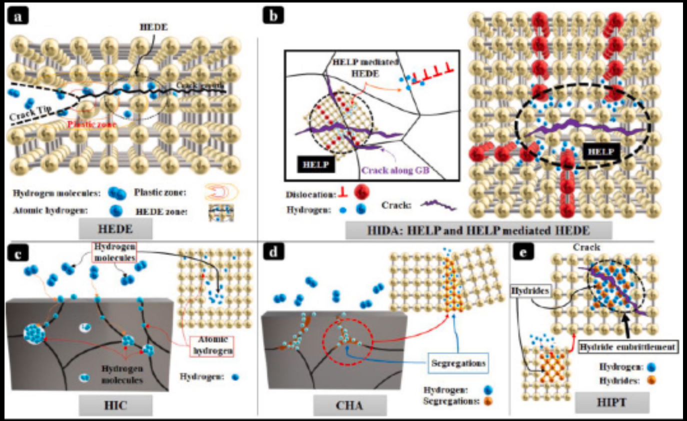
Solution

Replacing carbon with hydrogen as reducing agent.

Benefit

Hydrogen reduction produces water vapor instead of CO_2.





Challenges in Hydrogen Reduction

Hydrogen Embrittlement

Reduces ductility and toughness, increasing risk of unexpected fracture.

Microstructural Alterations

Changes in phase formation and alloying element behavior.

Process Adaptation

Significant technological changes required for hydrogen-based reduction.

Economic Challenges

High costs associated with green hydrogen production and infrastructure modifications.

International Journal of Hydrogen Energy, Vol: 58, Pages 1214-1239
International Journal of Hydrogen Energy, Vol. 47, Pages 32707-32731

Enhancing Material Characterisation using a combined ultra-high throughput examples

1

Integrated Analysis

Combining SAS, XRD, and PDF data for comprehensive understanding.

2

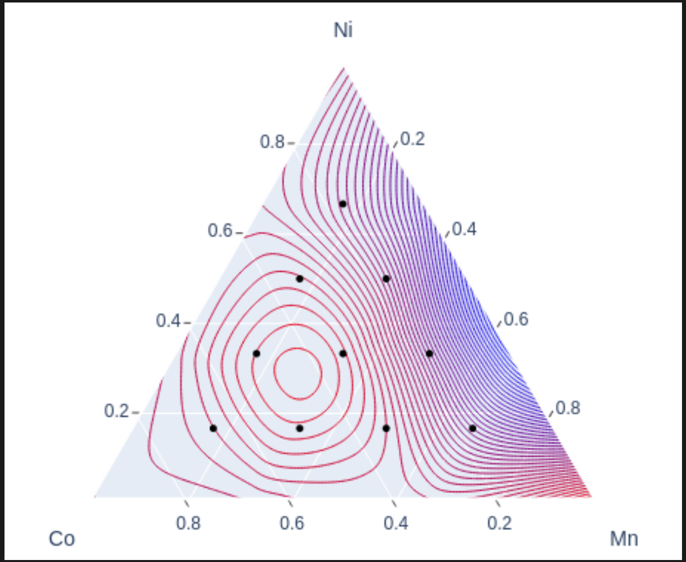
Microstructure-Property Correlation

Linking nanoscale features to macroscopic properties.

3

Tailored Properties

Adjusting processing conditions based on characterisation insights.



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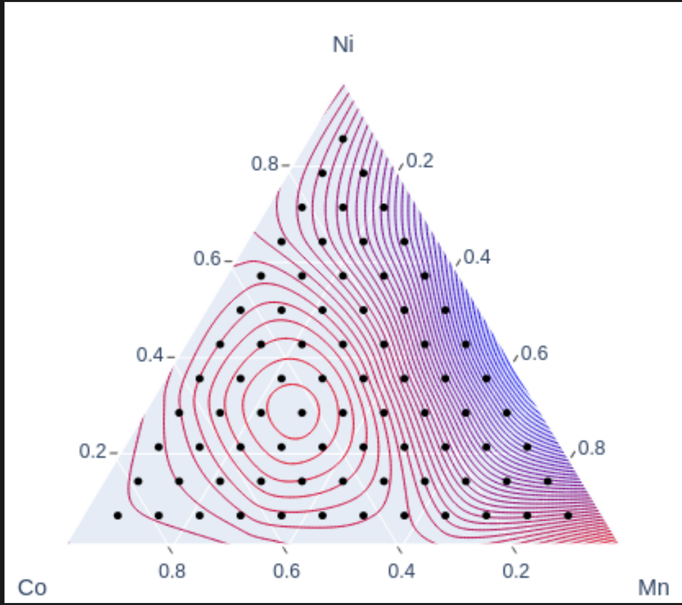

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