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Abstract

The transition towards a net-zero energy future heralds a groundbreaking shift away from carbon-based fuels and reducing agents, with hydrogen emerging as a key player in this revolution. Leveraging renewable energy to produce hydrogen through electrolysis unlocks its potential as a clean, versatile fuel and a sustainable reducing agent, especially in transformative processes like iron ore reduction. However, the journey is not without its challenges; hydrogen's tiny atomic size, high reactivity, and material compatibility demand innovative solutions for safe storage, transportation, and infrastructure development. Beyond these hurdles, its profound impact on metallurgical processes—from extraction to casting and fabrication—highlights the need for a paradigm shift in industrial practices. Successfully addressing these complexities promises a future where hydrogen fuels a cleaner, greener industrial era.

Introduction

Now, reaching net-zero carbon emissions has become of paramount importance to the entire world, which should compel one to abandon carbon-based fuels and reducing agents. This situation is especially dire in heavy industries, such as in metallurgy, in which carbon has so far been irreplaceable for production processes, including those of iron and steel. Hydrogen will be created by renewable energy-powered electrolysis and will change everything. Hydrogen, as a clean and sustainable fuel and reducing agent, stands to revolutionize industrial processes, especially for those industrial processes using carbon-intensive methods like the reduction of iron ore with coke. It could significantly reduce GHGs and would thus become an essential element in a greener and more sustainable industrial profile.

Despite the promise, there are several challenges that need to be overcome for hydrogen's wide-scale adoption. The small atomic size and high diffusivity complicate its storage and transportation due to such risks as leakage and material degradation, including hydrogen embrittlement. Such problems introduce further complications in infrastructural development such as pipelines and storage systems. Furthermore, metallurgical processing of hydrogen in every step-from extraction to casting and fabrication-involves huge adaptation and technological development. These are challenges that need a multidisciplinary effort in material science, engineering, and industrial innovation. Coupled with overcoming such hurdles, decarbonization will not only be driven, but hydrogen will establish itself as one of the cornerstones for the sustainable industrial revolution, changing energy systems and industrial processes worldwide.

The origins of hydrogen:-

Hydrogen exists both in its natural state as a diatomic gas, H_2 , and in various combined forms, each playing a vital role in its production and industrial use, especially in the context of a net-zero energy policy.

Natural State of Hydrogen:

Pure hydrogen will naturally occur as H_2 gas, a diatomic molecule comprising two hydrogen atoms. The universe is full of hydrogen as the most abundant chemical element, but it is barely found in its molecular form on Earth. This is because the H_2 molecule is light and small, hence over time, it escapes into space since Earth's gravity is not strong enough to retain more of it. Hence, free hydrogen does not accumulate in the atmosphere.

However, hydrogen is abundant in other forms on Earth. It is a major constituent of stars, such as our Sun, wherein nuclear fusion of hydrogen to helium is responsible for its enormous radiant energy output. In its natural form, this property of hydrogen is of no practical significance in the terrestrial/industrial context.

Combined Forms of Hydrogen:

On Earth, hydrogen, for the most part, is in combined forms, most noticeably in the following:

Water (H_2O): Hydrogen is a major constituent of water, which is about 70% of the Earth's surface. In this water, every molecule has two hydrogen atoms combined with a single atom of oxygen. Water is the most abundant compound with hydrogen, and this is very important in the generation of hydrogen gas by the process of electrolysis.

Hydrocarbons (e.g., Methane, Natural Gas): Hydrogen is also present in various forms in all fossil fuels, particularly hydrocarbons such as methane (CH_4) and coal. Most naturally occurring natural gas is methane, which has a single carbon atom bonded to four hydrogen atoms. Hydrogen extraction from hydrocarbons, sometimes referred to as steam methane reforming, or SMR, is presently one of the most common methods of producing hydrogen. However, the process generates carbon dioxide, and thus the source becomes less environmental unless combined with CCS technologies.

Organic Compounds: In all organic compounds, hydrogen is contained. Biomass, petroleum, and coal are all examples of organic compounds. Their extraction normally takes in complicated chemical reactions with steps such as gasification or pyrolysis.

Inorganic Compounds: Most of the inorganic compounds have hydrogen combined with different elements. For example, hydrogen sulfide, H_2S and other metal hydrides can be recognized as the source of hydrogen, though less predominately used than the water and hydrocarbons.

Relevance to Net-Zero Energy Transition:

Decarbonization within industry is highly relevant for transitioning towards net-zero energy systems, while hydrogen will revolutionize metallurgy. Conventionally, these processes in industries, such as the reduction of iron ore in steel production, utilize carbon-based agents like coke; this contributes greatly to CO_2 emissions. Hydrogen is a very promising clean substitute, being able to be used as a reducing agent to replace coke; hence, water vapor instead of carbon dioxide. This transition is an integral constituent in the industrial sector towards sustainability with low environmental impact.

However, each of these usages of hydrogen-in metallurgy and heavy industries-raises problems in terms of storage, transport, and integration with existing infrastructures. Hydrogen is very small in size, highly diffusive, and very reactive; it may induce leakage and material degradation, which requires sophisticated solutions for containment and delivery. Moreover, the production of hydrogen itself may have severe environmental impacts due to several of the methods involved and needs to be significantly improved if hydrogen is going to be a truly sustainable solution.

A detailed account of the structural changes that occur due to hydrogen absorption into metals in both the liquid and solid states.

Hydrogen absorption by metals-whether in the solid or liquid state-somehow drastically alters the structures of the metals and hence their properties. Indeed, as part of the roadmap for the transition to net-zero energy, such use of hydrogen as a reductant in metallurgical processes-especially in metal extraction, as with iron-requires an advanced understanding of hydrogen-metal interaction. Hydrogen absorption effects thus need to be well managed in the interest of the integrity of materials in industrial use, including storage systems, pipelines, and associated equipment in processing.

Structural Changes Due to Hydrogen Absorption in Metals

In the Solid State:

While hydrogen diffuses into metals in the solid state, various phenomena can occur at both the atomic and microscopic level. Hydrogen diffusion into the metal basically characterizes the major pathway of hydrogen entry into metals. In this process, hydrogen atoms diffuse into the metal lattice and normally go along either the grain boundary, dislocation, or defect, depending on the material's microstructure and hydrogen exposure condition, such as temperature and pressure.

1. **Hydrogen Embrittlement:** One of the most critical issues in the solid state is hydrogen embrittlement (HE). This phenomenon occurs when hydrogen atoms diffuse into the metal and interact with the crystal lattice. The absorbed hydrogen tends to occupy interstitial

sites within the lattice structure, which can reduce the metal's ductility and toughness. Hydrogen atoms can weaken atomic bonds, particularly in high-strength materials like steels, causing them to become brittle. This embrittlement leads to cracking and failure under stress, which is especially problematic in infrastructure like pipelines, storage tanks, and reactors that are exposed to hydrogen.

2. **Hydride Formation:** Another potential structural change is the formation of metal hydrides. Some metals, such as titanium, zirconium, and palladium, can form stable hydrides when exposed to hydrogen. These hydrides have a different atomic structure than the original metal, which can alter the material's mechanical properties. For example, hydride formation can increase the material's volume, creating internal stresses and further promoting cracking or failure.
3. **Phase Transitions:** In accompaniment to the absorption of hydrogen, phase transitions have been occurring in the host metal. For instance, there are host metals whose absorption of hydrogen results in changes in the crystal structure. It might subsequently change the general strength and stability of the metal or even performances under high-stress situations.

In the Liquid State:

In the liquid state, the hydrogen absorption into metals is qualitatively different but still impactful. Broadly speaking, liquid metals can have a certain amount of dissolved hydrogen dependent on the temperature and pressure conditions. Normally, though, the solubility of hydrogen in liquid metals exceeds that in solid metals; their behavior, however, is different because of the absence of a fixed lattice structure.

1. **Hydrogen Solubility:** The solubility of hydrogen in molten metals is a function of temperature, pressure, and composition of the metal. With rising temperatures, the solubility of hydrogen generally increases. The interaction of hydrogen with the metal is far less pronounced compared to the solid state, simply because there are no atomic lattice constraints exerted. It follows that hydrogen can much more easily be dissolved in the melt but probably promotes

gas bubble formation in the liquid metal, too, and therefore may cause defects such as porosity or gassing in the final product. Hydrogen, for example, generates gas defects in steel, reducing the quality of the cast metal.

2. Hydrogen-induced cracking may also, but less frequently, occur in molten metals. The hydrogen absorbed in liquid metal forms hydrogen gas bubbles inside the molten metal. These participate in the generation of certain defects, such as shrinkage cavities or gas porosity, particularly in the processes of casting and welding, where hydrogen might be present in such quantity as to affect the structural integrity of the final product.
3. Changes in Surface Tension: Dissolution of hydrogen in certain molten metals may result in variations in surface tension and wetting behavior of the liquid metal itself. That could affect casting operations where control over the surface properties of the molten metal is essential for obtaining the desired quality.

Impact on Metallurgical Processes

Understanding these structural alterations brought on by hydrogen absorption is essential for metallurgy in order to increase the safety and effectiveness of hydrogen as a reducing agent in procedures such as iron ore reduction. In the manufacturing of iron, for instance, substituting hydrogen for coke has a major positive impact on the environment by lowering carbon dioxide emissions; nevertheless, the difficulties caused by hydrogen's interaction with metals must be resolved.

1. The reduction of iron ore (FeO_3) to iron (Fe) can be accomplished by hydrogen substituting carbon, resulting in water vapour rather than carbon dioxide. The use of hydrogen in this process, however, presents certain difficulties, such as hydrogen embrittlement of steel infrastructure, which needs to be avoided by using alloys that are resistant to hydrogen and designing materials accordingly.

2. The design of materials for hydrogen storage and transit systems must take into account the difficulties posed by hydrogen absorption in metals, namely hydrogen embrittlement. Specialised coatings and metals are being created to withstand the harmful effects of hydrogen exposure, guaranteeing their safe and effective application in tanks, pipelines, and other infrastructure.

Metallographic examination, using both optical microscopy and electron microscopy showing evidence of hydrogen absorption:-

Hydrogen must be researched in relation to its impact on the structure of metals, as it is being adopted as a substitute for carbon in sustainable metallurgy, especially as a reducing agent. Optical and electron microscopy during metallographic examination play a very important role in determining how hydrogen absorption affects metals in material integrity and processing outcomes. These analyses are extremely important in overcoming challenges of hydrogen within a net-zero energy framework, where hydrogen in clean energy production and extraction in metals plays a very crucial role.

Evidence of Hydrogen Absorption in Metals

Optical Microscopy:

Optical microscopy provides a macro level perspective on hydrogen's effects on the metal structure. Common features observed include:

- **Hydrogen-Induced Cracking:** Optical microscopy may disclose surface and subsurface cracks resulting from hydrogen embrittlement. The associated cracking normally initiates at the local points of stress concentration and propagates along grain boundaries.
- **Porosity/ Voids:** Hydrogen may get absorbed in some metals during casting. This, then, forms gas bubbles and appears as pores or voids. These defects related to optical microscopy are useful in cross-section samples, which become vital for quality assessment.
- **Hydride formation:** In so-called hydride-forming metals, such as Ti or Zr, optical microscopy may reveal regions of hydride precipitation that differ in morphology and optical contrast.

2. Electron Microscopy:

All these methods-SEM and TEM alike-allow the high-resolution study of interaction between hydrogen and metal microstructure in great detail. Both SEM and TEM allow very detailed high-resolution studies of the interaction of hydrogen with the microstructure of metals.

- SEM analysis provides high resolution on the surface to determine hydrogen-related defects, such as intergranular and transgranular fractures. SEM usually shows the sites and paths for the nucleation and propagation of microcracks and thus gives clues on the operating mechanism.

TEM Analysis: TEM is crucial for understanding hydrogen's interaction at the atomic level. It can identify:

- Lattice Distortions: Lattice distortions due to hydrogen atoms occupying interstitial space are revealed by TEM images.
- Dislocation Movement: Solution hydrogen may provide the opportunity for easier dislocation movement that could be observed by TEM as localized strain regions in the crystal lattice.
- Nanoporosity: TEM can reveal, under certain conditions, the nanoscale voids or bubble-like features formed by hydrogen clusters in the metal matrix.

3. EDS, or energy dispersive X-ray spectroscopy, is frequently used in conjunction with SEM or TEM to identify elemental compositions and verify the existence of hydrogen in hydride phases or embrittlement regions. EDS can detect related chemical changes or compounds, even though direct hydrogen detection is difficult because of its low atomic number.

The Effect of Hydrogen Absorption on the Properties of Ferrous Metals in the Context of Net-Zero Energy Transition :-

Because hydrogen will replace carbon in many roles, as fuel and as a reducing agent, in the transition to net-zero energy systems, ferrous metals are those which will be significantly impacted due to hydrogen absorption-iron and steel are examples. Ferrous metals underpin construction, transportation, and energy infrastructure. Hydrogen can significantly affect the mechanical properties of these materials. For that reason, these mechanisms are very important with regard to system design, safety, and efficiency with regards to hydrogen handling for industrial processes such as iron ore reduction.

How Hydrogen Affects Ferrous Metals

1. Hydrogen Embrittlement (HE):

- **Impact on Mechanical Properties**

Reduced ductility—the metals, especially high strength steels, become less ductile and embrittle.

- **Reduced Toughness:** Energy absorption prior to fracture decreases for the metal, since it is highly prone to sudden failure.

- Lower Resistance to Fatigue: Hydrogen reduces the fatigue life of ferrous metals by increasing the initiation and growth of cracks under cyclic loading.

2. Infrastructure for Hydrogen Storage and Transport:

- Relevance: Ferrous metals are also in wide application in pipes, storage tanks, and reactors which may transport or store hydrogen.
- This is challenged by the fact that hydrogen embrittlement and cracking reduce the service life and reliability; either hydrogen-resistant steels or protective coatings must be used.

3. Strategies to Mitigate Hydrogen's Effects

- Material Selection: To reduce embrittlement, use low-strength steels or specifically made hydrogen-resistant alloys.
- Surface Treatments and Coatings: Hydrogen penetration into the metal is decreased by applying protective coatings or changing surface chemistries.
- Optimised manufacture Processes: Hydrogen-induced defects are decreased when inclusions and voids are minimised during manufacture.
- Real-Time Monitoring: By using sophisticated sensors to track how hydrogen interacts with metals, early indications of embrittlement or cracking can be found.

The consequential effect that hydrogen absorption has on processing, and in particular fabrication by welding :-

Effects of Hydrogen Absorption on Welding Processes:-

1. Hydrogen-Induced Cracking (HIC):
 - Hydrogen can enter the metal during welding by contaminating it with hydrocarbons, moisture, or shielding gases that include hydrogen. Hydrogen diffusion into the weld zone is encouraged by the high heat of welding.
2. Porosity in Welds:
 - As the metal cools and solidifies, gas bubbles may emerge from hydrogen absorbed into the molten metal during welding. These bubbles produce porosity if they become caught in the weld.
3. Alteration of Microstructure:
 - Weld and heat-affected zones' cooling speeds and microstructural changes can be influenced by hydrogen absorption during welding.

Mitigation Strategies for Hydrogen-Related Welding Issues:-

1. Treatments Before Welding:

Hydrogen cracking can be lessened by preheating the base metal, which lowers residual strains and decreases cooling rates.

Hydrogen contamination is reduced when surfaces are cleaned to get rid of moisture and hydrocarbons.

2. Heat treatment after welding :

Lowers residual stresses and the chance of cracking by expelling absorbed hydrogen from the weld zone.

The weld area's mechanical qualities and microstructural homogeneity are enhanced by normalising or annealing it.

Implications for Net-Zero Energy Systems

Welding procedures are essential for building infrastructure to generate, store, and transfer hydrogen in a hydrogen-driven net-zero framework.

In order to guarantee that hydrogen absorption does not jeopardise the performance and safety of hydrogen-based systems, advancements in welding processes, materials research, and quality control are crucial. A seamless shift to sustainable energy solutions is made possible by strong weld integrity.

Conclusion

Hydrogen is positioned as a crucial substitute for carbon-based fuels and reducing agents in the shift to a net-zero energy system, which is motivated by the pressing need to lower carbon emissions. A successful shift, however, requires addressing the substantial obstacles posed by the interaction of hydrogen with metals, from its absorption to its impact on material characteristics and processing.

In order to identify flaws and direct the creation of materials that are resistant to hydrogen, advanced metallographic techniques—such as optical and electron microscopy—are crucial for researching the effects of hydrogen on metals. Overcoming these obstacles requires the use of mitigation techniques, such as regulated welding conditions, pre- and post-processing treatments, and the choice of hydrogen-resistant alloys.

By substituting carbon and removing CO₂ emissions, the use of hydrogen as a reducing agent in metallurgy has positive environmental effects. To guarantee the dependability and safety of hydrogen-based systems, however, continued research, innovation, and material engineering are required, as highlighted by the structural and processing difficulties caused by hydrogen absorption.

Addressing hydrogen's effects on metals at every stage—from extraction to fabrication—is essential to achieving a sustainable, robust, and low-carbon future as we embrace it as a pillar of the net-zero energy transition.