ARTIFICIAL INTELLIGENCE IN SCIENTIFIC RESEARCH AND ITS ROLE IN THE GREEN AND DIGITAL TRANSITION

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Abstract: *The "twin transition" is a major global goal: making our world more digital while also making it green and sustainable. Artificial Intelligence (AI) has become a powerful tool to achieve both goals at the same time. This paper looks at how AI is changing scientific research to speed up digital updates and environmental solutions, with a special focus on materials science for the space industry. Developing materials for space requires balancing extreme performance with planet-friendly sustainability. We look at how AI helps discover new lightweight composites, improves radiation shielding, optimizes 3D printing, and reduces orbital waste. We also address a big problem: AI itself uses a massive amount of computer power, electricity, and water. Finally, we share a practical plan for "Green AI" to make sure the digital tools we use tomorrow do not harm our planet today.*

ИЗКУСТВЕНИЯТ ИНТЕЛЕКТ В НАУЧНИТЕ ИЗСЛЕДВАНИЯ: УСКОРЯВАНЕ НА ЕКОЛОГИЧНИЯ И ДИГИТАЛНИЯ ПРЕХОД

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Резюме: *„Двойният преход“ цели да направи света ни по-дигитален и същевременно по-зелен, като Изкуственият интелект (ИИ) е ключов инструмент за това. Този доклад разглежда как ИИ ускорява научните изследвания и екологичните решения в космическата индустрия. Анализира се ролята му в откриването на леки композити, подобряването на радиационната защита, оптимизирането на 3D принтирането и намаляването на орбиталния отпадък. Обърнато е внимание и на екологичния отпечатък на самия ИИ (консумация на енергия и вода).*

Introduction

The simultaneous global shift toward a green economy and a digital economy is built on the idea that sustainability and technology must develop together to reshape how societies produce and consume. This transition is referred to as the “twin transition”. Today, scientists face two major tasks: they need to use digital tools to handle massive amounts of data, and they need to find fast solutions to preserve our environment. Digital tools provide the analytical power required to solve complex ecological problems, while green priorities ensure that digital infrastructure grows responsibly without destroying our natural resources [1–3].

Nowhere is this balance more critical, or more difficult to achieve, than in the space industry. Building hardware for outer space introduces extreme operational challenges:

- Thermal Extremes: Materials must handle rapid changes between freezing cold shadows and blazing hot solar heat.
- Structural Stress: Rocket parts experience violent vibrations and heavy mechanical loads during launch.
- Vacuum and Radiation: Spacecraft face harsh cosmic rays and a vacuum environment that can cause standard materials to weaken or release toxic gases.

Historically, creating materials that could survive these conditions required decades of resource-heavy trial and error. The traditional loop relied on physically smelting metals, manual stress testing, and chemical treatments that left behind a massive carbon and toxic waste footprint on Earth.

Artificial Intelligence represents the fourth paradigm of science: data-driven discovery. By integrating advanced machine learning (ML), neural networks, and automated workflows into scientific research, AI acts as the connective tissue of the twin transition. It simultaneously satisfies the digital imperative by processing, structuring, and extracting insights from massive atomic datasets and the green imperative, by discovering lighter materials, optimizing manufacturing efficiency, and revolutionizing how we mitigate orbital waste [4–6].

This paper presents a comprehensive review and position analysis of current AI applications in space materials science, synthesizing recent case studies to propose an actionable framework for sustainable 'Green AI' adoption in the aerospace sector.

The Digital Transition: How AI Reshapes Scientific Inquiry

The digital transition in materials science extends beyond the mere digitization of analog records; it demands a fundamental shift in how hypotheses are generated, experiments are conducted, and data is synthesized at the atomic level [7–9].

Overcoming the "Curse of Dimensionality"

Scientific research frequently encounters high-dimensional spaces when mapping how different chemical elements interact. When designing a new aerospace alloy, a scientist must consider variations in temperature, pressure, elemental mixing ratios, and crystalline grain boundaries. The number of potential combinations quickly reaches into the millions, creating an informational bottleneck that traditional statistical models cannot handle.

AI algorithms, particularly deep neural networks, excel at non-linear dimensional reduction. They isolate latent variables and detect subtle atomic patterns within vast datasets that elude human analysis. This allows researchers to skip thousands of dead-end physical experiments by predicting material traits directly from digital models.

Autonomous Laboratories and Closed-Loop Systems

The integration of AI with robotics has given rise to autonomous laboratories, also known as "closed-loop" systems. In these environments, human intervention is minimized as software drives the physical research loop:

1. Hypothesis Generation: The AI system reads existing scientific literature and crystalline databases to suggest a new alloy combination.
2. Automated Synthesis: The AI instructs robotic platforms or specialized 3D printers to physically mix materials and create a test sample.
3. Real-Time Analysis: Computer vision systems and laser sensors monitor the sample's reaction to stress or heat.
4. Iterative Refinement: The algorithm processes the performance data and automatically adjusts the chemical recipe for the next round of testing.

This accelerates the cycle of digital scientific discovery by orders of magnitude, transforming materials research from a slow, manual endeavor into a highly scalable, continuous digital stream

The Green Transition: AI Applications in Space Materials Science

While AI drives digital methodologies, its ultimate value proposition within the twin transition lies in its application to pressing ecological and decarbonization challenges. In the space sector, this translates directly to reducing launch footprints, eliminating hazardous chemicals, cutting manufacturing waste, and preventing orbital pollution [7–9].

Lightweight Materials and Launch Fuel Optimization

Every single kilogram of payload launched into space requires an immense amount of rocket fuel, which releases substantial carbon dioxide and particulate soot into Earth's upper atmosphere. Therefore, the most direct way to green the space industry is to minimize the weight of the spacecraft itself.

AI disrupts traditional aerospace metallurgy through generative design and Graph Neural Networks (GNNs). By treating atoms as nodes and chemical bonds as edges, GNNs predict the physical, electrical, and thermal properties of hypothetical materials before they are physically created. This allows researchers to screen millions of candidate aluminum, titanium, and magnesium alloys in silico within days, isolating the strongest, lowest-density variants for rocket hulls, fuel tanks, and structural brackets.

Eco-Friendly and Safe Radiation Shielding

Astronauts and delicate flight computers require heavy shielding to survive the harsh radiation environment of deep space. Historically, this meant using heavy lead plates or toxic chemical composites that present severe environmental and handling hazards during manufacturing on Earth.

AI accelerates the discovery of alternative, hydrogen-rich polymer composites that block radiation naturally without ecological toxicity. By embedding fundamental subatomic physics laws directly into neural network architectures, these models simulate how cosmic rays smash through different molecular structures. This allows scientists to design clean, lightweight polymers entirely on a computer, bypassing the hazardous chemical waste streams typically generated during physical laboratory formulation.

Zero-Waste Additive Manufacturing (3D Printing)

Traditional aerospace manufacturing relies heavily on subtractive machining taking a large, solid block of titanium or aluminum and carving it away until only the finished part remains. This process is highly inefficient, often wasting up to 80% of the raw, energy-intensive material. The space industry is actively transitioning to additive manufacturing (3D printing) to build complex engine parts layer by layer, minimizing raw material consumption.

AI optimizes this green manufacturing method by monitoring the 3D printing process in real time. Specialized machine learning models process live video feeds, acoustic data, and thermal sensor metrics from the printer head [10].

Demisable Materials to Mitigate Orbital and Atmospheric Waste

When satellites reach the end of their operational lifespans, they present a dual environmental threat: they either remain in orbit as hazardous space junk, threatening future missions, or they burn up during atmospheric re-entry, leaving behind a trail of vaporized, toxic metallic pollution in the upper atmosphere. To solve this, space agencies require "demisable" materials compounds specifically engineered to break down completely, cleanly, and safely under the extreme heat of re-entry.

AI simulates the intense thermodynamic friction of atmospheric re-entry on experimental molecular blends. It predicts exactly how a satellite frame will fragment and vaporize. By using AI to design these self-consuming structures, space agencies can ensure that future satellite constellations leave zero physical footprint in orbit and zero chemical pollution in our biosphere.

Comprehensive Industrial Case Studies

To understand the real-world impact of AI on the twin transition in aerospace materials, we can look at three distinct case studies across government research, international space policy, and commercial engineering.

1. NASA Glenn Research Center and the GRX-810 Alloy

Material scientists at NASA's Glenn Research Center used artificial intelligence to develop a groundbreaking alloy called GRX-810 [9, 10].

The Problem: Components inside rocket engines must withstand temperatures over 2,000°F without melting or cracking under extreme pressure.

The AI Application: NASA deployed thermodynamic machine learning models to run thousands of virtual simulations. The AI predicted how adding microscopic particles would stabilize the metal matrix at extreme temperatures.

The Outcome: As detailed in the NASA Technology Transfer Program, the AI narrowed down the exact recipe 1,000 times faster than traditional trial-and-error laboratory work. The resulting material can survive extreme thermal stress, resists cracking, and lasts up to 1,000 times longer than standard aerospace alloys.

2. The European Space Agency (ESA) Clean Space Initiative

The European Space Agency has integrated AI into its "Clean Space" framework to systematically eliminate the long-term environmental hazards of space debris [11, 12].

The Problem: Ensuring that decommissioning satellites dissolve entirely upon atmospheric re-entry requires replacing rigid structural elements with custom aluminum-matrix composites that break down predictably under thermal stress.

The AI Application: ESA utilized deep learning models to conduct high-fidelity aerodynamic and structural testing on experimental satellite hulls. The AI tracked how mechanical stresses and high-speed plasma streams interact with complex material layups during descent.

The Outcome: The system successfully identified optimized structural designs that vaporize cleanly into the atmosphere without shedding dangerous fragments, supporting global mandates for zero-debris space missions.

3. Relativity Space and Intelligent Additive Manufacturing

In the commercial sector, private aerospace firms like Relativity Space are using generative AI to rethink rocket manufacturing from the ground up, utilizing giant, autonomous 3D printers to construct entire flight structures [13].

The Problem: Printing massive aluminum and titanium components can introduce hidden interior flaws or uneven cooling zones that ruin the structural integrity of a rocket fuel tank.

The AI Application: Neural networks are trained to analyze real-time video, acoustic, and thermal sensor data collected directly from the print head as it deposits molten metal.

The Outcome: The AI automatically corrects print parameters on the fly, eliminating raw material waste from failed prints and reducing the total time required to build a flight-ready rocket hull from years to less than 60 days.

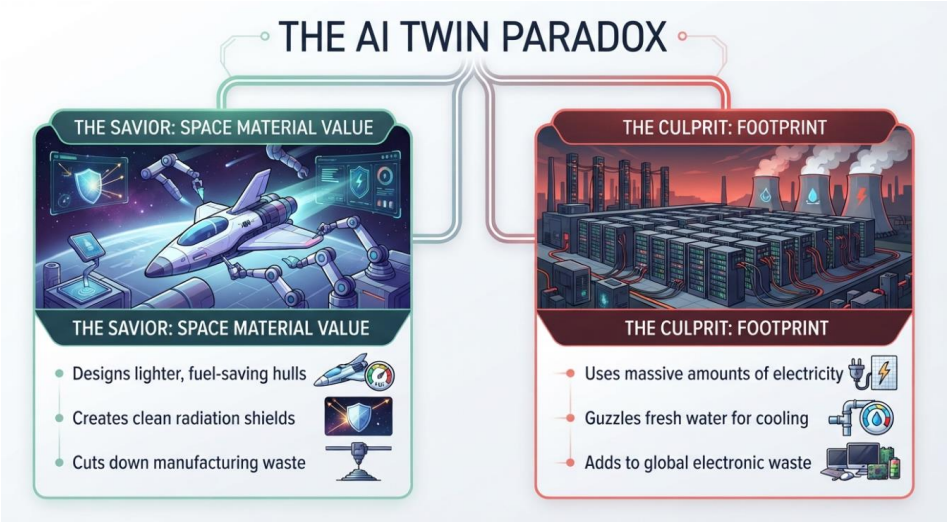
Comparative Analysis: Traditional vs. AI-Driven Materials Development

To clearly show how AI drives the digital transition while safeguarding green priorities, the following table compares traditional aerospace materials development with modern, AI-driven methodologies across key operational metrics.

Metric	Traditional Development	AI-Driven Development	Twin Transition Impact
Discovery Timeline	10 to 15 years of manual formulation and physical lab testing.	Days to weeks using high-throughput virtual screening.	Digital: Accelerates research cycles dramatically. Green: Deploys clean solutions faster.
Material Waste	High waste due to carving out metal blocks and physical trial-and-error smelting.	Minimal waste via real-time adjusted 3D printing and virtual prototyping.	Green: Preserves rare metals and reduces laboratory chemical waste.
Fuel Efficiency	Heavy or standard-weight materials increase launch vehicle fuel demands.	Generative design yields hyper-lightweight, ultra-strong parts.	Green: Directly reduces rocket fuel consumption and atmospheric carbon emissions.
Reliability	Inspected after production; hidden internal flaws can cause unexpected failures.	Monitored layer-by-layer via real-time AI computer vision.	Digital: Creates a continuous digital twin of the material. Green: Extends hardware lifespan.

The Sustainability Paradox: The Environmental Impact of AI Infrastructure

A complete analysis of AI's role in the twin transition must confront an inherent paradox: the digital tools driving environmental sustainability are themselves massive consumers of resources. The training and deployment of deep neural networks, large-scale simulations, and massive transformer architectures require substantial computational energy, introducing a potential conflict with green transition objectives if left unmanaged [15, 16].



To ensure AI remains a net-positive contributor to the twin transition, scientific research must pivot from prioritizing raw accuracy at any cost ("Red AI") toward computational efficiency and resource awareness ("Green AI").

Efficiency by Design: Model Compression Techniques

Researchers are actively developing methodologies to minimize the compute requirements of AI deployment without sacrificing predictive accuracy:

- Quantization: Reducing the numerical precision of weights and activations (e.g., from 32-bit floating-point to 8-bit integers), which dramatically lowers memory bandwidth and power consumption.
- Pruning: Systematically removing non-critical neurons or weights from a trained network, yielding compact models that run efficiently on low-power edge hardware.
- Knowledge Distillation: Transferring the capabilities of a massive, resource-heavy "teacher" model into a lightweight, streamlined "student" model tailored for sustainable deployment.

Algorithmic Innovations and Architectural Pivots

The scientific community is moving beyond dense, monolithic neural networks toward architectures that activate hardware conditionally. Spiking Neural Networks (SNNs), which mimic biological brains by processing data in sparse, event-driven bursts, offer a promising alternative to traditional continuous-activation models. Furthermore, the integration of analog neuromorphic hardware holds the potential to reduce operational energy requirements by several orders of magnitude compared to standard silicon architectures.

Future Outlook: Space Materials in the Next Decade (2026–2036)

As we look toward the next decade of space exploration, the deep integration of AI into materials science will likely move beyond individual lab experiments into a fully unified, global digital ecosystem.

- Fully Automated Off-World Manufacturing

The ultimate goal of combining AI and materials science in aerospace is to move manufacturing off Earth entirely. Future lunar bases and orbital manufacturing hubs will utilize autonomous AI loops to harvest local resources, such as lunar regolith or metallic asteroids. AI models will analyze the raw, unpredictable composition of space rocks in real time, automatically adjusting solar-powered 3D printers to construct habitats, radiation shields, and spare parts without needing supply shipments from Earth.

- Self-Healing Smart Materials

AI is accelerating the design of biomimetic, self-healing materials for long-duration deep space missions. These advanced composites contain microscopic networks filled with healing agents or shape-memory polymers. When a piece of space debris impacts a spacecraft hull, embedded AI micro-sensors instantly detect the pressure drop and trigger localized electrical currents to melt and reseal the puncture in seconds, ensuring astronaut safety while drastically extending the operational lifespan of the ship.

Conclusion

Artificial intelligence is a vital tool for the twin green and digital transition. It fundamentally improves how we do materials research for the space industry, cutting the time to find clean, lightweight composites from decades to days, improving manufacturing efficiency, and preventing orbital waste.

However, we cannot ignore the high environmental costs of computing. By using "Green AI" designs, making models smaller, and running them on clean energy, we can solve this paradox. Ultimately, we can make sure AI serves as a tool that doesn't just innovate for the stars, but actively protects our home planet.

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