High-Throughput Computational Search for Novel Ternary Superalloys

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Executive Statement:

This study uses high-throughput computational methods to identify novel ternary superalloys with superior mechanical properties.

Technology Overview:

The research focuses on the computational discovery of new superalloys, primarily nickel, cobalt, and iron-based systems, using the quasi-random structure (SQS-32) approach within the AFLOW computational framework. It evaluates the thermodynamic stability and potential of 2224 ternary systems, identifying 2111 compound-forming systems and highlighting 102 systems as particularly stable.

Key Advantages:

- Utilizes high-throughput computational techniques for efficient material discovery
- Employs a novel approach (SQS-32) to mimic random alloy statistics, enhancing the accuracy of predictions
- Identifies 2111 compound-forming ternary systems, significantly expanding the potential superalloy database
- Highlights 102 particularly stable systems, with 37 being novel, previously unreported systems
- Focuses on systems without experimental challenges, cost, or toxicity issues, streamlining further research and application

Problems Addressed:

- Overcomes the limitations of conventional nickel-based superalloys
- Reduces the time and expense associated with experimental trial-and-error methods for material discovery
- Addresses the need for materials suitable for high-temperature applications

Market Applications:

- Aerospace industry for turbine engines and other high-temperature components
- Automotive industry for advanced engine components requiring high performance under extreme conditions
- Manufacturing of industrial machinery and tools that operate at high temperatures
- Research and development in materials science, particularly for the development of

next-generation superalloys