Design and Development of Novel Alloys for the Energy Sector Based on Integrated Computational Materials Engineering (ICME)

QuesTek Innovations LLC of Evanston, IL uses its proprietary *Materials by Design*® expertise and technology in conjunction with its Integrated Computational Materials Engineering (ICME)-based methodologies to rapidly design, develop and qualify advanced alloys into demanding applications. Accelerating the historically slow and expensive materials design and development process, QuesTek's approach integrates extensive thermodynamic and kinetic databases with advanced computational modeling tools to develop and optimize precise chemical compositions and processing parameters, in order to ensure specified property targets and meet required performance goals.

QuesTek has computationally designed and developed many novel high-performance alloys, coatings, and materials including iron-, copper-, aluminum-, nickel-, cobalt-, molybdenum-, and titanium-based materials. As a global leader in the field of ICME, QuesTek has proven that these materials can be developed much faster and at lower cost, while providing unique, enhanced properties that directly meet user-defined material performance goals for demanding applications in energy, aerospace, automotive, oil & gas and other industries.

For the energy sector, QuesTek is currently involved in multiple ongoing Small Business Innovation Research (SBIR) projects funded by the Department of Energy (DOE), as well as other governmental departments, to design and develop novel high-performance alloys. Under one such ongoing, DOE-funded Phase II SBIR program, entitled "Computational Design of Weldable, High-Cr Ferritic Steel," QuesTek is applying its computational alloy design methodology and experience in high-Cr ferritic alloys to create a novel low-cost ferritic superalloy for applications to tubing components in Advanced Ultra-Super Critical (AUSC) steam boilers. With the performance goals of survivability at high operating temperatures (1400°F) and improved fuel and plant efficiency, the alloy is being designed to have enhanced mechanical properties to incumbent materials such as P92 alloy, specifically improved creep and corrosion resistance and eliminating the need for post welding heat treatment. In this SBIR QuesTek is partnering with Babcock & Wilcox, who serves as a technical advisor and voice of the OEM to ensure the alloy design considers all key requirements for steam boiler applications.

Under another ongoing, DOE-funded Phase II SBIR project entitled "Computational Materials Design of Castable Single Crystal Nickel-based Superalloys for IGT Blade Components," QuesTek is designing a highly castable single crystal Ni-based superalloy for large industrial gas turbine (IGT) blade components. By combining high castability with the superior creep performance comparable to state-of-the-art aeroturbine single crystal blades, QuesTek's new alloy promises to allow higher gas temperatures and increased thermal efficiency. In this SBIR, QuesTek is partnering with Siemens Energy Inc., who serves as the voice of the OEM, and PCC Airfoils LLC for technical input as well as production of both trial and full-scale IGT single crystal blade castings.

Additionally, QuesTek has been involved in multiple projects for the energy sector, including "Low Cost Alloys for High Temperature Solid Oxide Fuel Cell System Components," "Low Cost, High Strength, Low Loss Soft Magnetic Materials for Traction Drive Motor Applications," and "Tungsten Alloys with Improved Fracture Toughness and Lowered Ductile to Brittle Transition Temperature for Fusion Reactors."

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