Materials by Design®

QuesTek Innovations, LLC is a small business that specializes in computational materials design to rapidly and efficiently innovate, scale-up and deploy novel high-performance materials. Using Integrated Computational Materials Engineering (ICME) technologies, QuesTek integrates computational models within a systems engineering framework to model process-structure and structure-property interactions, allowing for microstructural design across a hierarchy of length scales to meet specific user-defined performance goals.

The *Materials by Design* methodology envisions materials as a system of inter-connected processing, structure and property subsystems, as show in Figure 1. At the beginning of each new materials design, a System Chart is developed by taking end-user defined material performance goals, translating them into quantitative property targets, and designing a hierarchy of microstructural subsystems that achieve those properties, while taking into consideration existing processing practices and constraints for the given alloy system.

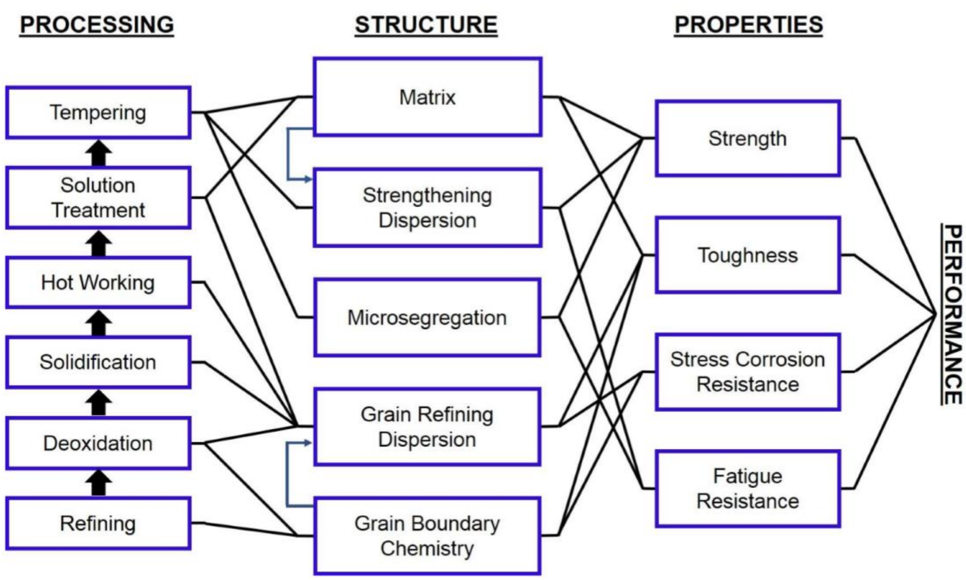

Figure 1. A System Chart for a high-performance structural steel that maps the inter-relationships between processing, structure, property and performance.

The foundation of computational materials design is embodied in the development of physics-based mechanistic models that accurately describe material process-structure and structure-property relationships. The models are integrated with extensive material parameter databases and executed through respective software platforms to inform the design process.

QuesTek applied its *Materials by Design* methodologies and ICME technologies to design, scale-up, and commercialize four high performance *Ferrium®* steels. The design and development of the Ferrium M54® steel, an ultra-high strength, high toughness, stress corrosion cracking (SCC) resistant structural alloy, is a leading example highlighting the effectiveness of a systems-based, targeted computational modeling approach to materials innovation. The M54 steel's development from a clean sheet alloy design to in-flight demonstration in a life-critical aerospace application was completed in less than seven years.

In designing M54 steel, which was engineered to be a fully martensitic, secondary hardening steel, a variety of computational tools were used. A CALculation of PHAse Diagrams (CALPHAD) based approach, using Thermo-Calc software, was used to generate composition-specific equilibrium step diagrams, as presented in Figure 2. These graphical representations detail the phases and phase fractions present at equilibrium as a function of temperature, informing microstructural design considerations and processing optimization.

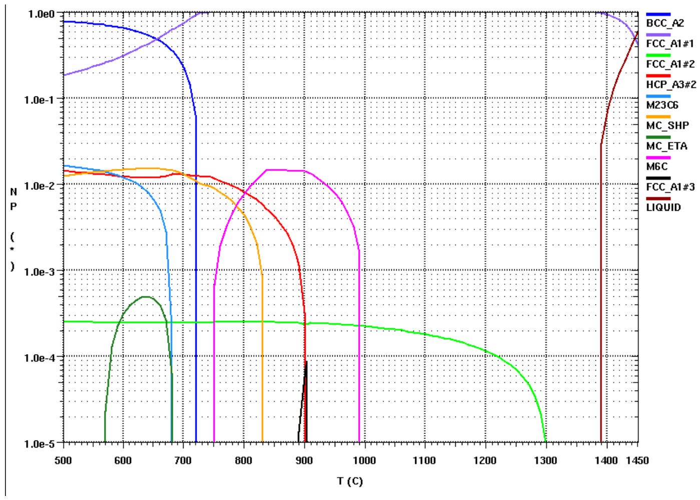

Figure 2. Schematic equilibrium step diagram generated by Thermo-Calc software representing phase fraction of equilibrium phases as a function of temperature for a specific composition.

Based upon compositions designed by the CALPHAD approach, mechanistic models relate calculated microstructures to properties relevant to the application of the alloy design. These structure-property models developed by QuesTek were used to optimize strength, fracture toughness and fatigue. Examples of these models, such as the modeling of ductile-to-brittle transition temperature (DBTT) and relationship of M_2C precipitate driving force to peak hardness, are illustrated in Figure 3.

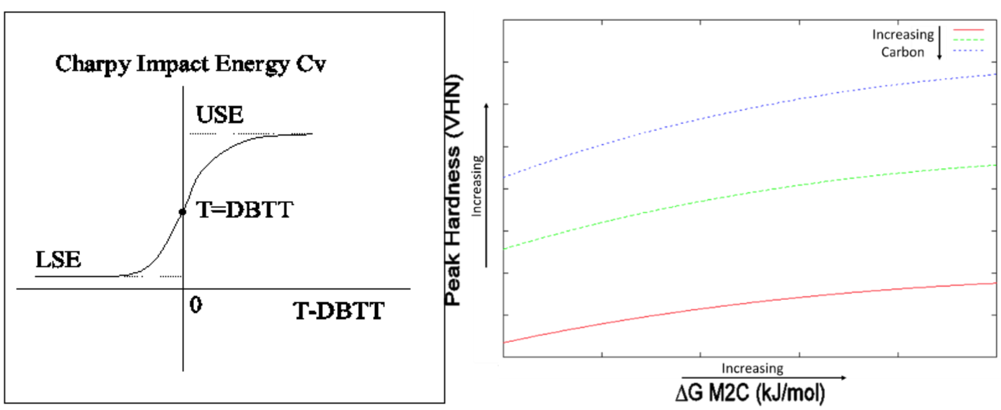

Figure 3. (left) Schematic representation of a master curve that has been calibrated for steels that factors in strength, upper and lower shelf energy, grain size and composition for optimizing toughness as it relates to temperature; **(right)** Schematic representation of M2C precipitate driving force and impact on hardness (strength).

Process-structure models, material databases, and thermodynamic and kinetic software such as DICTRA were used for processing optimization, further informed, calibrated and validated by advanced characterization techniques. As an example, Figure 4 details DICTRA solidification simulations, informed by secondary dendrite arm spacing measurements from a full-scale production ingot, that dictate homogenization cycle parameters.

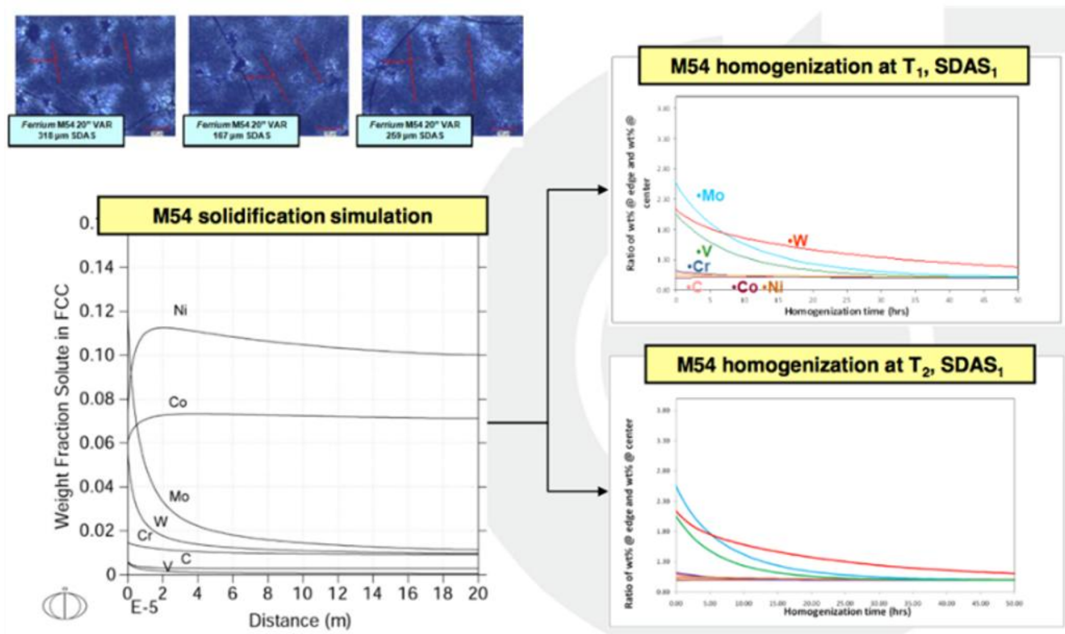

Figure 4. Example of solidification and homogenization calculations completed for Ferrium M54.

Through the integration of these process-structure and structure-property models in a systems-based design approach, QuesTek successfully accelerated M54's overall development from a clean sheet design in 2007 to a precise chemical composition in less than one year, with the production of the first 10-ton VIM/VAR ingot the following year. An Aerospace Material Specification (AMS 6516) was issued two years later, and inclusion in the MMPDS handbook for A- and B- basis design minima was approved in December 2013. QuesTek coordinated the production and qualification of hook shank components made from M54 for the U.S. Navy's T45 platform that were successfully flight tested in December 2014. The M54 hook shanks exhibited more than twice the component life of the incumbent Hy-Tuf steel hook shanks. This program led to a toll manufacturing contract to provide the Navy with 60 M54 hook shanks.