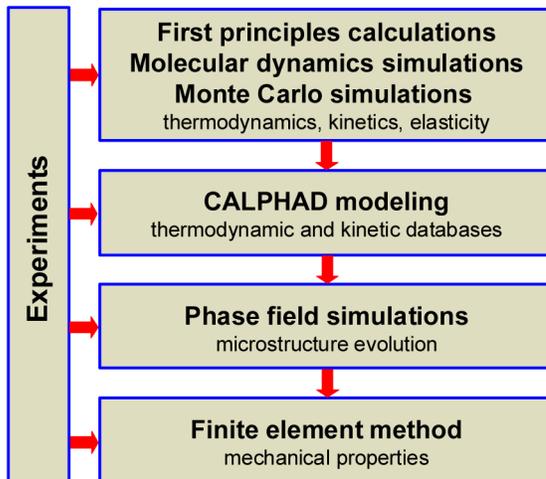




## An Integrated Approach To Materials Development

Traditional trial-and-error method in materials development is time consuming and costly. In order to speed up materials discovery for a variety of energy applications, an integrated approach for multi-scale materials simulations and materials design has been adopted at NETL. The core concept of this approach is that various computer simulation modules across a range of length and time scales are integrated and supported with critical experiments. These modules are first-principles calculations, molecular dynamics simulations, Monte Carlo simulations, CALPHAD modeling (acronym of Calculation of Phase Diagrams), phase field microstructure simulation, and finite element method (FEM). Ductile refractory metal-based alloys are being successfully designed with good creep and oxidation resistance for ultra-high temperature applications ( $\geq 1200$  °C) and for novel alloy membranes (PdCu-based crystalline and non-Pd based amorphous) for hydrogen separation from syngas.



*Multi-scale materials simulations supported by critical experiments.*

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First-principles calculations only require the atomic number and crystal structure as input and yield electronic and cohesive properties of solids. Therefore, they are widely used to predict physical properties of crystalline solids, including thermodynamic properties (enthalpy and entropy), elasticity, electronic, magnetic and optical properties without any experimental input. An unlimited number of alloys (binary, ternary and multi-component systems) can be “virtually” processed by computer, and only promising compositions that pass the property criteria are chosen and passed onto experiments for verification. Molecular dynamics and Monte Carlo simulations are used to predict structural and energetic evolution of large systems of more than one thousand atoms at finite temperatures. Composition dependence of atomic diffusivity can be theoretically calculated combining first-principles calculations and kinetic Monte Carlo simulations.

Upon verification, CALPHAD modeling is used to develop the corresponding thermodynamic and mobility databases. The CALPHAD method quantitatively models the Gibbs energy of a system based on experimental and theoretical data. It not only enables a user to readily determine the relevant phase field with respect to composition, temperature and pressure, but also can be directly used in conjunction with a mobility database to simulate temporal composition profile and microstructure evolution during a variety of processes, such as solidification, hot rolling, recrystallization, etc.

Microstructure simulations using phase field method and mechanical property simulations using FEM are other computational techniques. Phase field simulations are used to model phase transformations, grain growth and recrystallization in 1-D, 2-D and 3-D. Quantitative data sets of microstructure (e.g., grain shape evolution, grain size distribution, grain texture, interface composition, etc.) are readily obtained at various time scales at proposed temperature and pressure. The thermodynamic and kinetic databases for the alloy system developed using the CALPHAD method can be used as input for phase field simulations, which can then be directly compared with corresponding experiments. The digital microstructure obtained can be used as input for FEM simulations under applied thermal and mechanical constraints. Both elastic and plastic behavior of the as-built, multi-component, multi-phase structure are virtually examined without the need for costly experiments.

In order to verify these theoretical modeling results, key experiments are conducted in parallel to the calculations at each stage. The power of this integrated methodology is that experiments are limited to only those alloy compositions with the highest likelihood of success, thereby greatly speeding the process of alloy development and lowering development costs.

