D. Advanced Materials Development through Computational Design for HCCI Engine Applications

Vinod K. Sikka, G. (Murali) Muralidharan, and Rick Battiste
Materials Science and Technology Division
(865)574-5112: fax: (865) 574-4357; e-mail: sikkavk@ornl.gov
Bruce G. Bunting
Engineering Science and Technology Division
(865) 946-1512; fax: (865) 946-354; e-mail: buntingbg@ornl.gov

DOE Materials Technologies Team Leader: Jerry Gibbs
(202) 586-1182; fax: (202) 586-1600; e-mail: jerry.gibbs@ee.doe.gov
ORNL Technical Advisor: David Stinton
(865) 574-4556; fax: (865) 241-0411; e-mail: stintondp@ornl.gov

---

Contractor: Oak Ridge National Laboratory, Oak Ridge, Tennessee
Prime Contract No.: DE-AC05-00OR22725

Objectives

- Identify and catalog the materials operating conditions in homogeneous charge compression-ignition (HCCI) engines and use computational design concepts to develop advanced materials for such applications.
- Interact with designers of HCCI engines and manufacturers of components in order to identify the components that will be affected by the harsh operating conditions resulting from the HCCI design.
- Identify the highest-priority component(s) that are critical to the implementation of the HCCI concept.

Approach

- Identify engine components, currently used materials, and current operating conditions and compare them with the expected component operating conditions for HCCI engines.
- Demonstrate the feasibility of the "materials-by-design" approach for the highest-priority item. Improve material performance for HCCI applications through computational modeling and experimental validation.

Accomplishments

- Identified high-temperature fatigue as a critical property of interest in improving the performance of valve materials and identified weight percent (or volume fraction) of γ' as a critical microstructural characteristic that needs to be optimized.
- Identified eight commercially available compositions of nickel (Ni) -based alloys as potential candidates for further study in developing correlations between microstructure and properties.
- Completed thermodynamic calculations on all seven alloys and initiated microstructural characterization and mechanical property testing.
- Through discussions with suppliers of Ni-based alloys, identified one major supplier who has expressed interest in tracking progress in the project with regard to alloy properties and interest in active collaboration in the future.

- Based on computational approach for alloy design, obtained funding for a Work-For-Others project from a major automobile manufacturer to optimize compositions of cast irons for exhaust manifold applications.

Future Direction

- Communicate with automotive companies, Diesel Cross-Cut Team, FreedomCAR, and 21st Century Truck on the progress made through computational design.
- Develop data on mechanical properties of selected Ni-based alloys and correlate microstructure with properties. This will validate the computational design concept for design of advanced Ni-based alloys.

Introduction

There has been an increasing interest in HCCI combustion in recent years because of its potential to increase engine combustion efficiency and reduce emissions. However, the use of HCCI combustion will subject the engine components to significantly higher temperatures and pressures. The temperatures for diesel engines will reach over 1600°F, and pressure may reach > 2000 psi, which is approximately four times that of the normal combustion engine. Such severe engine operating conditions will require a significant improvement in materials performance in order to take advantage of the HCCI engine concept. This project deals with identifying materials requirements for HCCI engines for automotive and truck applications and the development of advanced, yet cost-effective, materials through computational design.

"Materials-by-design" is an Oak Ridge National Laboratory (ORNL) concept that encompasses a collection of materials-related techniques including modeling, correlation, and materials modification. The premise behind materials-by-design is that mechanical properties are correlated to microstructure and phase chemistry. The phase composition and microstructure can be achieved through thermodynamic equilibrium or through non-equilibrium techniques such as quenching, rapid casting solidification, or mechanical working. These characteristics can then be correlated to desired mechanical properties through equilibrium thermodynamics or through a variety of correlation techniques. The correlations allow untested compositions or treatments to be modeled so that desired trends can be rapidly established. Small heats of targeted materials can then be processed to confirm the modeled properties and to broaden the correlation data base.

Finally, there are several techniques, such as magnetic processing or low-temperature carburizing, that can be applied to allow further modification and optimization of desired properties. Materials-by-design is ideally suited to cast materials and heavily thermally processed materials (e.g., stainless steels, Ni alloys, cast irons, alloy steels, and brazed wrought aluminum alloys), and the concept has been successfully applied in such diverse areas as high-temperature furnace components, exhaust valves, exhaust manifolds, and tube fittings. Figure 1 and Table 1 provide an outline of the materials-by-design approach and a summary of the techniques that can be applied.

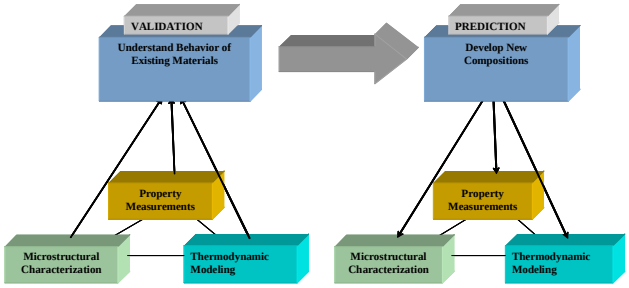

Figure 1. Overall approach for materials-by-design.

In our approach, we examined critical heavy-duty diesel engine materials and identified means to reduce their cost for acceptance in HCCI applications. This was accomplished through the following tasks:

Task 1. Identify critical material requirements for HCCI engines based on their operating conditions. This task will be accomplished through interactions with advanced engine and component designers. The interactions will include personal visits to six companies: Caterpillar, Cummins Engine, Deer, International Truck, Eaton Corp., and General Motors. Visits will be supplemented by a literature search, a review of advanced engine design studies, and follow-up discussions afterward. The key outcomes from this task will include (1) identifying

Table 1. ORNL materials by design toolbox

Modeling	Experimentation	Characterization
Thermodynamic modeling of material properties vs alloy composition	Ultra-high-gauss magnetic stabilization of alloy steels	Advanced microscopy techniques
Neural-network modeling of diverse, nonlinear materials properties and process variations	Low-temperature gas carburization of finished components	X- ray and neutron scattering
Detailed microstructure based empirical modeling	Ability to produce small quantities of materials and fabricate them into test bars for property measurements and production of prototype components by a variety of methods, including sand and die casting, extrusion, forging and rolling	Surface and bulk property measuring techniques
Non-equilibrium modeling of solidified structures		
Extrapolation of properties from simple alloy systems to complex systems using interaction parameters		

operating conditions for advanced engine concepts, with a focus on the HCCI concept; (2) identifying components most affected by these operating conditions; (3) identifying currently used materials, new requirements, and performance targets; and (4) ranking the highest-priority items for study by the materials by design approach.

Task 2. Demonstrate the feasibility of materials-by-design approach for the highest-priority item. In this task, we will identify the details of the currently used material for the highest-priority item. Specifically, we will examine material compositions, processing methods, mechanical properties, corrosion properties, and cost.

Based on the available mechanical properties data, microstructural analysis, and thermodynamic phase stability calculations, we will identify the underlying mechanism that delivers the current properties.

Task 3. Improve materials performance for HCCI application through computational modeling and experimental validation. In this task, we will use computational modeling (key basis for the material-by-design concept) to identify compositions that will deliver the desired phases for two purposes: (1) improving property performance and (2) finding alternatives to reduce cost for both current and improved performance. The outcome of the analysis will be validated through experimentation. The validation will be carried out in the following steps:

1. Prepare compositions identified based on computational design in 1-lb heats for microstructural analysis and very limited property determination; compare the results with output based on computational analysis for validation.
2. Scale up the validated composition into 20-lb to 100-lb heats and cast them into ingots for processing trials. In most cases, the material is expected to be used in the wrought condition. However, if it is to be used in the cast condition, we will save part of the ingots for analysis of as-cast properties.
3. Subject cast ingots to processing steps that are currently used by industry. Develop optimum processing and heat-treatment conditions to obtain the desired microstructure.
4. Carry out microstructural analysis and mechanical properties analysis on the material processed and heat-treated with optimum conditions.
5. Prepare autotype components for HCCI engine tests.

Extensive interaction with industrial partners will occur during all three tasks. This collaboration is expected to result in the rapid transfer of materials improvement from this project to industry for use in HCCI and other advanced engine concepts.

Results

Materials Development through Computational Design

Ni-based alloys have been identified as potential candidates for improved valve materials. There is particular interest in increasing the operating temperature of exhaust valves to about 1600°F (870°C). High temperature fatigue strength has been identified as a critical factor in determining the performance of these alloys in the valve application. An evaluation of the microstructure of various Ni-based alloys and correlation with limited information on the fatigue properties that are available show that the volume fraction of the γ' phase is likely to be a dominant factor in determining the performance of these alloys at high temperatures. Since the size of the strengthening precipitates is also critical, it is anticipated that the kinetics of coarsening this phase would also be influential in the long-term performance of the alloys in this application. Based upon discussions with various users and suppliers, a range of Ni-based alloys with potentially varying weight fractions (or volume fractions) of γ' have been identified in efforts to correlate the fatigue properties with the microstructure of the alloys. Table 2 shows a summary of these alloys and the compositions of specific heats procured for this study. IN 751 is the alloy currently used, and it has been added to the matrix as a reference.

To obtain initial information on the microstructures of these alloys at equilibrium, thermodynamic calculations have been carried out using JMatPro V4 for all the alloys shown in Table 2. Figures 2 to 9 show the phases present in the alloys as a function of temperature.

Comparison of the results of the calculations shown in Figures 4 to 9 shows that all alloys have a matrix of γ with the major strengthening phase as γ'. One or more carbide phases such as M23C6, MC, and M7C3 may also be present in different alloys. The primary difference between the microstructures of the various alloys is in the weight percent of the γ' phase at a given temperature and the highest temperature at which the γ' phase is stable in the different alloys. Table 3 shows a summary of the type and phases present at 900°C in the different alloys. The variation in γ' phase content is well illustrated in the table.

A survey of the data available on the high-temperature fatigue properties of these alloys was conducted. Results show that such data are available not for specific compositions of the alloys but for a broad range of compositions that could be associated with a particular grade. Thermodynamic calculations show that significant variations in the phase contents occur over this composition range. Thus it is not feasible to develop relationships between the microstructures of the alloys and their mechanical properties based on data available in the literature. The required high-temperature fatigue property data will be obtained as a part of the project, and equipment for testing has been assembled as outlined below.

Mechanical Property Measurement

To conduct fatigue tests on the selected Ni-based alloys**,** an existing material test system servohydraulic closed loop control material test facility has been upgraded to include high-temperature, low-cycle-fatigue testing capability for round bar type specimens. Test results will be reported next quarter.

Table 2. Compositions of various alloys selected for studying the correlation between microstructure and mechanical properties

Alloy	C	Si	Mn	Al	Co	Cr	Cu	Fe	Mo	Nb	Ni	Ta	Ti	W	Zr
X750	0.03	0.09	0.08	0.68	0.04	15.7	0.08	8.03	–	0.86	Bal	0.01	2.56	–	–
Nimonic 80A	0.08	0.1	0.06	1.44	0.05	19.6	0.03	0.53	–	–	Bal	–	2.53	–	–
IN 751	0.03	0.09	0.08	1.2	0.04	15.7	0.08	8.03	–	0.86	Bal	0.01	2.56	–	–
Nimonic 90	0.07	0.18	0.07	1.4	16.1	19.4	0.04	0.51	0.09	0.02	Bal	–	2.4	–	0.07
Waspaloy	0.03	0.03	0.03	1.28	12.5	19.3	0.02	1.56	4.2	–	Bal	–	2.97	–	0.05
Rene 41	0.06	0.01	0.01	1.6	10.6	18.4	0.01	0.2	9.9	–	Bal	–	3.2	–	–
Udimet 520	0.04	0.05	0.01	2.0	11.7	18.6	0.01	0.59	6.35	–	Bal	–	3.0		
Udimet 720	0.01	0.01	0.01	2.5	14.8	15.9	0.01	0.12	3.0	0.01	Bal	–	5.14	1.23	0.03

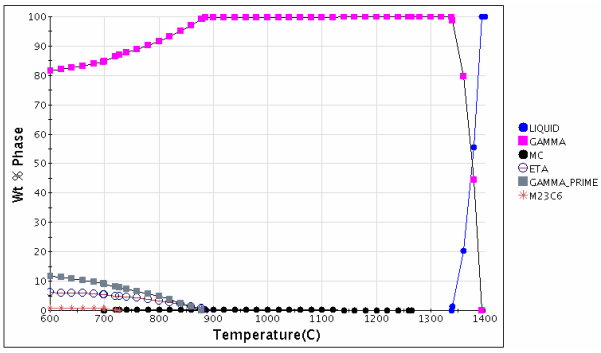

Figure 2. Phase equilibria in alloy X750.

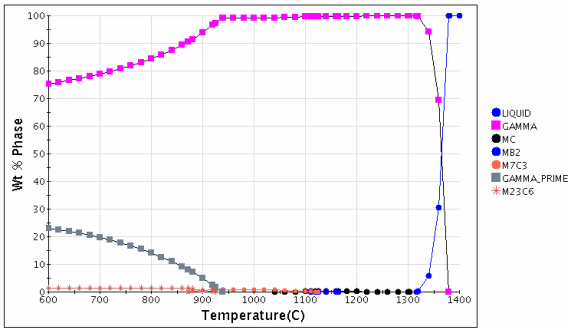

Figure 3. Phase equilibria in alloy Nimonic 80A.

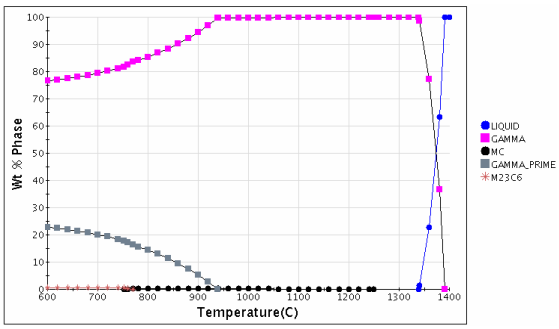

Figure 4. Phase equilibria in alloy IN751.

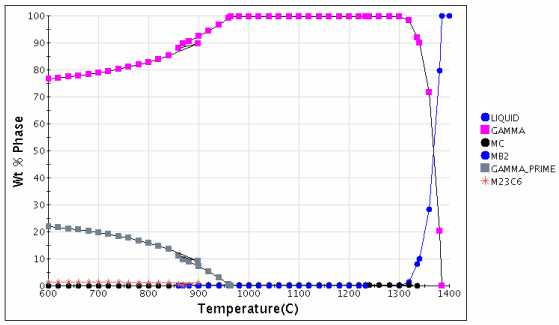

Figure 5. Phase equilibria in alloy Nimonic 90.

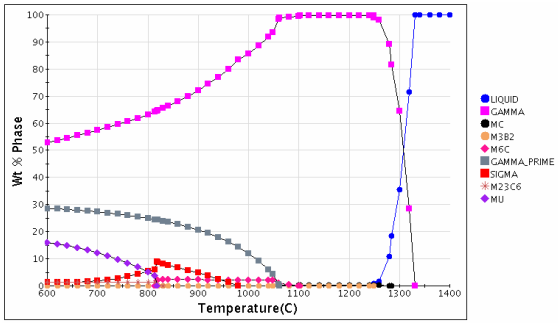

Figure 6. Phase equilibria in Waspaloy.

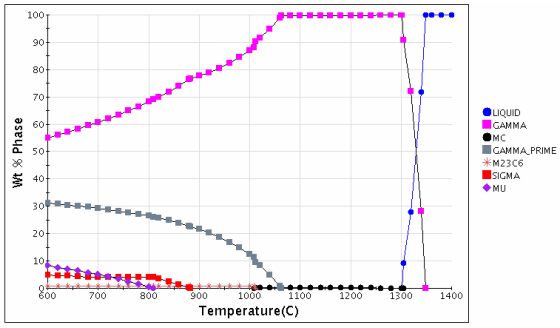

Figure 7. Phase equilibria in Rene 41.

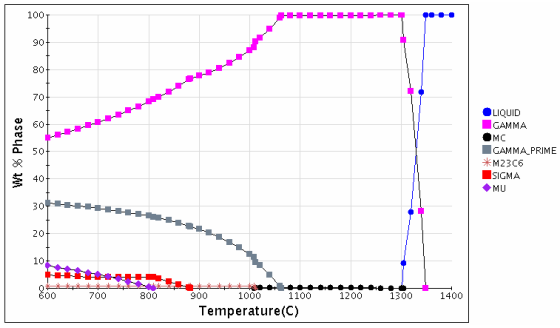

Figure 8. Phase equilibria in Udimet 520.

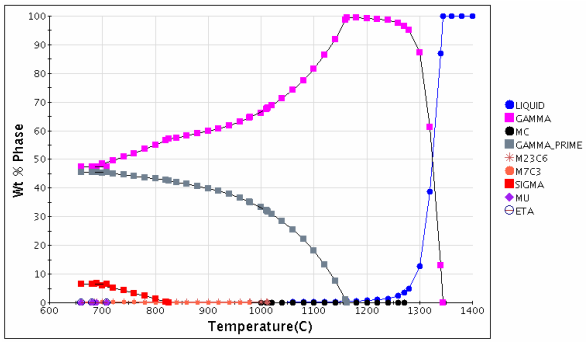

Figure 9. Phase equilibria in Udimet 720.

Table 3. Calculated major phase contents of various alloys at 900°C

Alloy	Wt % γ	Wt % γ'	Wt % carbides	Wt % other
X750	99.8	**0**	0.2	
Nimonic 80A	93.9	**5.0**	1.1	
IN 751	94.5	**5.3**	0.2	
Nimonic 90	89.8	**8.9**	1.3	–
Waspaloy	84.7	**14.7**	0.6	–
Rene 41	72.1	**20.7**	2.4	4.8
Udimet 520	77.6	**21.6**	0.8	–
Udimet 720	59.6	**40.0**	0.4	–

Conclusions

- Potential commercial Ni-based alloys that need to be evaluated for use in higher temperature exhaust valves were identified.
- Thermodynamic calculations show that the variation in the major strengthening phase spans a significant range and hence is appropriate for developing correlations between microstructure and mechanical properties.
- High-temperature fatigue data were identified as essential in the selection and/or development of Ni-based alloys for this application.

Publications/Presentations

Bruce Bunting, Govindarajan Muralidharan, V. K. Sikka, presentation at Cummins International.

Govindarajan Muralidharan, Steve Weber, Michael Pollard, and Haydn Chen, "Coarsening of Coherent Precipitates in Multi-Component Ni-Based Alloy Systems: Experiment vs Theory," a poster presentation at the Gordon Research Conference on Physical Metallurgy, July 23–28, Holderness School, Plymouth, NH.