2. MATERIALS DEVELOPMENT

A. Integrated Approach for Development of Energy-Efficient Steel Components for Heavy Vehicle and Transportation Applications

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Objective

- Develop methods and tools to achieve energy-efficient and environmentally benign steel components.
- Develop microstructure-level (often called mesoscale) simulation tools to capture the formation and influence of non-homogeneous (real-life) microstructures in steel processing. The tools will be used to understand and predict microstructure evolution during processing and ultimately to predict the resultant component performance.
- Use the information from the simulations to design steel microstructures and develop process roadmaps.
- Demonstrate the developed techniques on a pilot project at Caterpillar involving a defined structural component, namely a track roller shaft, that represents a steel component with high production volume that can potentially benefit from microstructure-level improvements.

Approach

- Develop microstructure-level models to accurately predict the evolution and behavior of steel microstructures during component processing and performance.
- Characterize thermomechanical properties of microstructural constituents as a function of temperature and composition for exact chemistries.

- Develop the tools to assess required environmental resources and integrate them into the modeling simulation endeavor.

Accomplishments

- Acquired 1045 and 15V45 steel material.
- Distributed the two alloys to be investigated to the project team members so that machining of the test specimens required for the tasks of microstructural characterization, machining experiments, and determination of strain-rate-dependent mechanical properties could be initiated during the first quarter of FY 2004.
- Acquired two track roller shafts and distributed segments of these to the project team members.
- Completed machining testing (round 1).
- Completed mechanical testing for 1045.
- Assessed resources for machining of track roller shafts.
- Assessed resources for processing of track roller shafts.
- Characterized ferrite and pearlite for the 1045 alloy.
- Received three ultra-pure materials from CRIM.
- Initiated simulation of heat treatment and machining operations.
- Compared machining model predictions for different microstructures and machining parameters with experimental results from precision-controlled machining experiments.
- Demonstrated that the machining model qualitatively predicts the adiabatic shear band formation and chip morphology observed in the machining chips obtained from the machining experiments.

Future Direction

- Develop and demonstrate a microstructure-level model incorporating phase transformation kinetics, but without chemical and microstructural inhomogeneities (to be implemented in year 3), for the heat treatment processes used by Caterpillar for the SAE 1045 and SAE 15V45 steel alloys (9/2005).
- For both types of steel, produce in the laboratory the microstructures that evolve during these heat treatment processes and thoroughly characterize them to provide quantitative input data for the heat treatment simulation models.
- Perform all mechanical tests on these microstructures that are required for inputs and validation of the heat treatment models.
- Characterize the influence of mill thermomechanical processing (TMP) variables on deformation and recrystallization behavior for incorporation into coupled polycrystalline and recrystallization models developed during years 2 and 3 of this project.
- Initiate development of coupled polycrystalline plasticity and recrystallization models to simulate mill TMP variable effects on austenite grain evolution behavior and characteristics.

Introduction

Product cost and performance are two major pressures influencing the acceptance of energy-saving technologies by manufacturers, suppliers, and users in the heavy vehicle and transportation industries. Energy cost has become a significant portion of total product cost for steel applications. Major reductions in energy use are potentially achievable for the transportation and heavy vehicle industries through development and optimization of cost-effective fabrication processes and enhanced product performance. The key enabling technologies to achieve these benefits are improved materials and realistic, microstructure-level simulations to predict manufacturability and life-cycle performance. Over the past two decades, steel mills and forge shops have successfully implemented numerous energy-efficient processes. The next logical step is to focus on the development of steel microstructures that are produced in such a way that they are energy efficient and environmentally benign over the entire manufacturing cycle.

Structural materials used in critical steel components of machines have evolved to the point where further improvements in performance can be achieved only through a fundamental understanding of the mechanisms driving material behavior during processing and service. Microstructural elements such as grain size, inclusion and precipitate distributions, and chemistry control the performance of engineering materials. Variation in these microstructural elements leads to variation in such critical properties as fatigue life, toughness, and wear resistance. Therefore, understanding and developing the capability to control the formation of steel microstructures, and predicting their functional and environmental performance, are critical to moving the industry closer to its energy-efficiency, resource-efficiency, and pollution-prevention goals. The full realization of these benefits, however, requires a design tool that optimizes the micro-structure with respect to the mechanical and environmental performance throughout the life cycle of a particular steel component.

To apply an integrated approach to development of energy-efficient steel components, the development of three major areas of research needs to be completed:

- Micro-structure-level models to accurately predict evolution and behavior of steel microstructures during component processing and performance
- thermomechanical properties of microstructural constituents as a function of temperature and composition for exact chemistries
- tools to assess required environmental resources

This project addresses activities required for the first of these three areas. The second and third tasks are either supported by current funding through the National Science Foundation (NSF) or are expected to be funded through the DOE Initiative for Proliferation Prevention. Through these integrated efforts, a design tool will be developed that optimizes the microstructure, manufacturability, and performance of components with respect to the mechanical and environmental performance required throughout the components' life cycles. The overall benefit of this research will be the development and demonstration of a design methodology that will enable the domestic transportation and heavy vehicle industries to compete effectively in future worldwide markets through improved product performance and energy savings. Furthermore, the proposed design tool can be extended to other materials—i.e., cast iron, aluminum, titanium, magnesium, nickel-based alloys, ceramics, and composites—thus impacting virtually all industries.

In addition to the significant energy and cost savings benefits that the transportation and steel industries will realize from microstructure-level modeling, virtually all industries will be impacted. Examples include aerospace (engines, transmissions, structural), marine (engines and drives), agricultural and construction equipment, oil and chemical processing (pumps and gear boxes), military vehicles, mining machinery, appliances (compressors, motors, gear boxes, shafts), power tools, and automotive aftermarket.

Project Deliverables

The deliverables for the project will be

- Microstructure-level methods for simulating the manufacturing cycle of steel products, coupled with material performance computations (Tasks 1, 2, and 3)
- A specific chemical composition and processing map for a 1500-series steel and a microalloyed steel suitable for the application under consideration (Task 4)
- A determination of the energy and environmental resources required to produce the selected steel component using at least two steels and processing schemes (Task 4)

Project tasks will focus on three critical areas in the development of these models: heat treatment processing, machining, and materials performance in specific applications. These three processes have been chosen because they are critical steps toward the goal of developing a specific steel for a particular application, with a heavy reliance on modeling and with energy requirements optimized as an integral part of the development process. Casting and forming processing have been modeled under other programs, and Caterpillar has shown successful application and commercialization of these models. These existing models will be used, along with the heat treatment, machining, and specific applications models described in this report, to complete a suite of models for the manufacture of microalloyed steels.

To accomplish the project objectives, a multidisciplinary team consisting of a national laboratory, a university, and a steel end-user has been assembled. The team will be supported by an international research institute for material characterization and by experts in environmental impact assessment.

Technical Tasks

Task 1: Heat Treating Process

This task will quantify the influence of chemical and microstructural inhomogeneities in the austenite phase on the final heat-treatment response. The microstructure-level models incorporating phase transformation kinetics, polycrystalline plasticity, and recrystallization dynamics will be developed collaboratively by the Oak Ridge National Laboratory (ORNL), Brown University, and Caterpillar. Validation will be accomplished using the unique experimental capabilities and expertise at ORNL for conducting kinetic and metallurgical characterization and using Caterpillar's capability to produce heat-treated specimens in precisely specified and controlled conditions. The modeling effort will draw on the programs at Brown and Caterpillar that have developed microstructural modeling capabilities.

The coupled mesoscale deformation and recrystallization models developed cooperatively by the three team members will be implemented to study the influence of mill TMP variables and mesoscale composition variation on the grain size, grain-size distribution, and austenite grain-boundary character prior to the decomposition of austenite. The coupled deformation and recrystallization models will be used to predict the evolution of austenite grain structure and grain-boundary character distribution during the TMP steps involved during secondary fabrication. The output of these simulations will feed directly into an austenite decomposition code that predicts phase transformation during the heat-treatment operation.

Task 2: Machining Processing

A microstructure-level model will be applied to machining simulation of steels to determine their machinability and material state after TMP. The model will consist of four main elements integrated into the finite element structure: microstructure simulation, material modeling, material characterization, and material flow and fracture. The microstructure simulation module will assemble individual constituents into a composite material based on microstructural composition, grain size, and grain-size distribution. This information, along with residual stress predictions for individual grains, will be obtained from Task 1.

The material modeling module will account for the response of each constituent to high strains, strain rates, temperature, damage, and effects of loading paths associated with machining. The material characterization module will provide the material modeling module with parameters to define strain rate and temperature-dependent behavior of individual phases. The material flow and fracture module will periodically examine each grain for damage, locate deformed grain boundaries, and generate new boundaries. This module will compute stress, strain, temperature, and damage in each phase based on initial microstructure, material state, tool geometry, and process parameters.

A concerted effort will be made to review and leverage all current developments in this materials and process-simulation field that is the scope of this project. Microstructure, residual stress, and cutting force measurements obtained by various research groups (e.g., ongoing research at Purdue University by S. Chandrasekar) will be used for model development and validation.

Task 2 and Task 1 will be augmented by a parallel project among Caterpillar, Brown, and the Central Research Institute for Materials in St. Petersburg, Russia, in which a detailed examination is being performed of the relationship between composition, microstructure, and mechanical properties of steels of highly controlled purity and microstructure.

Task 3: Material Performance and Application

After the materials have been processed and machined, the next concern is to predict their subsequent performance, that is, their strength and resistance to fracture. Thus the models for material performance need to be developed and validated. These models will explicitly include such microstructural elements as inclusions, precipitates, and grain boundaries and will be based on several finite element methods developed at Brown University.

The first step will be to develop predictive models of damage initiation by either cracking or debonding of second-phase inclusions and precipitates. This modeling will be performed using a cohesive surface framework to model the interface between the inclusion (or precipitate) and the matrix and to model the initiation and growth of cracks within the second phase. Parameter studies will be undertaken to identify measurable and controllable features of the microstructure that are key for damage initiation. The results for damage initiation will be used in a modified Gurson model[1] to predict material performance. Of initial interest will be the prediction of performance in a suite of test specimens that give rise to different plastic strain-stress triaxiality histories so that the predictive capabilities of this modeling can be compared with experimental observations. Three-dimensional calculations of more complex geometries will also be performed to demonstrate the capability of predicting failure in component-like geometries.

At the same time, experiments will be performed using specimens that have been carefully designed so that their mechanical response can be fully modeled. These specimens will be pulled in tension to various loads and then sectioned so that the microstructure can be observed. Particular attention will be given to identifying the second-phase particles that are present in the material and participate in crack nucleation.

Task 4: Pilot Project

The proposed research will focus on track roller shafts as a pilot component. The track roller shaft represents a component with high-production-volume steel at Caterpillar. It transmits the weight of a tractor through the undercarriage (see Figure 1) and can be produced from either conventional steel (heat-treated for strength) or microstructurally improved microalloy steel. The use of microalloy steel has been demonstrated to reduce the cost and environmental impact of the heat-treatment stage, making it currently the preferred material in regions with high energy costs (such as Japan). The use of microstructure-level simulation and sustainability metrics to evaluate and optimize its environmental performance throughout the entire life cycle may lead to further improvements and serve as an example of the effectiveness of integrated methodology.

Figure 1. The tractor undercarriage receives the weight of the tractor (a) through a track roller shaft (b).

First, the entire life cycle of a track roller shaft made with a conventional 1500-series steel will be modeled, and the environmental resources needed throughout a component life cycle will be assessed. The chemical composition and processing map will be optimized to minimize the environmental impact and cost of the component. Then the modeling process will be repeated for using a microalloyed steel, which will be optimized for the same requirements. This study aims to provide optimum chemical compositions and processing road maps for a track roller shaft made with a conventional 1500-series steel and a microalloyed steel. In addition, the pilot project will quantify energy and environmental resources required for the entire life cycle of a track roller shaft made with the steels and processes mentioned above.

A critical component in this task, as well as in the others, will be the quantification of energy use during production of a part, and optimization of the proposed process to minimize energy usage. Caterpillar has already established a project called "Bridges to Sustainability," and NSF interns at

Brown worked in the summer of 2003 on this project. The tools developed by the NSF-sponsored project will be applied in this project to assess energy usage and savings for the processes used here.

Current Period Progress

Microstructure-Level Modeling of Machining

At the microstructural level, steel can no longer be treated as a homogeneous material. Different types of microstructures due to chemical composition and heat treatment cause the material to appear as a composite on the microscale. Thus material heterogeneity must be considered. Different microstructures—namely ferrite, pearlite, martensite, bainite, and tempered martensite—as well as inclusions, porosity, and precipitates, will have combined effects on the material behavior. By looking at deformation at the microstructural level, much detailed information can be obtained. Thus microstructure grains or colonies will be built into the model explicitly. A plasticity model based on dislocation interaction and evolution called the BCJ model will be used to describe the single-phase behavior of each microstructure. Owing to the nature of local high temperatures caused by mechanical deformation and high strain rate near the contact between tool and part, a material model should also be a function of temperature and strain rate.

Since material behavior is a function of temperature, the thermal field also turns out to be very important for this current simulation. A coupled thermal-mechanical scheme is adopted in the analysis methodology. It shows significant impact on chip formation. Friction-generated heat is assumed to be important traditionally; therefore friction-generated heat and heat transferred between the contact interfaces of the tool and part are also included in the model.

Machining test modeling input. Several orthogonal cutting tests have been done on different microstructures generated by different heat treatment operations. Microstructures before the machining operation have been recorded as modeling input. Microstructures in the chips and the machined surface after machining have also been checked for validation purposes. (These results were shown in this project's prior semiannual report.)

Microstructure evolution results. During the machining operation, individual microstructure grains and colonies will change significantly as a result of large shear deformation and even be broken into smaller grains or colony size. This microstructural change will affect the cutting process and the material properties after machining. The simulation results show steel with a ferrite/pearlite microstructure. The volume fraction of ferrite is about 30%, and the rest is pearlite. In an optical micrograph image, pearlite colonies are shown in black and ferrite grains are shown in white. Cutting was simulated for two speeds, 2m/s and 3.33m/s. Results for microstructure in the chip and the machining part from the simulation and test are shown in Figure 2 for the first speed. In the chip, grains are deformed in the direction of shear localization. Similar patterns of this deformation can be seen in both the simulation and the actual machining test. On the machined surface of the part, grains are separated by the cutting process and form a thin-layer shear zone. The simulation shows good agreement with testing.

Chip morphology. Different chip shapes can have an impact on the machining operation. Figures 2 and 3 show the chip shape under two different cutting speeds, for simulation and test. For the higher cutting speed, the chip appears to be more segmented. Also, chip thickness is reduced compared with the low cutting speed. Those changes are mainly due to different shear localization behaviors at the different cutting speeds. At high speed, the temperature increases locally because of the short transit time, which causes large local softening and a segmented chip. At low speed, heat generated by deformation will spread out and cause a more uniform temperature field. At the same time, the local temperature cannot go very high. A larger amount of material is softened to form the chip; this will cause the chip thickness to increase.

Temperature field. Material response during machining is highly dependent on the temperature. The temperature field is also very important for cooling during machining. In some cases, material can become welded onto the tool, a behavior that can be related to the temperature field. Simulation results for the temperature field are shown in Figure 4 for the two different cutting speeds. It can

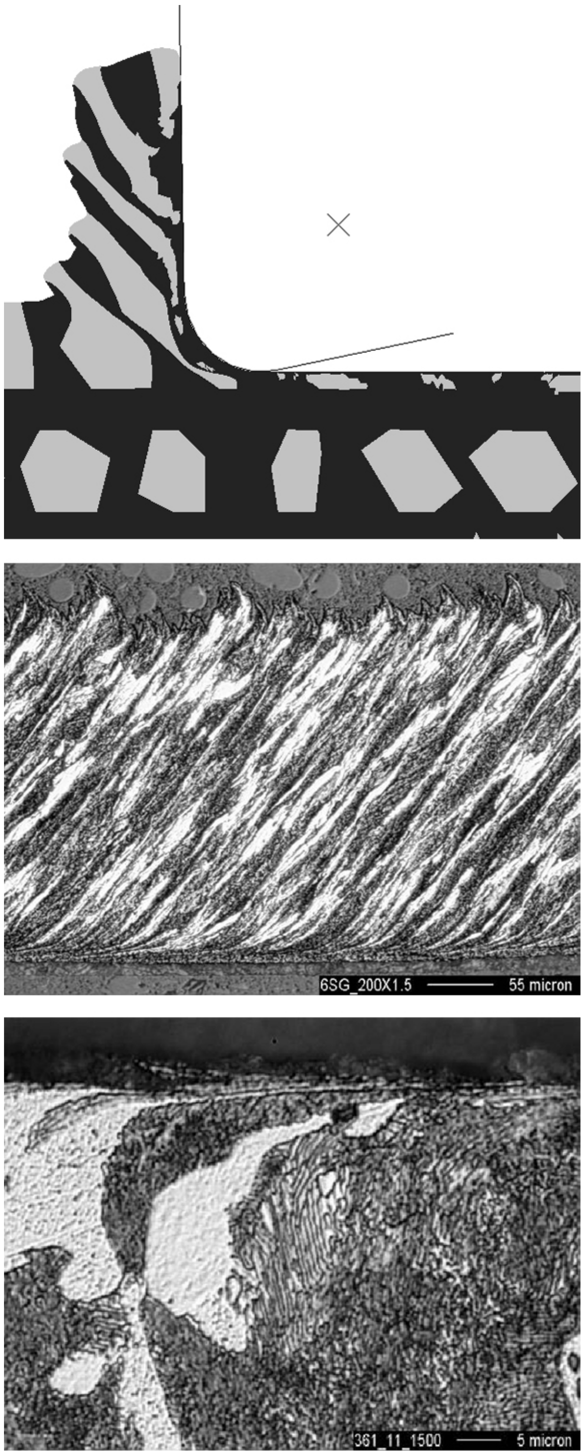

Figure 2. Microstructure evolution during cutting at 2 m/s: (top) simulation shows microstructure in chip and part; (middle) microstructure in chip after testing; (bottom) microstructure for part after testing.

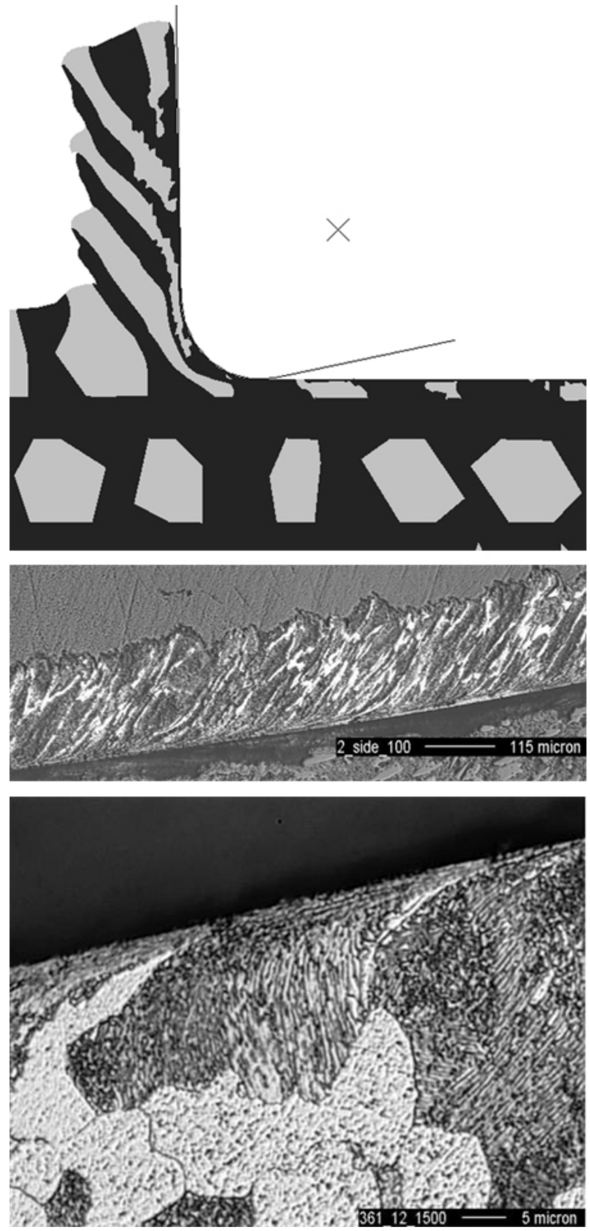

Figure 3. Microstructure evolution during cutting at 3.33 m/s: (top) simulation shows microstructure in chip and part; (middle) microstructure in chip after testing; (bottom) microstructure for part after testing.

be seen that the maximum temperature occurs slightly above the tool nose. This is normally where welding of material onto the tool can occur. For high-speed machining, temperature is more localized and has a higher maximum value.

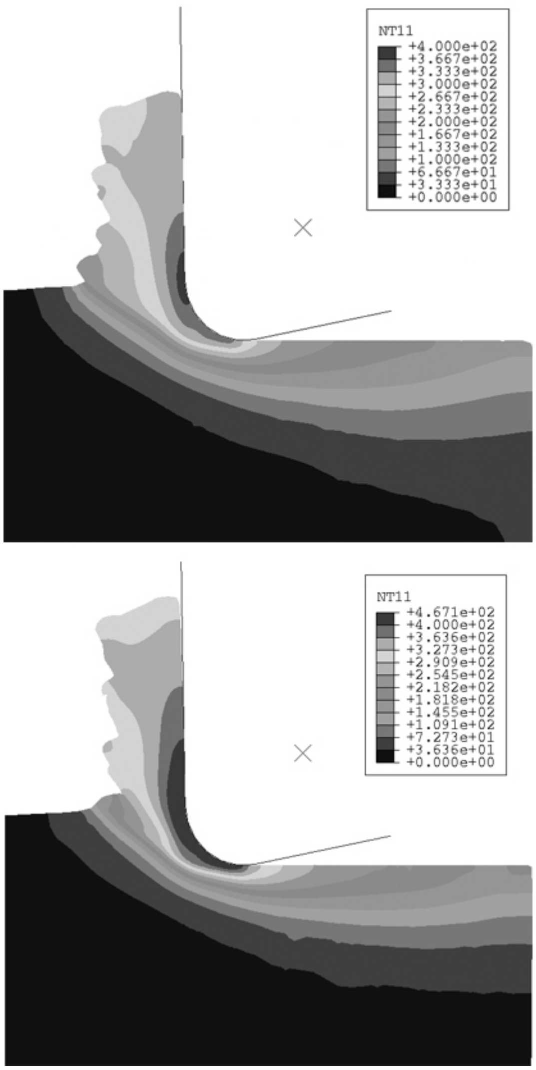

Figure 4. Temperature field for two different cutting speeds: 2 m/s (top) and 3.33 m/s (bottom).

By comparison, chip shape is shown in Figure 5 for an adiabatic situation. It shows a significant difference from the case with heat conduction. The segmented chip shape shows an indication of adiabatic shear band formation. It can be concluded that at this cutting speed, heat conduction must be considered.

Friction heat generation. Friction is another source of heat generation. A model was set up to account for heat generation by friction and account for the heat conduction between tool and part. A temperature field is shown in Figure 6 for cases with friction-generated heat and without. It can be seen that temperature increases directly as a result of the friction-generated heat.

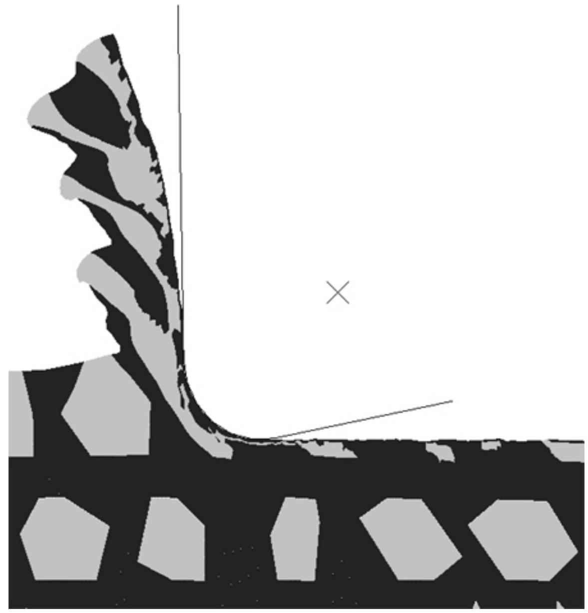

Figure 5. Chip formation for adiabatic condition at a cutting speed of 2 m/s.

Effects on cutting force. Figure 7 shows several cutting force predictions and testing results resulting from different conditions of cutting speed and friction.

The cutting force predicted in the simulation with a friction coefficient of 1.2 is in good agreement with testing results. In machining operations, the friction coefficient can vary from 0.6 to 2.0. Here, a constant value is assumed throughout the whole cutting time. Higher friction will increase the cutting force. At the extreme case of infinite friction, the cutting force goes up by about 10% compared with the friction coefficient of 1.2. The cutting force will also be affected by cutting speed; higher cutting speed results in a lower cutting force for the same material.

Conclusions. A simulation model of the machining process at the mesoscale microstructure level has been set up. The model includes microstructural features such as grains and colonies. The material model is related to dislocation motion and interaction. A fully coupled thermal mechanical setup gives more realistic thermal field and chip formation. This model shows its capabilities in accurate prediction of chip shape, temperature field, and cutting force directly based on material microstructure. This simulation tool can also be extended

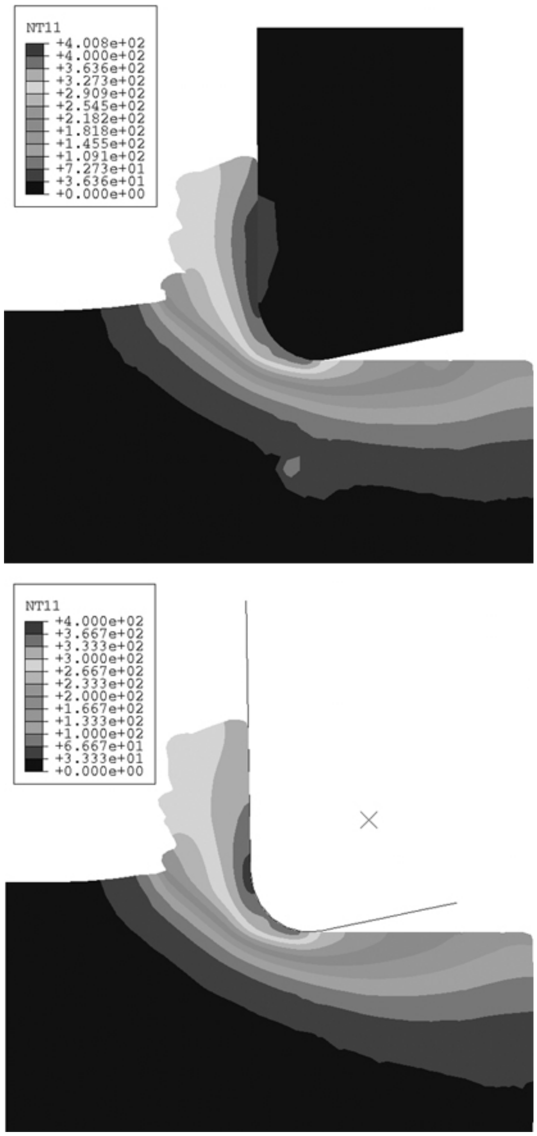

Figure 6. Temperature field with friction-generated heat (top) and without (bottom).

to simulation of other manufacturing processes fairly easily.

Future work. Currently, material properties have been characterized for only two types of microstructures, ferrite and pearlite. More material characterizations are needed; they are already included in another parallel material characterization project. A proper model for friction is needed for accurate predictions.

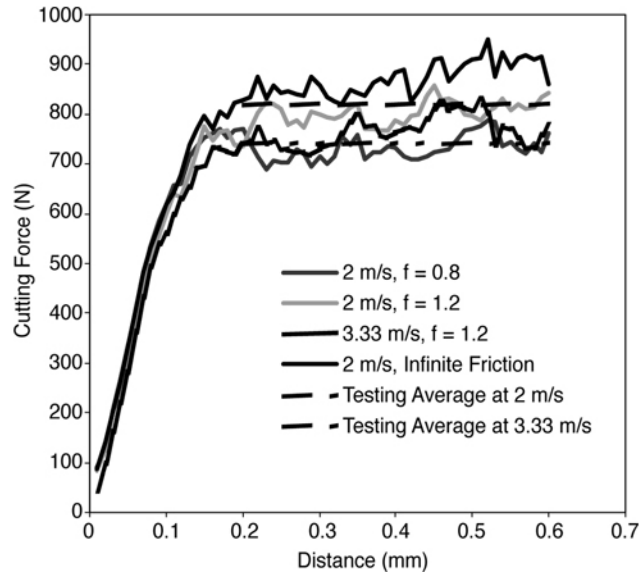

Figure 7. Cutting force vs. distance.

Development of Microstructure Evolution Module Using Cellular Automata

As the first step in developing a robust microstructure evolution module for simulation of heat treatment, a single austenite grain transforming to multiple ferrite grains upon cooling was studied using cellular automata (CA) techniques coupled with a Monte Carlo approach. The cellular automation used in this study has been developed in two dimensions on a square grid, representing an austenite grain. The computation domain is one austenite grain with an 'average' grain size. The general approach is to calculate the total energy for a given cell in the austenite phase and the ferrite phase first. Then a probability is determined for that given volume to change from austenite to ferrite. The probability is calculated using Boltzmann statistics. Initial results (Figure 8) have shown that the CA modeling technique can be successfully used for phase transformation modeling that will provide information on microstructure evolution. This information can be combined with an MLS model to provide explicit microstructure information for material properties calculation in the heat treatment simulation.

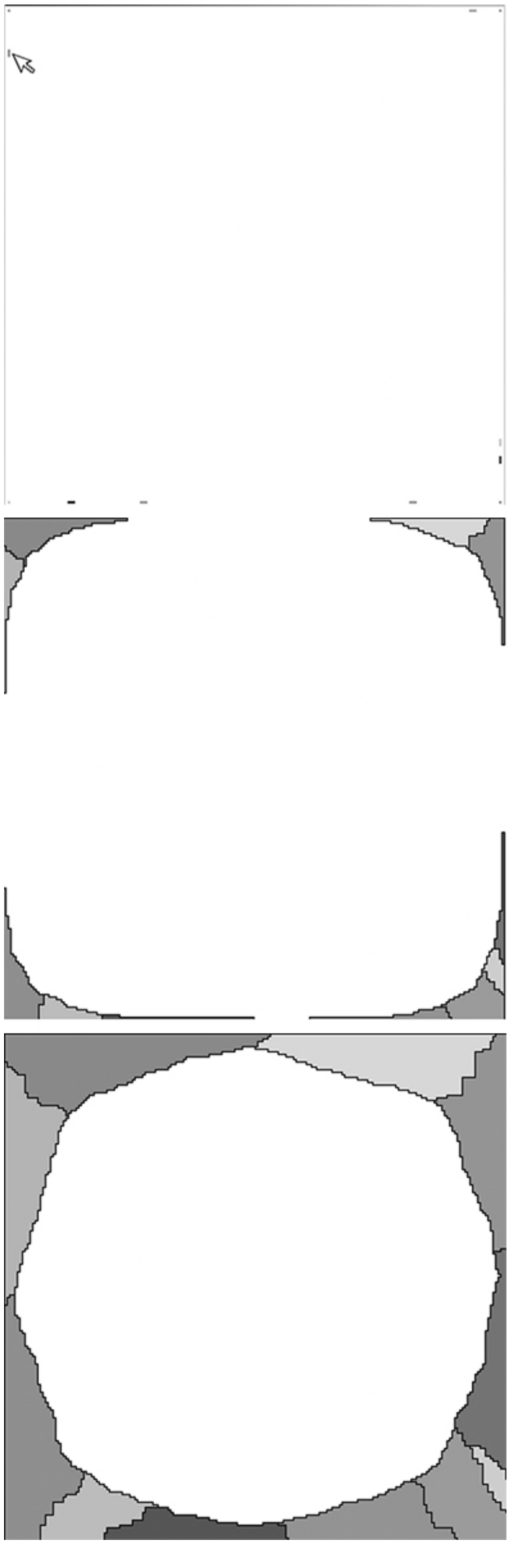

Figure 8. Initial nuclei site of ferrite in austenite grain (top); ferrite grain growth (middle); ferrite grains when eutectoid temperature is reached (bottom).

Material responses during quenching of steel. The most critical issue in modeling heat treatment is the multiphase material constitutive relationship on a highly heterogeneous material found in a heat treatment process. The traditional approach has been to use an elastic-plastic or elastic-viscoplastic model based on a liner rule of mixtures (RM) or an average material property model. For microscale-level simulation, material properties for each individual phase can be accurately described according to the result of each individual phase characterized in a parallel project. Explicit microstructural descriptions can also be obtained from a microstructure evolution simulation based on stochastic modeling of microstructure. Using a macro/micro modeling technique, material properties for the multiphase structure during heat treatment can be calculated according to the MLS model. As an initial step, effective yield strength for 1045 steel with different constituent fractions of martensite and austenite phases was evaluated. These material properties for the martensite and austenite phases are given in Table 1.

Table 1. Material properties for martensite and austenite

Phase	E(GPa)	ν	σ_y@ ε=0(MPa)	σ_y@ ε=0.04(MPa)
Martensite	214	0.3	1550	2339
Austenite	196	0.3	189	289

A 2-dimensional finite element model (FEM) with random shape and orientation was created for the martensite and austenite phases. The mesh for 31% martensite (dark grey) + 69% austenite (light grey) is shown in Figure 9. Periodic boundary conditions were prescribed at the edges by considering (1) symmetry along the left and bottom edge, (2) constraint of the nodes on the top edge to exhibit the same Y-displacement, and (3) constraint of the right-edge nodes to exhibit the same X-displacement. Displacement loading was applied to the right edge. The mechanical analysis was performed at room temperature using plane stress quadrilateral elements in ABAQUS.

Figure 10 shows the stress-strain plot for different fractions of martensite and austenite. The solid line depicts the results from the FEM study, and the dotted line represents the yield strength values calculated using the linear RM. Figure 10 shows clearly that the composite of martensite and austen-

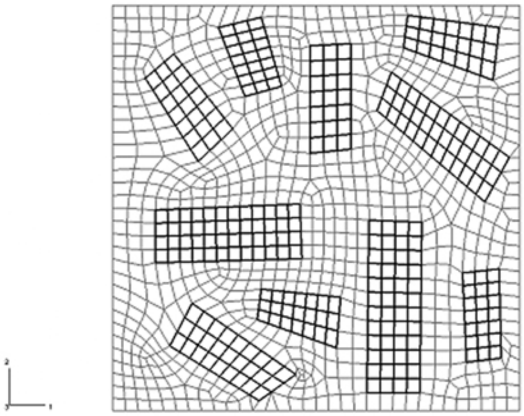

Figure 9. Finite element mesh.

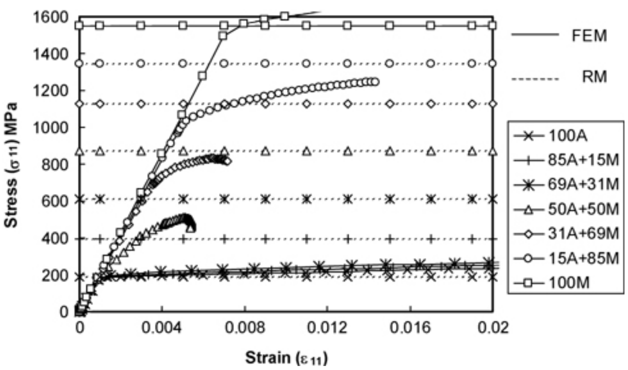

Figure 10. Stress-strain plot for different fractions of martensite (M) and austenite (A) phases. FEM results are represented by the solid line and dotted line shows the yield strength calculated using rule of mixtures (RM).

ite shows considerably lower values of yield strength from FEM than the RM values. The difference is significant (200 to 300%) at higher fractions of austenite (85% A, 69% A and 50%A). At higher fractions of martensite (85% and 69% M), the difference between the yield strength values is around 50%. This difference decreases at higher fractions of martensite, primarily because of the high yield strength of 100% martensite compared with 100% austenite.

With this MLS approach to describe each individual phase explicitly, transformation-induced plasticity, a concept generally used in continuum models, can be explicitly modeled with great accuracy. The next step would be to incorporate material characterization results with the microstructure evolution model to implement an MLS scheme to provide material properties for a heat treatment simulation with a macro/micro model approach.

Integrated heat treat model development. Heat treatment simulation tool development is a key enabling part of the road map for resource-efficient steel components, as heat treatment provides the necessary material properties for many steel parts with great efficiency and minimum resource costs. In the case of the track roller shaft, quenching and tempering is applied after the forging process. Then induction heat treatment is applied again after the quenching and tempering process to create material properties that meet roller shaft design performance requirements. The manufacturing process is completed with a finish grinding after the induction process. To provide the final microstructure and predict roller shaft performance, an integrated computation method was developed to simulate the quenching/tempering process and the following induction hardening process. Microstructure and residual stress predicted from the quenching/tempering process were fed into an induction-hardening simulation model as input. The final microstructure, residual stress, and distortion could be predicted after the induction hardening process.

Conclusions

This research has successfully accomplished its first-year goals. The microstructural characterization and mechanical property tasks are proceeding on schedule. These efforts have been completed for the initial microstructures of the SAE 1045 and 15V45 steels in support of the heat treatment and machining simulation code development activities. In addition, the machining tests at two machining speeds for both alloys were accomplished. Finally, preliminary machining modeling results have been shown to qualitatively predict the chip morphology, including adiabatic shear band formation, for the as-quenched microstructure of the 15V45 steel alloy.

References

1. A.L. Gurson, “Continuum Theory of Ductile Rupture, Void Nucleation and Growth,” *Journal of Engineering Materials Technology*, **99**(2) (1977).