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Using Simulation for Heat Treat Process Design: Matching the Quenching Process with Steel Grade and Product Geometry

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Abstract

The performance of steel parts is heavily dependent on the heat treat process applied. The alloy content of the steel establishes the steel hardenability. The severity of the quench establishes the local temperature history throughout the body of the part. In combination, the steel hardenability and the quenching process determine the final microstructure, mechanical properties, residual stress state, and the performance of the part.

The residual stress state, especially the surface stress state is a significant factor in affecting fatigue life of the part. The steel hardenability and quenching practice can be adjusted to enhance residual surface compression and improve the fatigue life of a component. Computer simulation of the heat treat process that includes calculation of the metallurgical phase transformations during the heating and cooling processes offers a method for scientifically designing the heat treat process and selecting the steel alloy to optimize the performance of a particular product. In this paper, the DANTE® heat treat simulation software will be used to demonstrate this design methodology for a spur gear.

Keywords: *quantitative characterization, heat treat simulation, phase transformation kinetics, dilatometry, residual stress*

1. Introduction

Alloy selection for a particular part is dependent on the application – this is a known fact, but how is the selection actually decided upon? Experience with similar parts and the alloy(s) used in those parts typically is the basis of selection. This also is the basis of process definition for producing the part. A particular steel alloy is heat treated using a particular recipe. The metallurgical bases for alloy and process selection are commonly the Jominy hardenability test and the ideal diameter calculation (DI) for the steel chemistry [1-3]. There is difficulty of using DI values and Jominy hardness data quantitatively in actual part design because they are meant to check the response of the chemistry to specific quench conditions. In part manufacture, the geometry, process conditions and the steel alloy are all important in determining the hardness, stress state and final dimensions.

Finite element based tools such as DANTE that include phase transformation calculations as well as thermal, stress and displacement calculations provide results that are useful for alloy selection, part design, process specification and final part performance predictions. Because the simulation tools have not been widely used, there is not a wealth of data available for applying these powerful tools. This paper discusses some of the necessary material models for simulating heat treatment of steel parts, the data and sources of data that are needed for the models, and the model results. The software used in this paper is DANTE. The models and the material parameters that drive the models are specific to DANTE, but the tests and data from which the parameters are derived are generic to heat treat simulations.

2. Phase Transformation Kinetics Models and Data

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The phase transformation kinetics equations in DANTE have been presented in detail [4, 5]. The kinetics equations are rate based, and the general form includes a temperature based mobility term, an exponent that is material and phase dependent, and multipliers of the remaining austenite phase fraction. For heating transformations, the main aspects are austenite formation from any mixture of tempered martensite, bainite, pearlite, and ferrite. For cooling transformations, the main aspects are austenite decomposition to any mixture of martensite, bainite, pearlite and ferrite.

Inherent in these calculations is either the dissolution or the formation of carbides and the effects of prior microstructure on both the temperature and rate of transformation. The data contained in the DANTE database is a set of parameters that drive the kinetics equations for transformations on heating or cooling, and these can be derived from either dilatometry experiments or published TTT/CCT data. The parameters derived from dilatometry are preferred because the experiments include transformation strain data, thermal expansion data, and TRIP effect, and most likely, the experiments are more accurate than published TTT/CCT data. The phase transformation models effectively encompass the DI and Jominy hardenability calculations and provide additional details about the sequence, rate and magnitudes of the transformations that occur during the heat treatment process.

Dilatometry is used to determine critical temperatures and coefficients of thermal expansion for the metallurgical phases. Two types of tests are used to characterize phase transformation behavior during cooling. ASTM specification A1033 describes these tests and the data that are collected from these test procedures. It does not, however, describe how to determine model parameters from the raw data since available software packages use different equations to mathematically describe the phase transformations. The specification focuses on collecting data for austenite decomposition transformations, but the principles apply equally well to determination of austenite formation kinetics. Both types of tests start by heating a sample into the austenite range and holding at temperature for a representative time period. For isothermal tests, the austenitized sample is quenched or cooled rapidly to the test transformation temperature, quickly stabilized at that temperature and held for a particular time period, and finally rapidly cooled to ambient. The data collected are time, temperature and strain; the strain represents the volume change due to phase transformations if the temperature is well controlled. As the austenitic sample is held at the test temperature, nucleation and then growth of a diffusive phase will occur as evidenced by strain. From the recorded strain and time data, the rate and amount of the phase transformation are determined.

The other type of dilatometry test involves continuous cooling at a controlled rate from the austenitizing temperature to ambient. In this test both diffusive and martensitic transformations may occur. The phase transformations are evidenced by changes in the slope of the strain vs. temperature curve as shown in Figure 1.

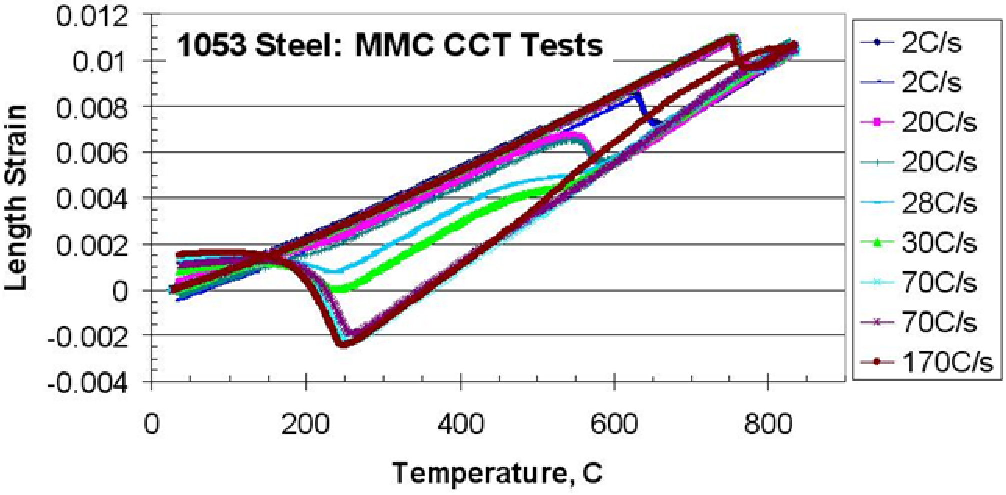

Figure 1: Continuous cooling dilatometry tests of AISI 1053

The strategy used by DCT to determine the parameters that drive the DANTE kinetics equations is based on optimization as shown in Figure 2. First the data are segregated by type of phase formed. This is most easily done using isothermal test data where the test temperature can be used as the phase identification agent. Phase transformation model parameters are determined for these segregated data sets. Then, all of the data are co-mingled and a final fitting is performed. Because there is no unique solution in determining the equation parameters, a considerable amount of checking is required to ensure that the determined parameters are reasonable. For DANTE, the final result is a data set for the alloy being characterized that includes parameters for all the diffusive and martensitic transformations likely for that steel and the processes used to harden it.

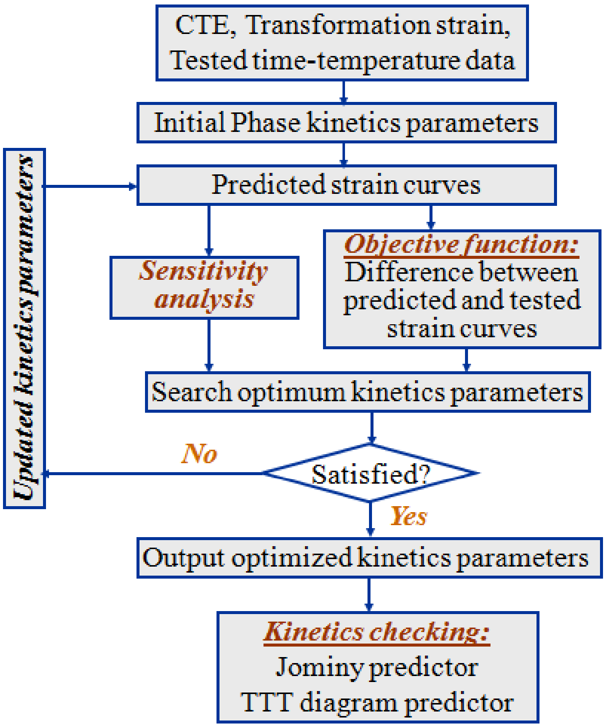

Figure 2: Schematic flow chart for fitting phase transformation kinetics

If it is not possible to perform dilatometry tests, the kinetics parameters must be derived from some other data source such as published TTT/CCT diagrams. These diagrams are incomplete in terms of the data that is needed, so some necessary assumptions are required. First, there is no strain data available in the TTT/CCT diagrams, so thermal and transformation strains from a similar steel grade must be used as estimated data. Second, the amount of information for phase evolution is typically sparse, i.e. 1%, 50% and 99% lines and no others, so estimates of rates of phase fraction development must be made. Then, parameter determination can proceed as described above.

The final checks on model parameter accuracy include simulating the actual dilatometry tests to document that the predictions accurately reproduce the test data, and simulation of a well known test such as the Jominy test to determine that the results are reasonable. The Jominy test, in particular, is good because all of the kinetics parameters are normally exercised because of the wide range of local cooling rates in the Jominy test bar.

3. Mechanical Behavior Model

Because the material state and the accompanying physical properties change during heat treatment processes, the mechanical model in heat treatment simulation software must be capable of describing all of the possible combinations of metallurgical phases that may occur during heat treatment. As discussed in reference [4], the mechanical model in DANTE is based on the Bammann-Chiesa-Johnson (BCJ) internal state variable (ISV) model. A mixture methodology is used to describe the behavior of multiple phase interactions during the heat treatment. The ISV parameters are fit from conventional isothermal and strain rate controlled tension and compression tests. These parameters, in combination with the phase transformation kinetics parameters drive the FE calculations and determine the accuracy of the heat treatment simulation in terms of residual stress and distortion.

It may be difficult to get clean separation of phases for the mechanical tests. For low hardenability steels, it is often not possible to determine stress-strain data for austenite at intermediate and low temperatures because ferrite and pearlite form too rapidly as the austenitized sample is cooled to the test temperature. For many steel grades, bainitic samples may also have amounts of ferrite and pearlite. This means that certain assumptions must be made in order to determine the plasticity parameters used in the mechanical model. These problems are true for any mechanical model used for heat treating simulation.

During the quenching process, the steel part will experience localized thermally induced stresses, and transformation induced stresses. The surface of the part will experience initial tension as it cools faster than the core of the part. As the surface or near-surface layers transform, the tension will be relieved and may transition to surface compressive stress due to transformation and restriction of the surface layer volumetric expansion by the underlying interior. As the subsurface transforms and volumetrically expands, the surface layer may again reverse its stress state to tension. Stress reversals are inherent to the quenching process for steels, and, if possible, stress reversal tests and interrupted loading tests should also be part of the mechanical test program. These tests allow hardening of the phase yield surfaces to be accurately characterized.

From the experimental tests, DANTE uses a sensitivity based optimization method to determine the mechanical parameters for each phase. The procedures for determining the mechanical model parameters are similar to the kinetics fitting procedures. Test data are segregated by phase and parameters are determined. Because the solution is not unique, the parameters that are determined must be checked to see that they accurately predict the test data and also produce reasonable behavior for known cases, including residual stress values and dimensional change. The parameters determined from the fitting are stored in a file that will be accessed during DANTE simulations. Besides mechanical parameters, the thermal conductivity and specific heat data, thermal expansion data, and latent heat data are also contained in these database files.

4. Heat Transfer During Quench Hardening

The third main process variable is heat transfer boundary conditions, focusing on the quench hardening process. Much has been written about the phenomena during immersion quenching in oil, polymer or plain water, i.e. film boiling, nucleate boiling and convective cooling. The heat transfer during high pressure gas quenching has also been getting attention in recent years. It is sufficient to say that an accurate characterization of the heat transfer on all the surfaces of a part is necessary for accurate simulation. The surface heat transfer establishes the internal cooling of the part and the sequence and nature of the phase transformations that occur.

Accurate heat transfer data can be derived from thermal probes and parts instrumented with thermocouples. Either inverse FE methods or sensitivity-based optimization methods that run forward FE simulations iteratively with modification of heat transfer coefficients occurring between iterations may be applied. However, care must be taken to ensure that the thermocouple wires are not influencing the local heating and cooling, and that the locations of the thermocouples are appropriate to capture the steep thermal gradients that occur. Probes and real parts with multiple thermocouples at various depths are preferred for the characterization.

5. Comparison of 9310 and Pyrowear 53 Steel Gears for Two Quenching Processes

AISI 9310 and Pyrowear 53 are high hardenability, carburizing grades of steel, see Table 1.

Table 1. Steel Chemistries

	C,w/o	Mn, w/o	Si, w/o	Ni, w/o	Cr, w/o	Mo, w/o	Cu, w/o	V, w/o
9310	0.08/0.13	0.45/0.65	0.2/0.35	3.0/3.5	1.0/1.4	0.08/0.15	-	-
Pyrowear53	0.1	0.35	1.0	2.0	1.0	3.25	2.0	0.1

Spur gears used to evaluate tooth bending fatigue strength are being manufactured from these steelsfor a current project. The tip diameter of the gear is about 95mm, the tooth thickness is about 6mm. The gear has 28 teeth, and the gear geometry is shown in Figure 3.

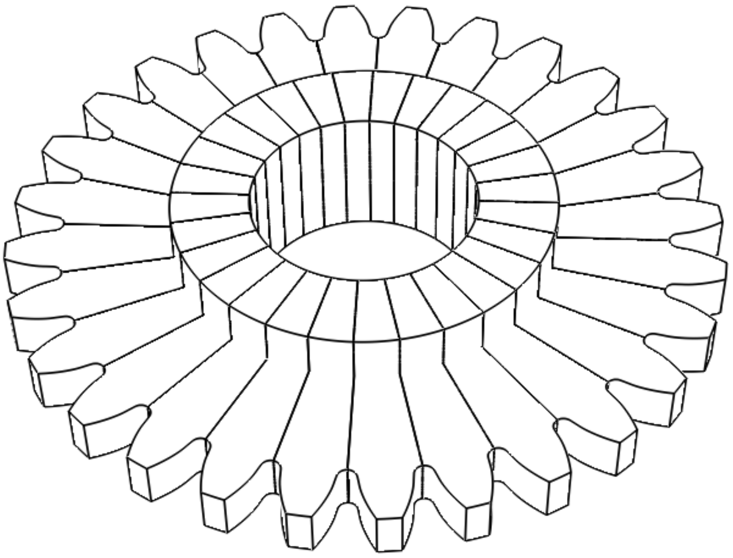

Figure 3: Gear geometry with 28 teeth: tip diameter 95mm; tooth thickness 6mm.

The gear tooth surface is carburized, and all other surfaces are copper plated during carburization. Two quench processes are being evaluated and both are discussed in this paper, conventional oil quenching and intensive quenching. The two heat treatment schedules that were modeled are given in Table 2. For comparison, all other process steps are the same. The only difference is the quenching method. Note that the lower temperature tempering was not included in the models. Important results include hardness and residual stress profiles and distortion. Because improved tooth bending fatigue strength is a goal, residual compressive stress around the tooth root are especially critical.

Table 2. Heat Treat Practice

	9310	Pyrowear 53
Carburize	8 hrs. at 927° C	8 hrs. at 927° C
Subcritical Anneal	4 hrs. at 621 C	4 hrs. at 621 C
Austenitize	912 C	912 C
Quench	80 C Oil or Intensive Water Quench	80 C Oil or Intensive Water Quench
Deep Freeze	-80 C for 1 hr.	-80 C for 1 hr.
Double Temper (not modeled)	150 C	230 C

The tangential surface stresses are reported in Table 3 because this is the direction most highly stressed during tooth bending and has the most significant effect on bending fatigue*[6]*. For both grades, the stress in the root fillet is more compressive that at the root center due to the geometry effect. Interestingly, the predicted magnitude of compressive stress in the Pyrowear 53 gears is higher than that in the 9310 gears.

Figure 4 shows the hoop (tangential) residual stresses after quench and deep freeze at the root fillet location. The X-Axis in Figure 4 is the depth from surface of the fillet, and Y-Axis is the hoop or tangential stress plotted using a local cylindrical coordinate system. Figure 4 shows that the two steel grades have significant difference in responding the quenching process. Pyrowear53 gear ends up with deeper and higher residual compression comparing with the 9310 gear.

Table 3. Tangential Surface Residual Stress (Unit: MPa)*

Process Quench Method	9310 Spur Gear		Pyrowear 53 Spur Gear	
	Root Center	Root Fillet	Root Center	Root Fillet
Oil Quench (predicted)	-506	-784	-775	-1099
Intensive Quench (predicted)	-552	-707	-1061	-1349

* at room temperature after deep freeze

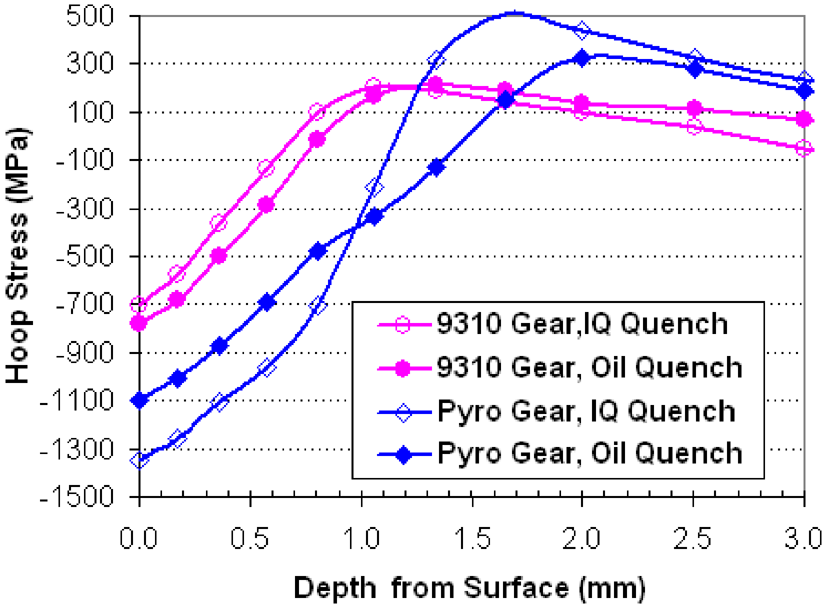

Figure 4: Hoop residual stresses in terms of depth at the gear root fillet location

There are some differences between the steels in terms of response to quenching. The data in the DANTE database for martensite transformation starting temperature (Ms) reports that Pyrowear 53 has a wider range of Ms over the carbon levels from core to case than 9310 by 50 °C. The martensitic phase transformation finishing temperatures (Mf) of the two steels with base carbon also have significant difference. This will cause a difference in the microstructural evolution and resultant stress state. The low martensite finish temperature in the high carbon carburized case for both steels results in retained austenite at room temperature. Table 4 contains the retained austenite volume fraction amounts for the high carbon case of both steels after quench practices. Before deep freeze, oil quenched gears have higher retained austenite than intensively quenched gears for both steels. Also, Pyrowear 53 gears have almost double the retained austenite content of 9310 gears before deep freeze. After deep freezing, both steels have less that 4% retained austenite. Possible reasons for the differences in predicted residual stress are being investigated, and XRD measurements to determine stress levels will be performed for theses gears. For other spur gears of similar face widths and steel grades, stress measurements based on XRD and those predicted using DANTE have been in close agreement.

Besides chemistry and its effects on phase transformation behavior, the geometry and its effect on cooling non-uniformity also affect both dimensional change and stress state. For a spur gear, radial and circumferential dimensional changes vary from the root center to the tooth tip center. Simplistic thinking about the direction of dimensional change upon cooling dictates that the root center should move toward the gear center while the flank faces on the tooth will move toward the centerline of the tooth and toward the gear center. Reality is more complex as heat transfer from the faces of the gear will add thickness dimensional change, and the volumetric expansion that accompanies martensite formation will add reversals in part movement. Differences of the martensitic transformation timing between the two steel grades will result in both dimensional differences and stress differences.

Table 4. Predicted Retained Austenite Volume Fractions in Carburized Case

Steel & Quench	At Room Temperature After Quench	At Room Temperature After Deep Freeze
9310 – Oil	8 to 9%	3.0 to 3.4%
9310 – IQ	8 to 9%	3.3 to 3.5%
Pyro53 – Oil	14.7 to 19%	3.4 to 4%
Pyro53 - IQ	12.5 to 16%	3.5%

For the intensive quenching simulation, only one quenching condition is reported in this paper. From Table 3, the benefit of intensive quenching for Pyrowear 53 is evident by the higher compressive stress in the gear root and fillet regions. For 9310, there is insignificant difference between oil quenching and intensive quenching. Just judging by the root fillet residual stresses, oil quenching would be the preferred method. With simulation, alternative quench practices can be investigated, and, indeed, an alternative intensive quenching practice was predicted to produce higher surface compressive stress in the entire root region than oil quenching.

6. Summary

- In addition to the main variables of mechanical behavior, phase transformation kinetics and heat transfer, geometry plays a significant role, not just in terms of section thickness, but also in terms of part features.
- The quench hardening process must be matched with the steel's hardenability and part geometry for optimum performance. The difference in response for the two steels to the same quenching conditions demonstrates this principle.
- While complex in terms of process physics and data requirements, simulation of quench hardening of carburized steel parts provides great insight into metallurgical events that occur, and also provides part conditions that can be carried forward for accurate performance prediction.

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