Material Data Requirements for DANTE Modeling

To model heat treatment processes for any steel alloy, a lot of data is required for that alloy because of the wide range of temperatures, rates of change and the resulting metallurgical phase possibilities that must be addressed by the models. If a process like carburization or nitriding is involved, the chemistry gradient and its affect on properties must also be characterized. The critical properties include metallurgical phase transformations, and the mechanical and thermal properties of each phase over the range of temperatures that the phase may exist.   Of these properties, characterization of the solid-state phase transformations that occur in the steel alloy are most important.

At this time, DANTE considers these steel phases: ferrite, pearlite, upper bainite, lower bainite, martensite, tempered martensite, and austenite. Spheroidization of carbides is not considered, so a spheroidize-annealed microstructure would be considered pearlite. Grain size is addressed indirectly by modification of alloy mobility parameters. The same is true for variations of alloy content for variations within a steel grade. For more dramatic variations, such as Mn modified steels, either mobility or carbon level or both can be adjusted to account for changed hardenability.

Dilatometry Data to Determine Phase Transformation Parameters & CTE

The phase transformation kinetics models in DANTE predict the effect of heating and cooling on the microstructural make-up of steel parts during heat treatment. Both diffusive and martensitic transformations are modeled. The preferred method for characterizing the phase transformation behavior of steel alloys and determining the parameters in DANTE's transformation kinetics database is by fitting dilatometry test data.   Key data that are determined are the temperature ranges over which the transformations occur, the related transformation strains, the rates of transformations, and the coefficient of thermal expansion of the individual phases.   The parameters stored in the database allow metallurgical phase fractions, dimensional change, and stress state to be calculated throughout the heat treatment process.

There are several types of lab machines that can be used to produce dilatometry data. The equipment must be able to heat and cool the test coupon under controlled conditions so that thermal gradients and resultant stress gradients and phase gradients are minimized. Each type of equipment has sensors to measure either length or diameter or both while the sample is being heated or cooled at controlled rates. Because the steel alloy is being characterized for heat treatment, i.e. quench hardening, temperature changes must cover fairly high rates. Data collected include time, temperature and dimensional change.   From dimensional change the strain is calculated.

For diffusive phase formation characterization, i.e. ferrite, pearlite, bainite and austenite formation, isothermal tests are favored.   A dilatometry sample is stabilized at one temperature and then quickly heated or cooled to a particular temperature and held at that temperature for a period of time to determine if a phase change will occur.   The data collected includes time, temperature and dimensional change, especially during the holding

period. For example, by testing over a range of isothermal holding temperatures at 25 C temperature intervals during cooling from austenite, the phase transformation parameters for ferrite, pearlite and bainite can be determined.

Martensite formation requires that cooling be continuous, so tests with cooling at well controlled rates from say 2 C/s to 150 C/s need to be performed. These data will also provide additional data for diffusive phase formation, as the slower cooling rates will typically experience a partial transformation to one or more of the diffusive phases before reaching the martensite start temperature.

The isothermal and continuous cooling tests will determine the transformation types, temperature dependence, formation rates, and transformation strains for both diffusive and martensitic phase formations for the alloy being characterized. Approximately 24 samples of a size 100 mm long x 6 mm diameter (4"L x 0.25"ϕ) will be needed.

We have developed utility software for determining phase transformation parameters from dilatometry data. While the mathematical form of our kinetics models is complex, there is no unique solution in determining the kinetics parameters. User experience followed by considerable testing of the datasets are required to produce a good set of kinetics parameters for a material.

Determining Mechanical Datasets for DANTE Analysis

DANTE uses an internal state variable mechanical model that balances hardening and recovery. Mechanical constants that characterize each phase are determined from isothermal tension and compression tests that are strain rate controlled. Many laboratories and universities have the equipment needed for these tests. The main difficulty is controlling the microstructure so that only single phases are being tested.

For each phase of consequence, tests must be run. Austenite can easily be tested at high temperatures, but it may be difficult to get test data at temperatures below A_{E1} if the diffusive phases form quickly. Also, it may not be possible to isolate ferrite and pearlite phases from each other. Testing of the combined phases can be done, with the results analyzed as a composite. Bainite properties are highly dependent on the temperature of formation, so this must be included in the test matrix if bainite is a dominant phase in the part that will be modeled using DANTE. Martensite can usually be tested at room temperature and temperatures up to typical tempering temperatures to determine its mechanical constants.

For steel grades, the internal state variable constants fit from the tension and compression tests are determined using a DANTE utility program called MCFIT. There is a total of 27 constants for each phase, and these constants describe basic yielding, rate dependent yielding, local and global hardening and softening mechanisms, and creep behavior. Temperature, strain rate and carbon dependencies are covered by these parameters. The fitting is automated using MCFIT, but fitting is not trivial. There is no unique fit, so many variations of datasets for the same test data are possible, and experience is required to

determine the most appropriate dataset. Because of this complication, most DANTE users should not fit mechanical test data without assistance from DANTE Solutions. For this reason, the standard database files, which are contained in the STD subdirectory of the supplied database DATABASEDB3_6, cannot be modified.

The basic procedure for these tests is to first austenitize the test sample, and then quickly cool to a test temperature. If the test is for austenite properties, it should be performed immediately. If the test is for a transformation product, the sample should be held at temperature until the transformation has finished. For this reason, kinetics testing should precede mechanical testing. Testing of martensite requires that the austenite completely decompose to martensite prior to testing. Also, it can be difficult to avoid tempering of the as-quenched martensite to get properties above room temperature of as-quenched martensite.

Both elastic and plastic mechanical properties need to be determined for the steel phases. Because the elastic properties do not change appreciably with changes in phase, DANTE treats Young's modulus and the elastic Poisson ratio as functions of temperature only. However, the plastic properties of each phase must be determined over the range of temperatures, strain levels, and strain rates experienced during heat treating processes. We recommend that at least two strain rates be tested for austenite, pearlite and bainitic microstructures. Martensite testing will require compression tests. To minimize costs, the number of tests can be reduced to a bare minimum - three isothermal tests for austenite at the two strain rates (3 temps. x 2 rates x duplicate tests = 12 samples). Tests for pearlite, upper bainite and lower bainite can be conducted at two temperatures, again at two strain rates (3 phases x 2 temps. x 2 rates x duplicate tests = 24 samples). Martensite can be tested using compression tests at room temperature and at a representative tempering temperature (2 temps. x 1 rate x duplicate tests = 4 samples). The 40 test bars are each 127mm long x 12.7mm diameter (5"L x 0.5" ϕ).

Ideally, the elastic modulus and elastic Poisson's ratio should be determined over the range of pertinent temperatures.

For further information on the Bammann-Chiesa-Johnson state variable model see the following paper:

D. Bammann, et al., "Development of a Carburizing and Quenching Simulation Tool: A Material Model for Carburizing Steels Undergoing Phase Transformations," **2nd International Conference on Quenching and Control of Distortion**, eds, G. Totten, et al., ASM International, Materials Park, OH, pp 367-375, 1996.

Other papers by Doug Bammann, Mike Chiesa, Mark Horstemeyer, or Vince Prantil can also be found that discuss this model.

A final word is necessary since the steel alloy during heat treatment often exists as a composite, that is, it is a mixture of phases. DANTE contains a mixture law that calculates the mechanical behavior of the composite alloy. This law cannot be the

simplest form, a linear rule of mixtures, since the mechanical behavior of the individual phases is so different.

Thermal Property Determination

Thermal conductivity and specific heat capacity should be determined for each microstructural phase present during quench hardening. Again, to minimize testing costs, values for thermal conductivity and specific heat can be estimated from values for similar alloys or from handbook data. For example, the thermal conductivity of ferritic ductile iron is approximately 36 W/(m*K) and pearlitic ductile iron is about 20% lower.   Knowing differences in thermal behavior for steel phases and the effect of temperature on these properties can aid us in estimating the values for ductile iron phases.