# MULTI-SCALE FINITE ELEMENT MODELING AND MICROSTRUCTURAL OPTIMIZATION OF CAST HIGH SPEED STEEL FINISHING ROLLS <sup>1</sup>

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### **Abstract**

A detailed microstructural evaluation was conducted on a series of radial samples from the shell of high speed steel (HSS) work rolls produced by centrifugal spin casting. Continuous local transformations were simulated using FEM and Microstructural observations from production rolls thermodynamic predictions. validated non-linear heat transient results and actual thermo-processing data. FEM sub-structuring and image processing techniques were implemented to aid in the development of a multi-scale model to simulate the local response of an individual microstructural constituents, i.e. carbides and/or matrix, under heat treatment (HT) conditions. The proper as-cast structure is a necessary precursor to facilitate microstructural evolution and optimization during subsequent final hardening. Fine as-cast microstructures promote increased kinetic response during final hardening. Preliminary HT offers an additional degree of microstructural conditioning, accelerating the kinetics during final hardening. Austenitization temperatures and times were adjusted, facilitating increased dissolution and decomposition of carbides, ultimately enriching the alloy content of the matrix. As a result, the matrix hardness and strength were increased in comparison to conventionally hardened cast high speed steel roll material. A non-conventional approach was designed to optimize the response of the high speed material to HT.

**Key words**: HSS rolls; Carbide dissolution; Austenitization; Multi-scale modelling.

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# 1 INTRODUCTION

The heat treatment process plays a vital role in the processing path of a ferrous based component. The properties of steel are a function of the material microstructure, which is determined by the heat treatment.

High speed tool steels are heterogeneous and hypereutectoid by nature, consisting primarily of a mixed tempered martensitic-bainitic matrix, eutectic interdendritic carbides, and secondary carbides. During heat treatment a certain quantity of undissolved or excess carbide particles remains. They are only consumed at appreciably high temperatures, which are not used in commercial heat treat practice. Classic tool steel hardening practices employ high temperature heat treatments. These types of high speed steel materials dissolve approximately 10 to 12% total amount of carbides on heating. The decrease in total carbide's quantity is almost entirely due to the dissolution of the chromium-rich M<sub>23</sub>C<sub>6</sub> carbides, which disappear completely at 2000°F (1093°C). Continued heating above 1900°F (1038°C) produces a relatively steady solution of tungsten-molybdenum-rich carbide M<sub>6</sub>C. In contrast, vanadium-rich eutectic MC carbide is very stable, dissolving at a much slower rate, which is increasing slightly only as the melting point is approached. Figure 1 shows an example of the effect of austenitizing time and temperature on the hardness of a T1-type high speed steel. (1) Hardness reaches a maximum due to the dissolution of carbides, enriching the surrounding matrix.

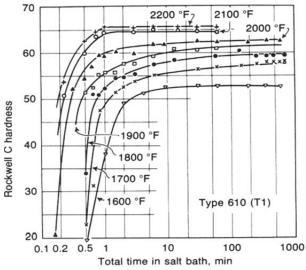


Figure 1. Effect of Austenitizing Temperature and Time on Hardness (HRC). (1)

To achieve high red hardness levels in high speed steel tooling, high austenitizing temperatures are used. The theory of tool steel hardening is applicable to heat treated high speed steel (HSS) rolls. However, the application of the classical heat treat practice to HSS rolls is not directly applicable since there are fundamental and equipment limitations presented to the roll manufacturer.

Cast bi-metallic rolls, specifically HSS work rolls, pose challenges when attempting to achieve high austenitizing temperatures commonly used for HSS material. The core of the cast HSS roll is comprised of iron material possessing a relatively low melting point. High temperature austenitizing treatments used on commercial high speed steel material must prevent the liquation of core material and possible de-bonding between the shell and core. The nature of the bi-metallic product potentially limits both the material response during heat treatment and, as a consequence, resulting

performance. One can appreciate the range of performances reported for HSS rolls. Unfortunately, sub-optimization of the heat treated roll microstructure limits the performance capability that cast high speed steel material inherently possesses. One of the most common tests used to rate the quality of high speeds steels, or rolls for that matter, is the room temperature hardness test (HRC, HRB, VHN) which differs from the "hot hardness" or "red hardness" describing the hardness value at elevated temperatures replicating service conditions. As surfaces are in contact during the use of tool steels or rolls, thermal contact and friction initiate a softening response of the material reducing wear resistance. A material with high hot hardness and good oxidation behavior are desired.

# 2 MATERIALS AND METHODS

In order to characterize and optimize the response of cast HSS roll material to heat treatment, a complex multi-physical multi-scale approach was utilized based on experimental, computational and approximation methods. The range of chemical compositions evaluated is listed in Table 1. HSS rolls were produced by the centrifugal horizontal spin cast process then subjected to varying heat treatment routes described in Table 2. Continuous local transformations and thermal gradients that occur during heating and quenching were simulated using finite-element method (FEM) and thermodynamic, kinetic predictions. Microstructural observations were compared to non-linear heat transient results and actual thermo-processing data. FEM sub-structuring and image processing techniques were implemented to aid in the development of the model and simulate the local response of individual microstructural constituents, i.e. carbides and/or matrix, under heat treat conditions. P0-group represents a relatively high carbon group, whereas S0- lower carbon. S9 roll was subjected to a relatively high austenitization temperature enabling dissolution of eutectic and secondary precipitated carbides (e.g., M<sub>2</sub>C, M<sub>6</sub>C, and M23C6), dispersed in the matrix, and altering interdendritic solute-rich regions. The P9 sample is an optimized roll (Synergy100) with a finer grain size, and uniform high hardness profile, due to non conventional routes.

 Table 1. Typical Chemical HSS Composition (wt%)

С	Si	S	Mn	Р	Ni	Cr	Мо	V	W
1.7-2	2 0.50-0.90	0.020 max	0.50-0.75	0.030 max	0.10-1.0	3.5-5.5	5.0-7.0	3.0-6.0	0-6.0

Table 2. A Series of HSS Radial Roll Samples

ID	Condition	Carbon, wt%	COMMENT
P0	As -Cast	2.0 - 2.2	Troostite around M2C; MC, M7C3, M23C6, M6C etc.
P0	P	2.0 - 2.2	Spheroidized matrix, partial dissolution of M2C
P0	A+DT	2.0 - 2.2	Martensitic, bainitic, pearlitic matrix, MC, M2C, M7C3 etc.
P0	P+A+DT	2.0 - 2.2	Mixed behavior of matrix, micro-segregation in matrix
S0	A	1.8-2.0	Martensitic, pearlitic matrix with dispersed M6C, M23C6
S0	P	1.8-2.0	Spheroidized matrix, partial dissolution of M2C
S9	P+A+DT	1.8-2.0	Intense dissolution of M23C6, M6C with increased T <sub>y</sub>
S-Shell	As-cast (no core poured)	1.8 – 2.0	Troostite present in less amount nearby M2C; finer grains to inner surface; higher concentration and uniform distribution of globular MC; fine Mo-Cr-V carbides in the matrix
P9 Synergy100	P+A+DT	1.8-2.0	Optimal dissolution T <sub>v</sub> and accelerated cooling: refined grains, uniform distribution of fine MC, discontinuous and partially dissolved M2C, mostly dissolved fine M23C6, M6C in matrix

Note: P- preliminary heat treatment; A- austenitization; DT- double tempering

Thermodynamic and kinetic predictions were made for several alloys and compositions with the aid of commercial software packages Pandat 8.0 and JMatPro 4.0. Equilibrium and non-equilibrium (Scheil-Gulliver) models were used. A simulated equilibrium carbon diagram is shown on Figure 2 with the zoomed region, representing high temperature phase fields. The general microstructure and precipitation sequence of carbides was analyzed with the aid of advanced experimental, physical and numerical methods. It was found that continuous local transformations take place due to compositional variations and thermal gradients, yielding to microstructural variability.

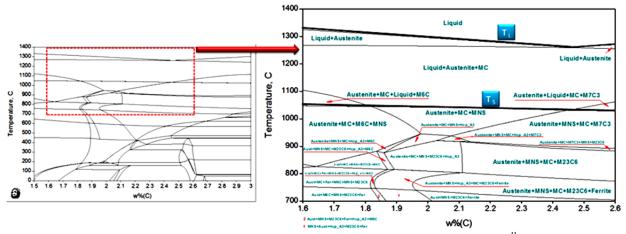


Figure 2. Equilibrium Carbon Diagram %C Variations vs. Temperature, °C

# **3 RESULTS AND DISCUSSION**

Using scanning electron microscopy (SEM) with energy-dispersive X-ray spectroscopy (EDS), a detailed microstructural analysis was carried out on radial shell samples, Figure 3. Identification of the carbides and matrix in terms of type

(crystal structure), volume fraction, composition, and morphology as a function of radial depth in the shell was completed. The main eutectic carbides such as MC,  $M_2C$ ,  $M_6C$ ,  $M_7C_3$  etc. were found and compared between conventional and non-conventional HT approaches. EDS analysis includes, but not limited to: detailed individual carbide analysis; local segregations via line scanning in the matrix (Figure 4a) and eutectic interdendritic boundaries (Figure 4b); 2D compositional mapping of the local area.

According to the preliminary observations of HSS material subjected to conventional heat treatment, the interdendritic eutectic carbides are not considerably affected due to their stable behavior at relatively high temperatures. However, the matrix was found to be more responsive. Hence it was concluded that the main eutectic carbides have to be initially refined and uniformly distributed during the casting stage in order to avoid formation of brittle carbide networks yielding to brittle intergranular cracking. (2-6) Structural refinement during the solidification process also influences material response during HT.

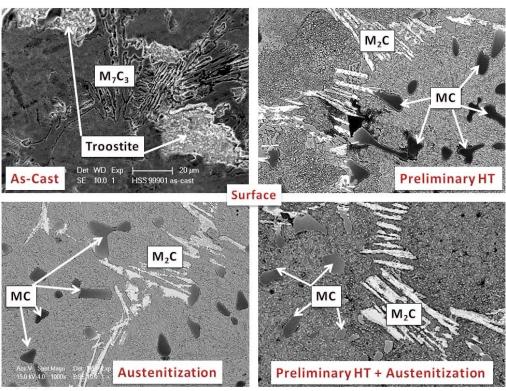
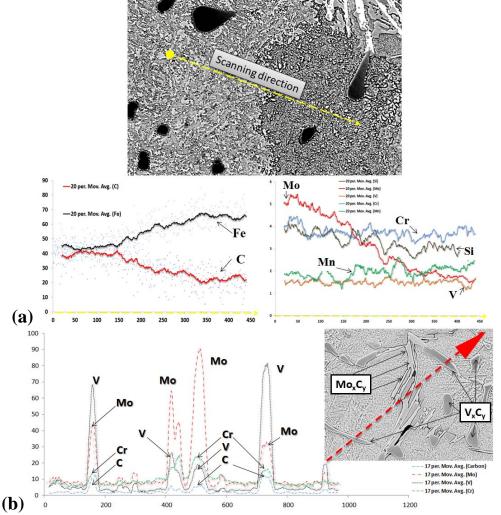


Figure 3. Effect of Different Heat Treatment on HSS Shell (Conventional Case)

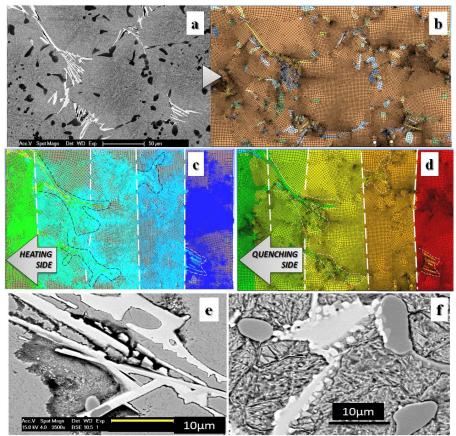


**Figure 4.** Example of Micro-Segregations in the Conventional Preliminary HT Matrix (a), and in As-Cast Eutectic Solute-Rich Boundaries (b)

In order to analyze the response of the roll to heating-cooling cycles, three-dimensional finite element (FE) simulations were evaluated using ANSYS taking into account non-linear material properties generated with JMatPro, based on measured chemical compositions with the spectrometer. The FE HSS roll model is composite, consisting of the three main domains: shell, intermix zone and ductile iron core. Additionally, the shell is modeled as a multi-layered structure, accounting for possible compositional variation due to its as-cast nature. Each individual layer is considered in detail revealing observed microstructural behavior before and after heat treatment. In order to control a volumetric distortion of the roll body, which takes place because of thermal gradients and phase transformations, a coupled thermal-stress analysis was performed. Actual infra-red data acquisition during roll production was used for result verification.

A more detailed attempt was made to investigate local microstructural response. Figure 5 displays an example showing micro-scale heat transport analysis, where a part of as-cast microstructure (Figure 5a) is divided into finite elements (Figure 5b) and time-varying boundary conditions are applied, simulating heating (Figure 5c) and cooling cycles (Figure 5d). In the model there are three main isotropic, homogenized constituents considered: 1) martensitic matrix (bright grey), 2) eutectic MC carbides, V-rich, in petal-like and idiomorphic morphologies (dark grey), and 3)  $M_2C$ , Mo-rich,

eutectic interdendritic carbide networks (white). It was found that the supplied energy advances faster through the Mo-rich zones than the main propagating heat front. During quenching the heat dissipation is being retarded in Mo-enriched zones, which can be attributed to the higher thermal conductivity and lower heat capacity of Moregions respectively in comparison with V-rich carbides. Advancing or retarded heat fluxes are highlighted with the curved dash lines, and the temperature gradient fronts are shown with vertical dashed lines. In the case of the heating cycle the total heat flux is higher at the Mo-carbide-matrix interface and moreover, it propagates within Mo-rich zones faster than the heating front itself. During the quenching cycle it is noted that, there is a residual heat flux concentrated at separate Mo-rich areas behind the cooling front. This transient analysis resembles observed M<sub>2</sub>C carbide's decomposition, which starts at the carbide-matrix interface (Figure 5e, before HT, and Figure 5f- after HT) and reflects the possible sequence of transformations.



**Figure 5.** Example of nonlinear FE micro-scale heat transport simulation (a), (e)- SEM images of ascast microstructure; (b) meshed FE model of actual SEM image given in (a); (c) total heat flux during heating cycle; (d) dissipation of energy while quenching the left edge (vertical dash lines- propagating heat flux (negative direction); curved lines – residual retarded flux in Mo-rich zones, leaving the front behind; (e) zoomed as-cast Mo-rich eutectic interdendritic carbides with troostite pearlite (dark area); (f) resulted decomposed  $M_2C$  into  $M_6C$  and MC after high temperature hardening

The wear behavior is a function of the material's red hardness.<sup>(7)</sup> It is very important to maintain relatively high hardness of the matrix throughout the shell thickness which can be achieved by proper dissolution of solute-rich interdendritic eutectic boundaries and secondary carbides having a size of less than 500 nm. The nature of secondary precipitates in the as-cast condition is found to be strongly dependent on alloy composition. During conventional heat treatment of HSS rolls such secondary carbides remain and coarsen. Hence, a classical high temperature tool steel

hardening approach was adopted for cast HSS rolls. A non-conventional approach is focused on the dissolution of precipitated secondary Cr-rich carbides in the matrix and transient "peanut-like" Mo-V epitaxial carbides in order to improve oxidation and wear resistance. At the same time the non conventional approach ensures modification of the eutectic interdendritic solute-rich interconnected boundaries, increasing fracture toughness of the shell material.

The role of a preliminary heat treatment was also investigated. The optimal preliminary high temperature treatment was found to have several main preconditioning effects: 1) matrix homogenization (elimination of local segregation, shown in Figure 4); 2) as-cast stress relieving; 3) modification of eutectic interdendritic brittle networks by localized diffusion; 4) spherodization of the matrix producing spherical alloy carbides increasing surface energy for the following high temperature austenitization; 5) the "roughening" of the coarse sharp eutectic  $M_2C$ .

In most cases, a partial dissolution of  $M_2C$  was observed, which can be described as fine epitaxial "peanut-like" Mo-V carbides<sup>(5,8)</sup> which were found in the vicinity of  $M_2C$ . After non-conventional high austenitization, the amount of such carbides is considerably reduced.

The carbide-forming elements (Mo, V, Cr etc.) are substitutional, causing a local distortion of the crystalline lattice, but with proper tempering a secondary precipitation is observed (<200nm) with uniform distribution inside eutectic γ-cells.

The matrix is the most responsive, compared to the various types of carbides. Fine sub-grain structures can be developed inside prior austenite grain boundaries, which are not mobile due to the presence of carbides stable at high temperatures. The sub-grain's size is a function of quenching from austenite region.

The refined as-cast microstructure properly responded to the developed heat treatment (preliminary pre-conditioning of the matrix, high temperature austenitization and double tempering) with adjusted soaking times, accelerated cooling paths and optimal dissolution temperature, facilitating the formation of relatively fine sub-grain development and fine precipitation hardening. Figure 6a, 6b, 6e compares the developed microstructure with advanced continuously poured for cladding (CPC) material, Figure 6c, 6d, 6f, respectively. In regards to heat treatment the proper ascast structure is a necessary precursor to facilitate proper microstructural evolution and optimization during subsequent final hardening. The eutectic cell sizes are almost the same in the final hardened product as in the cast state. With a new alternative heat treatment the eutectic interdendritic brittle solute-rich networks were altered and became less connected.

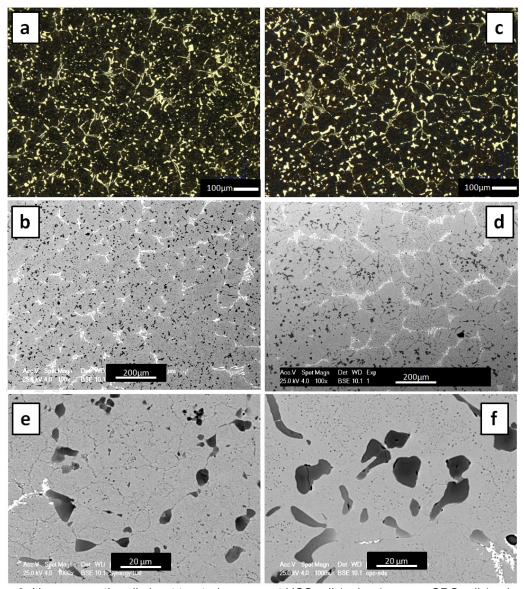
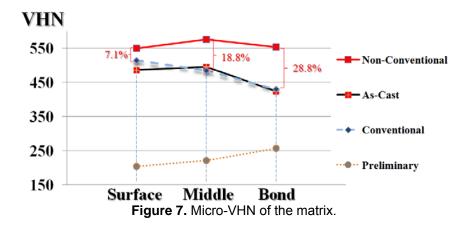


Figure 6. Non-conventionally heat treated spun-cast HSS roll (a, b, e) versus CPC roll (c, d, and f)

The matrix was enriched with alloying content and homogenized, which demonstrated uniform and increased micro hardness (VHN) profiles of the matrix, Figure 7 (top line), where the increase is approximately 18% with standard deviation 10% depending on location in the shell compared to conventionally heat treated HSS shell matrix.



Moreover, the radial bulk Rockwell-C (HRC) hardness measurements at room temperature through the HSS shell thickness also exhibit uniform, stable hardness values from the surface to the core (Line I, Figure 8), validating the efficiency of a new alternative HT process.

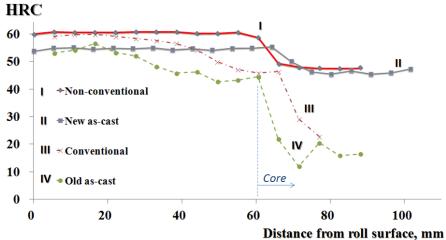


Figure 8. Bulk HRC hardness of HSS shell in radial direction.

# 4 CONCLUSIONS

- 1) Refined as-cast structure promoted faster kinetics during high temperature hardening HT. Preliminary HT homogenized the matrix, reducing compositional variations, and spherodized fine alloy carbides in the matrix facilitating increased kinetics during hardening steps.
- 2) Austenitization temperature and time were adjusted, yielding to increased dissolution and decomposition of transient carbides, enriching alloy content of the matrix. The eutectic interdendritic boundaries were modified and less interconnected. Thus, the matrix hardness and strength were increased in comparison to conventionally hardened cast HSS shell, promoting high temperature stability of the material, improved oxidation behavior and toughness.
- 3) The proposed multi-scale computational approach is based on sub-structuring and microstructural image-based FE modelling. The fundamental interpretation of the multi-layered structure helps to understand kinetics phenomena associated with carbides-matrix decomposition, i.e. continuous local transformations in HSS shell. The developed model provides more insight into a complex non-liner heat transfer phenomena and related microstructural features in the material.

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