



## Mathematical modelling of austenite decomposition during the quenching

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**Abstract:** Mathematical modelling of austenite decomposition has been investigated. Phase portion in steel are predict based on hardenability curve of Jominy-specimen. The kinetic of phase transformations and hardness distribution have been estimated based on time relevant for structure transformation. The designed inverse method of prediction austenite decomposition is used in computer simulation of microstructure transformation during the austenite decomposition of steel C 45 (DIN). The kinetic of austenite decomposition and IT-diagrams of steel can be successfully predicted by proposed method.

**Keywords:** Austenite decomposition, Computer simulation, Quenching, Steel

### 1. INTRODUCTION

Phase transformations usually are predicted by isothermal transformation (IT) diagram or continuous cooling transformations (CCT) diagrams [1]. IT and CCT diagrams are irreplaceable in the clear presentation of structural transformation during the steel cooling in order to predict structural constitution and hardness after cooling. Moreover, preparing of these diagrams is rather expensive. They are prepared for strictly determined elemental composition and austenitizing temperature and they could be used with accuracy only for simulation of quenching of steel with same elemental composition, austenitizing temperature and history as were of steel for it the IT and CCT diagrams are made.

In practice numerous phase transformations calculations are based just on statistic correlation between chemical composition and final microstructure as result of quenching. From another point of view, the kinetic of phase transformations, i.e., IT and CCT diagrams can be simulated by mathematical modelling. But, mechanism of phase transformations is not fully understood and interactive influences of different elements, austenitizing temperature, etc. on results usually are not easy to take in account. The kinetic of phase transformations and hardness distribution can be estimated by inverse method based on time, relevant for structure transformation measured on Jominy specimen [2].

### 2. PHASE PORTION PREDICTION

The austenite decomposition results can be estimated based on time, relevant for structure transformation. The characteristic cooling time, relevant for structure transformation for most

structural steel is the time of cooling from 800 to 500 °C (time  $t_{8/5}$ ) [1]. Involving the time  $t_{8/5}$  in the mathematical model of steel quenching, the Jominy-test result can be involved in austenite decomposition model [2]. It could be written for Jominy-test that phase hardness depends of chemical composition (CC) and cooling rate parameter (CRP) that corresponds to actual distance (d) of Jominy-specimen quenched end. It was adopted that  $CRP = t_{8/5}$ .

$$HV_d^M = f_M(CC, CRP) = HV_{max}^M - K_M \log \frac{t_{8/5d}^M}{t_{8/5max}^M} \quad (1)$$

$$HV_d^B = f_B(CC, CRP) = HV_{max}^B - K_B \log \frac{t_{8/5d}^B}{t_{8/5max}^B} \quad (2)$$

$$HV_d^{P+F} = f_{P+F}(CC, CRP) = HV_N^{P+F} + K_{P+F} \log \frac{t_{8/5N}^{P+F}}{t_{8/5d}^{P+F}} \quad (3)$$

where N is normalising, Bmax is lower bainite. Characteristic values of HV, K and  $t_{8/5}$  in equations (3), (4) and (5) have to be evaluated based on chemical composition for investigated steel, combined by Jominy-test results. Hardness of quenched structures with 100%, 90% or 50% of martensite can be predicted by using the diagram of hardness at different percentages of martensite vs. carbon content after Hodge and Orehsoki [3][4] and Jominy-curve. The influence of chemical composition of steel has to be taken in account.

Distances of quenched end Jominy-specimen with martensite fraction of 90% and 50% can be predicted by the diagram of Jominy-curve by conversion hardness results to distances. Distances of 100% martensite and 100% of pearlite can be predicted by the diagram of Jominy-curve. The regression relations between the cooling time from 800 to 500°C for cooling structures of 100%, 50%, 10% and 0% (pearlite + ferrite) can be established [5].

If both, hardness (HV) of cooling microstructure with specific content of martensite or (ferrite+pearlite) is known and if the hardness of microstructure constituents separately is known it is not difficult by equation (4) and (5) to predict content of two other microconstituents:

$$HV = ((\% \text{ ferrite}) HV(F) + (\% \text{ pearlite}) HV(P) + (\% \text{ bainite}) HV(B) + (\% \text{ martensite}) HV(M)) / 100 \quad (4)$$

$$((\% \text{ ferrite} + \% \text{ pearlite}) + \% \text{ bainite} + \% \text{ martensite}) / 100 = 1 \quad (5)$$

### 3. ALGORITHM FOR PREDICTION OF KINETIC OF PHASE TRANSFORMATIONS

When the additive rule holds for the progress of transformation and approximating continues cooling by step cooling in accordance with R. W. Cahn, a fraction of the transformed austenite in the pearlite or bainite during the time step  $\Delta t$  generally is equal [6]:

$$\Delta X_i \approx K f(T, D) f_2(k_i, A, \Delta T_u) \left( \ln \frac{1}{1 - X_{i-1}} \right)^{\frac{n-1}{n}} (1 - X_{i-1}) \Delta t_i \quad (6)$$

where  $K$ ,  $k_1$  are the coefficients,  $D$ -diffusion coefficient,  $\Delta T_u$ -austenite undercooling,  $A_1$ -eqilibrium temperature of austenite decomposition. In a task of simulation of microstructure transformations and IT-diagram for the concrete steel, coefficients  $K$ ,  $k_1$  and exponent  $n$  have to be calibrated using the Jominy-test results of steel.

#### 4. APPLICATION

An own computer software program was used for estimation of phase portion of Jominy-specimen of steel C 45. Elemental composition of investigated steel C45 was 0.44 % C, 0.28% Si, 0.60% Mn. Jominy-test results of investigated steel C45 are shown in Figure 1. Austenitizing temperature was equal 850 °C. Diagram of microstructure portion for Jominy-specimen of steel C 45 is shown in Figure 2.

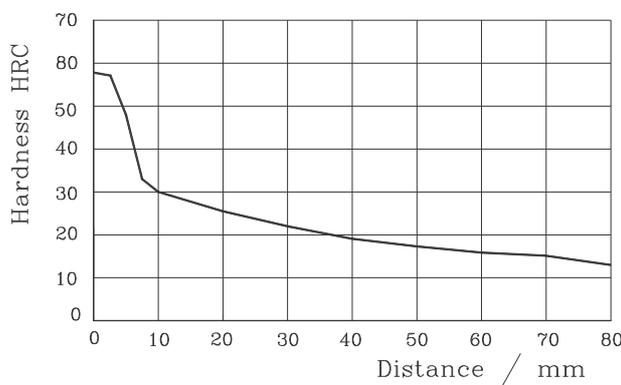


Figure 1. Jominy-test result of steel C45

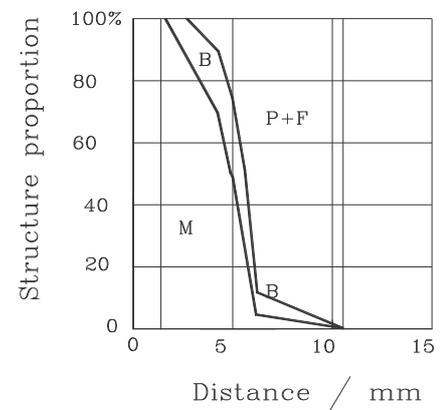


Figure 2. Simulated structure composition vs. Jominy-distances of steel C45

The calculated hardness distribution and phase distribution in quenched cylindrical steel specimen of 50 mm Dia. of steel C 45 is shown in figure 3. Heat treatment of quenching was: heating to 850 °C for 30 min and quenching in agitated water with severity of quenching  $H=1.4$ . The heat transfer coefficient is predicted by calibration [5].

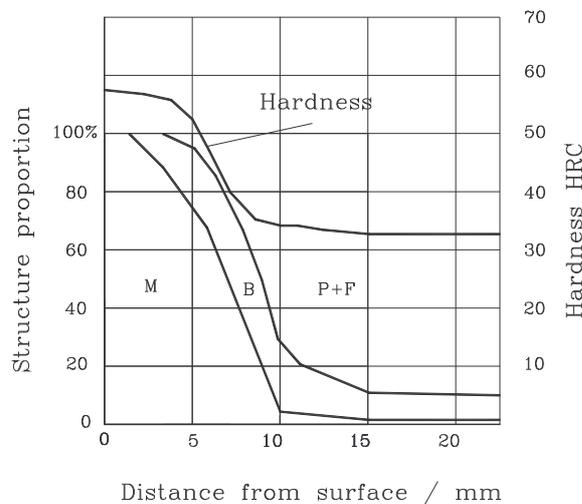


Figure 3. Simulated structure composition of cylindrical specimen of steel C45

Characteristic curves of IT-diagram of steel C 45 were calculated by the calibrated equation (6). Figure 4 shows the experimental and predicted IT-diagram of steel C 45.

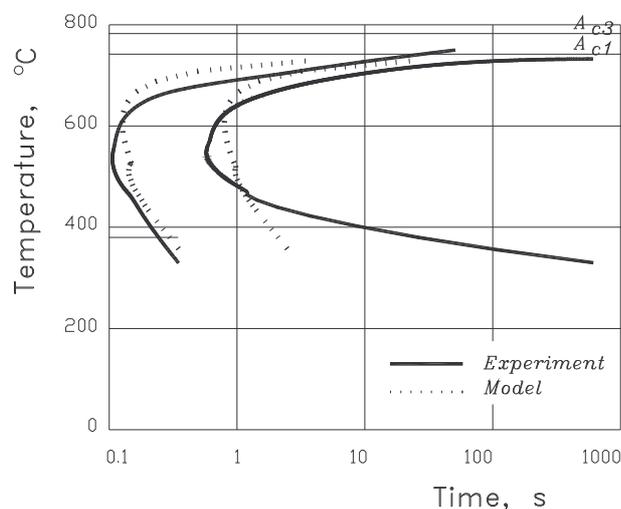


Figure 4. Experimental and predicted IT-diagram of steel C 45.

## 5. CONCLUSIONS

The inverse method of computer simulation of austenite decomposition and evaluation of quenched phase portion was established. In the established mathematical model the numerical measure of specimen cooling kinetic was time  $t_{8/5}$ . For the calculation of microstructure composition Jominy-test results and chemical composition of steel must be known.

The established mathematical model was applied in computer simulation of microstructure transformation in *Jominy*-specimen and cylindrical specimen of steel C 45. It can be concluded, that microstructure composition in quenched steel specimen can be successfully calculated and IT-diagrams of low alloyed steel can be successfully predicted by proposed method of computer simulation.

## REFERENCES

1. A. Rose et al, Atlas zur Wärmebehandlung der Stähle I, Verlag Stahleisen, Düsseldorf, 1958.
2. B. Smoljan, Computer Simulation of austenite decomposition, International Conference on Advanced Materials processing technologies (AMPT'01), Madrid, 2001.
3. S. Hoyt, Metal Data, Columbus, Ohio, 1952.
4. ... Theory and Technology of Quenching, eds. B. Liščić H. Tensi and W. Luty, Springer Verlag, (1992).
5. B. Smoljan, Computer Simulation of Microstructure Transformation during the Quenching, 13<sup>th</sup> IFHTSI Congress/ ASM Surface Engineering Congress, Columbus, OH, 2002.
6. B. Smoljan, Computer Simulation of IT-diagrams of Steel, 14<sup>th</sup> IFHTSI Congress, Shanghai, China, 2004.