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SIMULATION OF MICROSTRUCTURE – TRANSFORMATION – KINETICS OF UNALLOYED CONSTRUCTIONAL STEEL IN CASE OF FAST THERMAL CYCLES

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Abstract

All laser processes lead to very fast heating rates up to 10.000 K/s and are followed by very fast cooling rates. It is still unknown yet, whether the normal Weld – CCT – diagram is able to describe the transformation in case of this fast thermal cycles or not. Because of the fast heating rates the solution and diffusion processes are uncertain and take place in non – equilibrium conditions. But the state of the microstructure at the peak temperature determines the transformation character at the cooling process.

The grain coarsening at maximum temperature in case of laser processes is slow and the high heating rate acts like a brake. This fact seems to be positive regarding to the transformation of the austenite during cooling.

The authors developed a computer aided model to simulate especially the transformation of metal structure during fast heating processes and to estimate the microstructure at peak temperature. A macro model, based on the mathematical description of the diffusion processes during heating and cooling, connected with a micro model, based on the Monte – Carlo – Simulation of the formation of the new austenitic phase can help us to understand the metallurgical processes in case of fast thermal cycles.

Keywords: austenite transformation, diffusion processes, mathematical simulation

1 Introduction

The transformation behaviour of constructional steel is decisively influenced by the distribution of alloying elements and precipitations. They are responsible for the formation of nuclei and so they influence the following precipitations and transformations.

The carbide dissolution during the heating process is the most important process to the homogenisation of the austenite. It can be expected that with an increasing heating rate the dissolution of the carbides will be incomplete. Especially in welding processes with reduced heating time, e.g. laser beam welding or electron beam welding, such a behaviour is conceivable, which is not detectable by practical experiments in case of very fast heating rates. Resulting from fast heating experiments for building Time – Temperature – Transformation – Curves with a "GLEEBLE 3500" – system it is shown (*Fig. 1*), that the formed martensite after passing a fast thermal cycle at a heating rate of 6000 K/s has a lower hardness after a cooling time $t_{8/5}$ = 2,0 s than after a cooling time $t_{8/5}$ = 3,0 s [1].

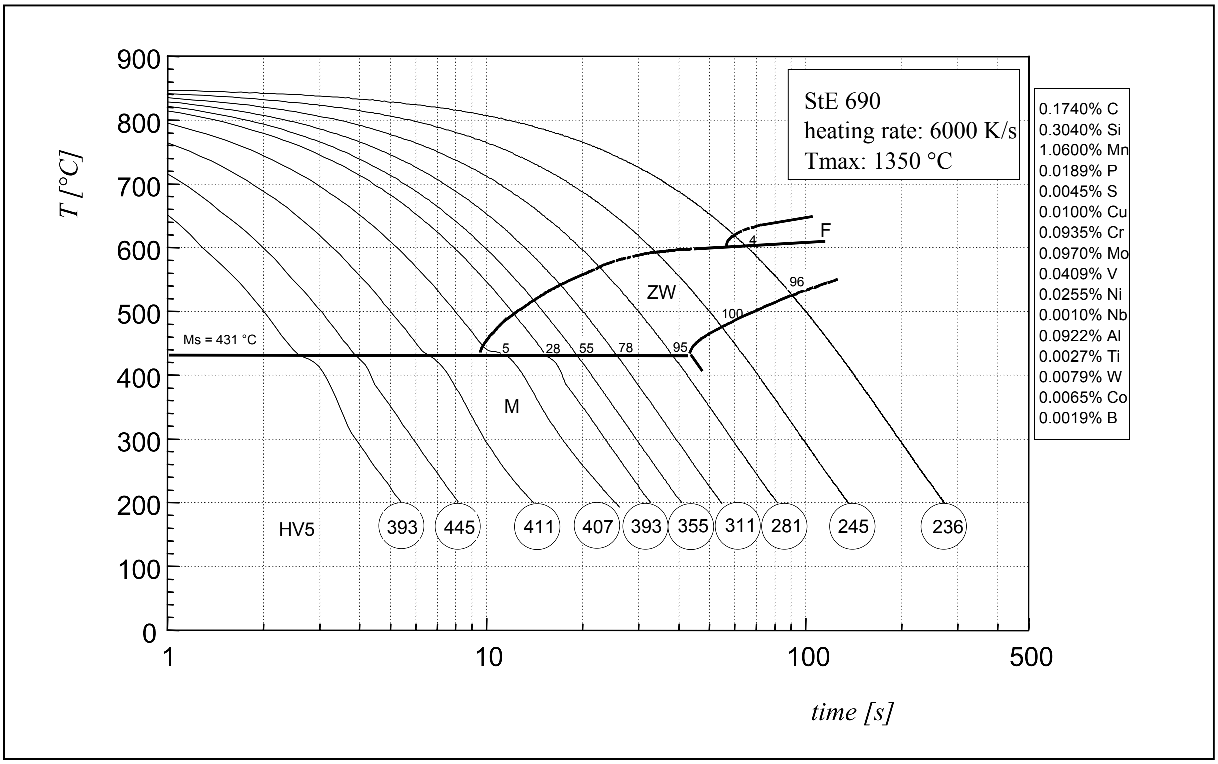


***Fig. 1**: Time – temperature – transformation – curve of a steel StE 690 [1]*

Such a phenomenon has never been observed in case of heating rates typical of arc welding processes. The described phenomenon allows the presumption, that during very fast thermal cycles the degree of homogenisation of austenite is low and the growth of the austenitic grain is braked with positive effects to the resulting material structure and its properties. Unfortunately it is not possible to quantify the different degree of homogenisation and its effects on the material structure after finishing the transformations in practical experiments in case of very fast thermal cycles.

The presented mathematical models, valid for the binary system Fe – C, said to be the first step for a mathematical description of the transformation behaviour between the A_{c1} – and the A_{r3} – temperature for unalloyed constructional steel.

2 The general model

It is well known from experiments [2], [3], that an increasing heating rate results in a shift of the A_{c1} – temperature and the area of existence of carbides to higher temperatures. For heating rates above 2400 K/s an experimental procedure is not feasible. The calculation of the transformation temperatures and the area of carbides' existence including the degree of the austenite homogenisation is a chance to predict them for welding processes with very fast thermal cycles.

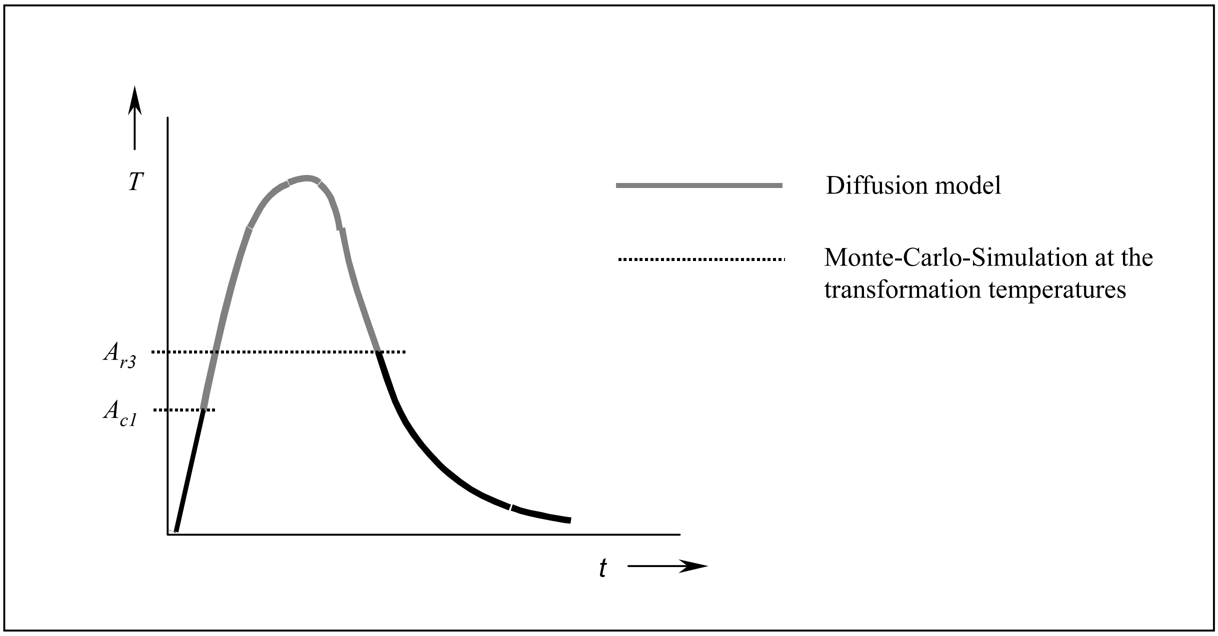


Fig. 2*: Thermal cycle in the HAZ, schematically*

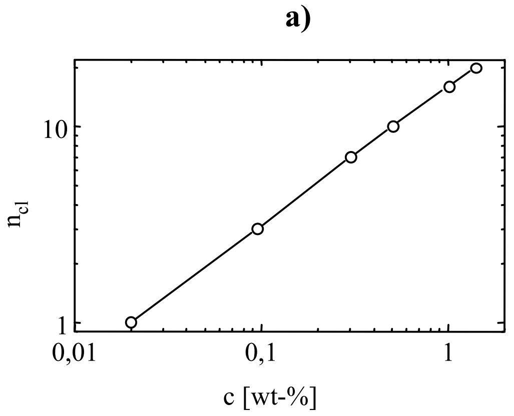
In *Fig. 2* a typical thermal cycle in the HAZ of a welding process is shown. The two critical points and the critical area for the transformation process are marked.

At the A_{c1} – and the A_{r3} – temperature the formation of nuclei are the decisive reactions, between these two temperatures diffusion processes are the most important reactions. For the description of the whole process it is necessary to combine mathematical models, each of them is valid for a different model area. For this combination only the temperature is a suitable parameter.

The Monte – Carlo – Simulation is used in a micro – model for the calculation of the formation of nuclei for the austenitic and the ferritic phase and for the calculation of the A_{c1} – and the A_{r3} – temperature. Furthermore these temperatures are the connectors to the macro diffusion model that is used.

3 Calculation of the A_{c1} – temperature

For the transformation from ferrite into austenite a restructuring of iron atoms is supposed [4]. The carbon stabilizes the austenite, its existence area moves to lower temperatures. Below the A_{c1} – temperature the carbon is bonded in the cementite. Therefore there is a stable growth of the austenite above the A_{c1} – temperature, if the cementite decomposes and the released iron atoms diffuse into austenite.



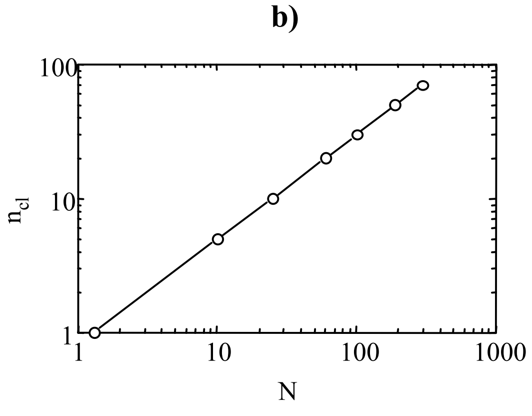


***Fig. 3a**: Number of particles for the formation of an austenitic nucleus depending on the carbon concentration [5]*

***Fig. 3b**: Carbide size n_{Cl} depending on the number of steps N; wt-% carbon c_0 =0,1%, [5]*

For the used mathematical model it is supposed, that the cementite decomposition dominates the transformation behaviour and that the number of particles for the formation of an austenitic nucleus depends on the carbon concentration (*Fig. 3a*). The starting point in this figure is equivalent to the point P (c_0=0,02 wt-% C) in the iron – carbon – equilibrium – diagram with the least number of particles n_{Cl}=1, formed by decomposition.

The A_{c1} – temperature is calculated with:

$$T_{Ac1} = 723 + \sum_{i=1}^{N} v_{heating} \cdot \Delta t(T)_i \tag{1}$$

The correlation between the decomposed cluster size n_{Cl} and the required steps N for any heating rates $v_{heating}$ is known from calculation experiments [5] (*Fig. 3b*). So the data for n_{Cl} and N depending on any carbon concentration, are fixed. For the calculation of the time element [5], [6] is used:

$$\Delta t = \frac{\exp\left(\frac{E_0}{k \cdot T}\right)}{\Gamma_0}, \tag{2}$$

where Γ_0 is a factor for the simple cubic lattice and E_0 is the summarized decomposition energy $E_0 = E_{iron} + E_{carbon}$.

It is known from calculations of diffusion [4],[7], that the onward cementite decomposition results in a layer of unbounded carbon atoms, which obstructs the further decomposition. This decisively influence of the carbon only can be compensate with the growth of the austenitic area. With the implementation of this criteria all model calculations finishes on a maximum temperature from 791°C, independent from the heating rate. This results agrees excellent with experiments [2].

***Tab. 1**: Calculated A_{c1} – temperatures depending on variable heating rates for a carbon content of 0,1 wt-%*

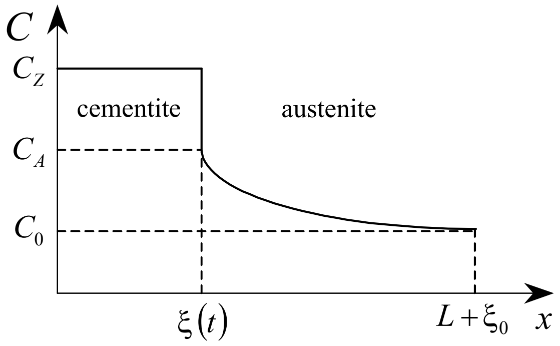
$v_{heating}$ [K/s]	2000	3000	4000	5000	6000	7000	8000
A_{c1} [°C]	751	761	769	776	782	788	790

With the described mathematical model the A_{c1} – temperatures for a system with 0,1 wt-% carbon were calculated (*Tab. 1*). These temperatures were used for further calculations described in chapter 4. Despite the very high heating rates, typical for laser processes, the austenite growth, the cementite decomposition respectively, starts below the temperature of 791°C.

With a similar mathematical model, based on the same fundamentals it is possible to calculate the A_{r3} – temperature depending on different cooling rates, in case of a homogenized austenite as well as in case of different welding conditions.

4 Diffusion model for the austenite homogenisation

With the aim of a first estimation of the dissolution behaviour of the cementite and the degree of austenite homogenisation after passing a welding thermal cycle a diffusion model *(Fig. 4*) based on the second law by Fick was used.



C_Z = carbon concentration in the cementite = 6,67 %

C_A = carbon concentration at the cementite/austenite-boundary

C_0 = carbon concentration in the general system

ξ_0 = starting dimension of the carbide

$\xi(t)$ = dimension of the carbide at the time t

$L+\xi_0$ = dimension of the model area

***Fig. 4**: Diffusion model for the calculation of the dissolution of cementite inclusions in the austenite*

The second law by Fick is used in the following way for the calculation of the dissolution of cementite inclusions with variable geometry:

$$\frac{\partial C}{\partial t} = \frac{1}{x^n}\frac{\partial}{\partial x}\left(x^n D \frac{\partial C}{\partial x}\right), \qquad \xi(t) < x < (L+\xi_0) \tag{3}$$

The index n in this equation describes the variable geometry: n=0 describes a flat inclusion, n=1 describes a cylindrical and n=2 describes a spherical inclusion. As marginal conditions one has to consider, that the carbon concentration at the cementite – austenite – boundary corresponds with the concentration along the line SE in the iron – carbon – equilibrium – diagram and that at the end of the model area ($L+\xi_0$) there is no concentration gradient ($dC/dx = 0$).

The description of the austenite dissolution is realised with a mass balance on the move of the cementite – austenite – boundary. The balance describes the transport of the carbon depending on the concentration profile in the austenite.

For the estimation of the degree of dissolution, the carbon removal respectively, it was used the spherical model of a cementite inclusion. So the dissolved volume can be calculated with:

$$V_{dissolve} = \frac{4}{3}\pi \cdot (\xi_0^3 - \xi^3)\,. \tag{4}$$

The results of some calculations are shown in *Fig. 5*. With decreasing temperatures, increasing cooling rates respectively, the dissolved volume of cementite is decreasing. On the other hand the dissolved volume is increasing with an increased dimension of the cementite inclusion.

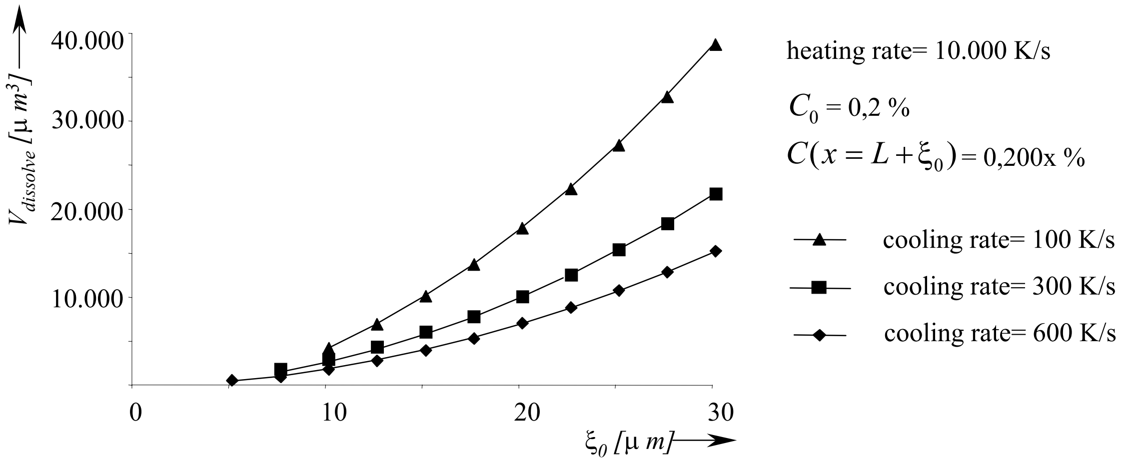


Fig. 5: *Calculated dissolved volume of cementite depending on the starting dimension of a cementite inclusion [8]*

Depending on the dimension of the cementite inclusions and the time staying in the austenite area, *Fig. 5* can be showed as an dissolution diagram (*Fig. 6*). This diagram allows an estimation whether a cementite inclusion with a given starting dimension will be dissolved during variable thermal cycles or not. Although the very fast thermal cycles used in this diagram are more theoretical, it is essential to know an estimation of not dissolved cementite inclusions, which are available for the formation of a fine grained structure in the HAZ.

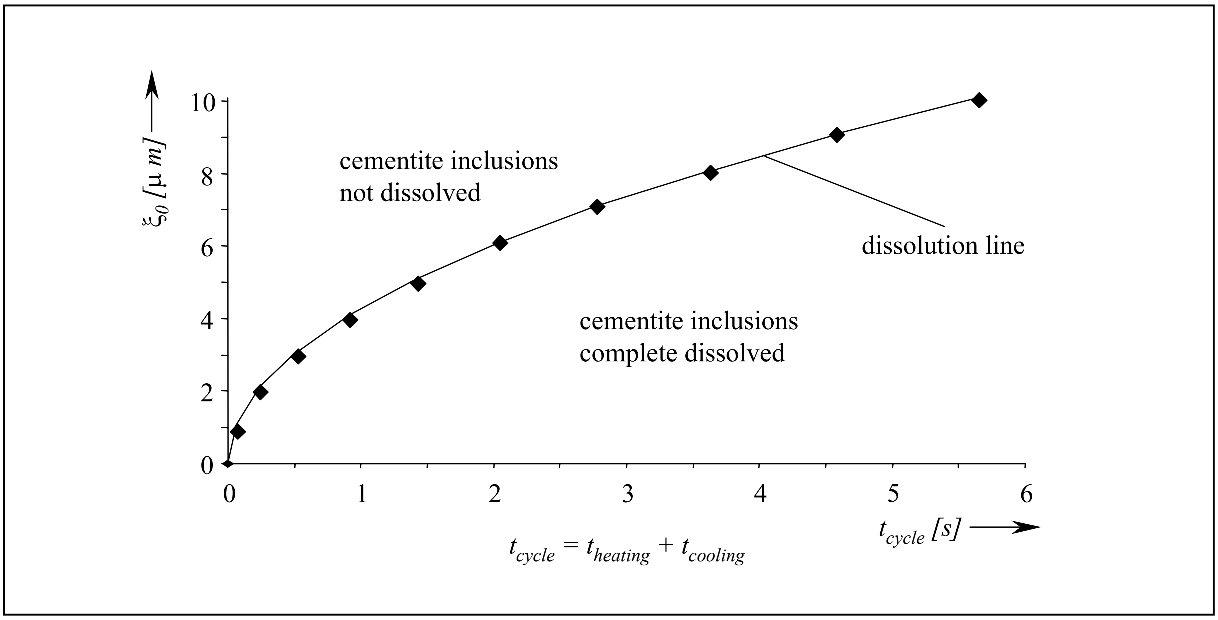


***Fig. 6**: Calculated dissolution of spherical cementite inclusions with variable dimensions [8]*

With a further developed diffusion model it is possible to consider the calculated A_{c1} – temperatures according to paragraph 3 in case of high heating rates as well as the peak temperatures in the thermal cycle. The consideration of overheating depending on the actual heating rate, allows it to calculate the transformation of a lamellar or a globular perlitic structure into austenite. The first results can be shown in the form of the well known Time – Temperature –Austenitization – Diagrams as a Perlite – Transformation – Diagram in case of very high heating rates (*Fig. 7*).

The calculations for the diagram in *Fig. 7* were done for a lamellar perlitic structure. The A_{c1} – temperatures, the amount of overheating respectively, were calculated with the Monte – Carlo – Simulation for the binary system Fe – C with a carbon content of 0,1 wt-%. The width of a ferrite lamella was 1µm, the width of a cementite lamella was 0,125 µm.

The Perlite – Transformation – Diagram allows an estimation of the degree of austenite homogenisation in case of very fast thermal cycles. With the complete dissolution of the cementite inclusions and the following constant carbon distribution everywhere in the model area, the requirements for an intensified growth of the austenitic grain are given. With the knowledge of the A_{r3} – temperature and the other conditions in the HAZ during welding (e.g. heating and cooling rate, peak temperature) it is possible to calculate the conditions for the growth of the austenitic grain and to estimate the material structure, that will be formed.

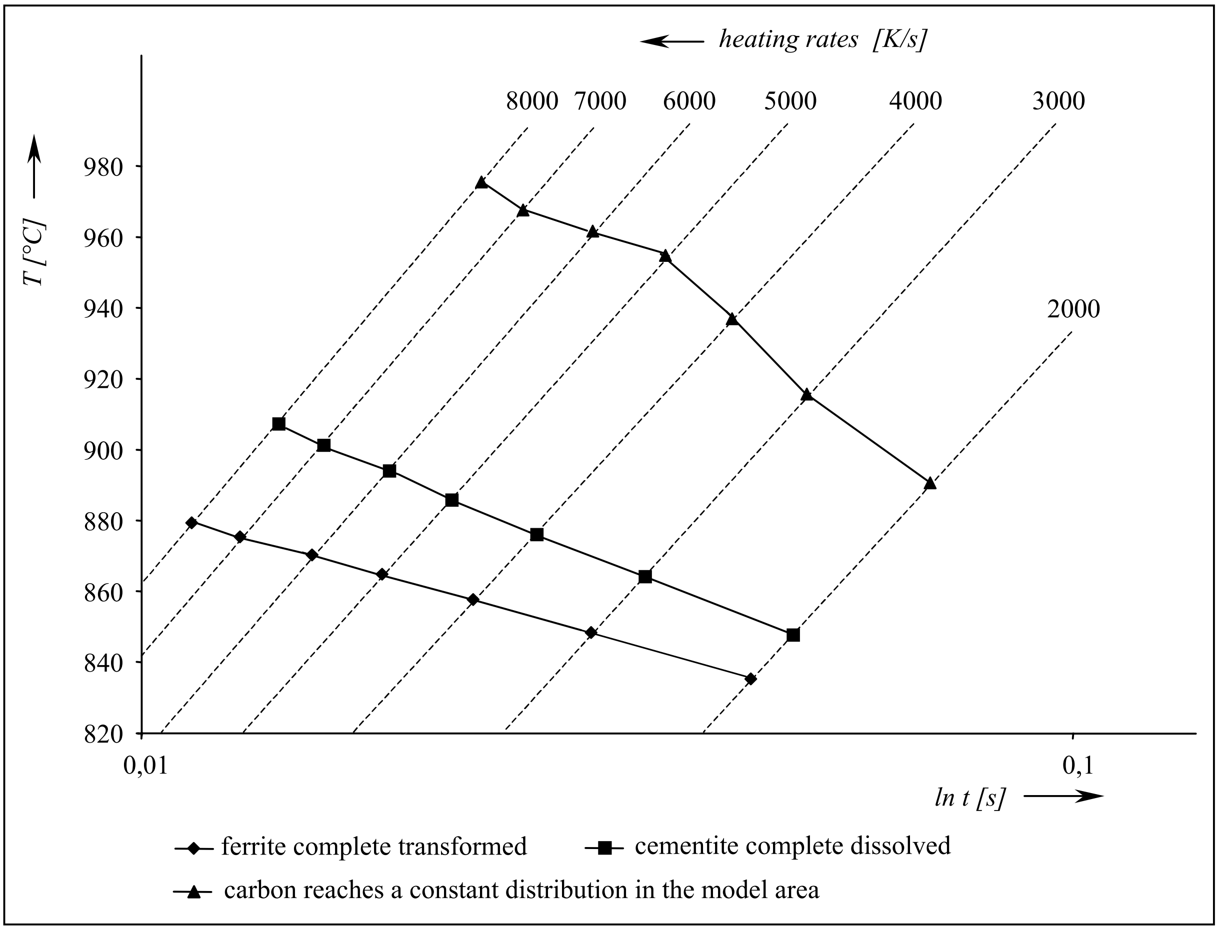


***Fig.** 7: Calculated Perlite – Transformation – Diagram*

5 Conclusions

The presented diagrams and calculations make clear the great dynamics of the transformation kinetics in the binary system Fe – C in case of very fast thermal cycles. The connection between the micro Monte – Carlo – model and the macro diffusion – model at a certain temperature allows an theoretical estimation of the transformation behaviour of unalloyed constructional steel under welding conditions.

In connection with the results from fast heating experiments using a “GLEEBLE 3500” – system, which show the real material structure after very fast thermal cycles with heating rates up to 6.000 K/s, a method exists to help us to understand the transformation behaviour in case of laser welding.

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