

METRO

MEtallurgical TRaining On-line



Computer modelling of phase transformation of cast alloys in solid state especially taking into consideration ADI castings

Lecture I: ADI, Austenitization

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AGH



Education and Culture



AUSTENITIZATION

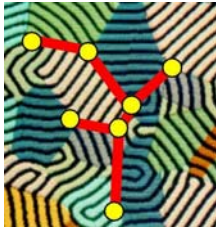


Abstract of Lecture

In computations of the kinetics of austenitizing, a one-dimensional model of austenite growth assuming a diffusion-related mechanism acting between the lamellae of ferrite and cementite was used. The diffusion-related mechanism of transformation was coupled with the transient field of temperature, resulting from preheating of the casting (sample) in a salt bath. The results of modeling were compared with the values of temperature measured in the preheated sample. For comparison, the Kolmogorov equation was also used to determine volume of the transformed phase, where the kinetics of the austenite grains nucleation and growth was related to overheating above the A_1 temperature in the Fe-C system (allowing for an effect of Si and Mn) and to the kinetics of sample preheating. The Kolmogorov equation was compared with the Johnson-Mehl-Avrami equation (for constant coefficients).

Keywords:

modeling, austenitization, pearlite, ductile iron, ADI

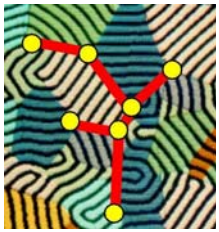


AUSTENITIZATION



Austenitizing as a first stage of the heat treatment of castings to obtain ADI (Fig. 1) consists in holding of castings at a temperature in the range of 800-950°C, to obtain austenitic structure of the matrix, considered to be a starting point for ausferritic structure. According to data given in literature, the temperature and time of austenitizing have certain effect on the parameters of both structure and mechanical properties of this cast iron after its final treatment, i.e. after austempering.

Too short time of austenitizing may cause incomplete transformation of pearlite into austenite, and consequently retain the untransformed structure, which has an unfavorable impact on ADI parameters. The necessary and optimum time of austenitizing greatly depends on the type of matrix (pearlitic, ferritic, or holding both of these structural constituents), and also on the degree of structure refining.



AUSTENITIZATION

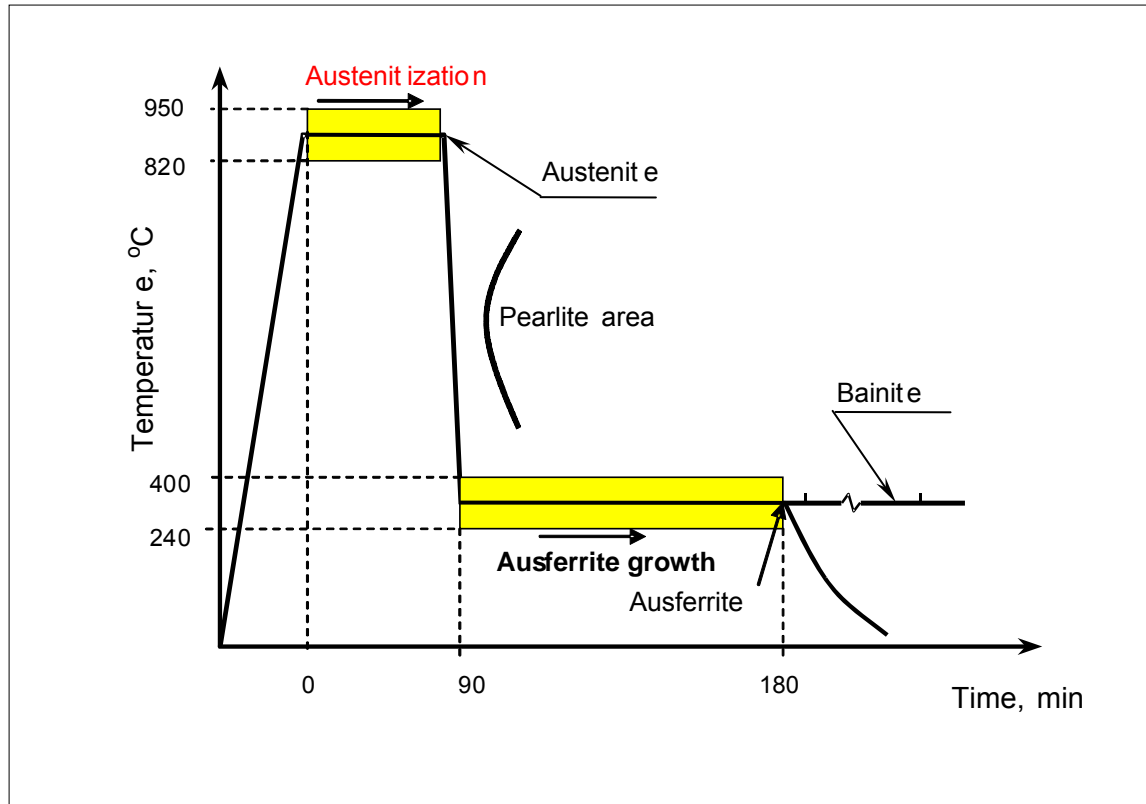
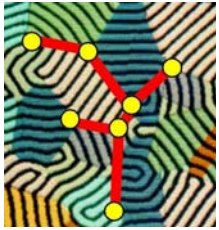


Fig. 1. Austenitization - the first step for ADI technology



Austenitization – process models



According to the data quoted by literature, three groups of models can be distinguished; they approach the process of austenitization through:

- diffusion-related mechanism acting between the lamellae of ferrite, cementite and austenite [Akbay, Reed, Atkinson 1994-96, Mancini, Budde 1999, Caballero, Capdevila, Garcia de Andres 2000];
- diffusion field in the growing grain of austenite on the front of ferrite and cementite lamellae [A. Jacot, M. Rappaz, R.C. Reed 1997-98 – numerical model , Gaude-Fugarolas, Bhadeshia 2003 - analytical model];
- Avrami equation (Johnson-Mehl-Avrami or Kolmogorov-Johnson-Mehl-Avrami equation) for volume-related relationship between the growing phase of austenite and time [Roosz, Gacsi, Fuchs 1983, Nihli Ahmadabadi, Parsa 2001, Elmer et al. 2003, Szeng, Shi 2004, Kumar et al. 2005].



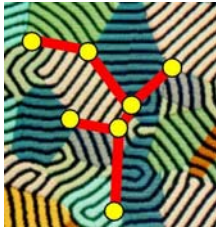
AUSTENITIZATION



In this study, the first from the above mentioned models of austenite growth in pearlite (a lamellar 1D model) was used, where the diffusion-related lamellar mechanism of transformation was coupled with transient field of temperature (3D), resulting from preheating of casting (sample) in salt bath (seemingly isothermal process).

The results of modeling were compared with the results of temperature measurement in preheated sample. For comparison, Kolmogorov equation was also used (as a model from group second mentioned above) to determine volume of the transformed phase, where the kinetics of the austenite grains nucleation and growth was related to overheating above the temperature A_1 in Fe-C system (allowing for an effect of Si and Mn) and to the kinetics of sample preheating.

Kolmogorov equation was compared with Johnson-Mehl-Avrami equation (for constant coefficients).



Austenitization – profile of model



Modelling was performed on a half-lamella of cementite and a half-lamella of ferrite which, when put together, were conventionally claimed to form a lamella of pearlite of the thickness X_{prl} .

The model considers the following problems:

- kinetics of sample (casting) preheating in an austenitizing bath;
- carbon diffusion caused by changes in conditions of phase equilibrium on preheating of the sample (casting) in an austenitizing bath;
- migration of phase boundaries caused by carbon diffusion;
- variations in carbon diffusion coefficient in austenite and ferrite in function of temperature;
- effect of Si and Mn content on the orientation of equilibrium lines in an Fe-C alloy.

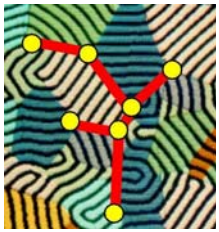


Austenitization – profile of model (cont.)



It is assumed that austenite nucleates in the form of lamellae along the whole length between cementite and ferrite, at the onset of the austenitization process, upon exceeding the boundary line in phase equilibrium diagram.

The point of departure for further considerations will be an Fe-Fe₃C system (Fig. 2a), where some typical points of phase equilibrium have been plotted. The same points are also visible on a schematic representation of a pearlite lamella (Fig. 2b) in which, at a certain stage of growth, a lamella of austenite is present, too.



Austenitization – profile of model (cont.)

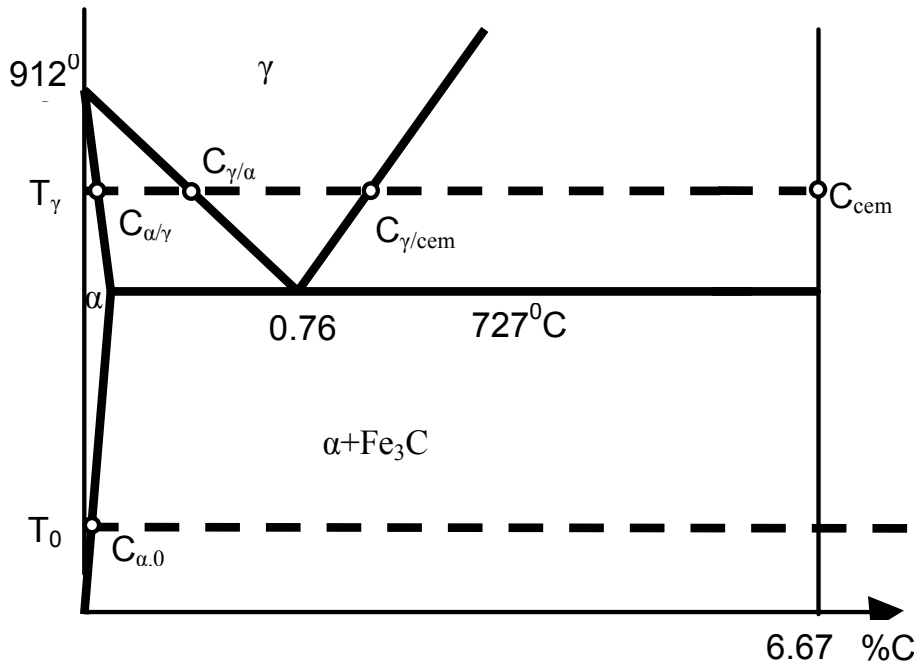


Fig. 2a. Scheme of metastable equilibrium diagram for Fe-Fe₃C.

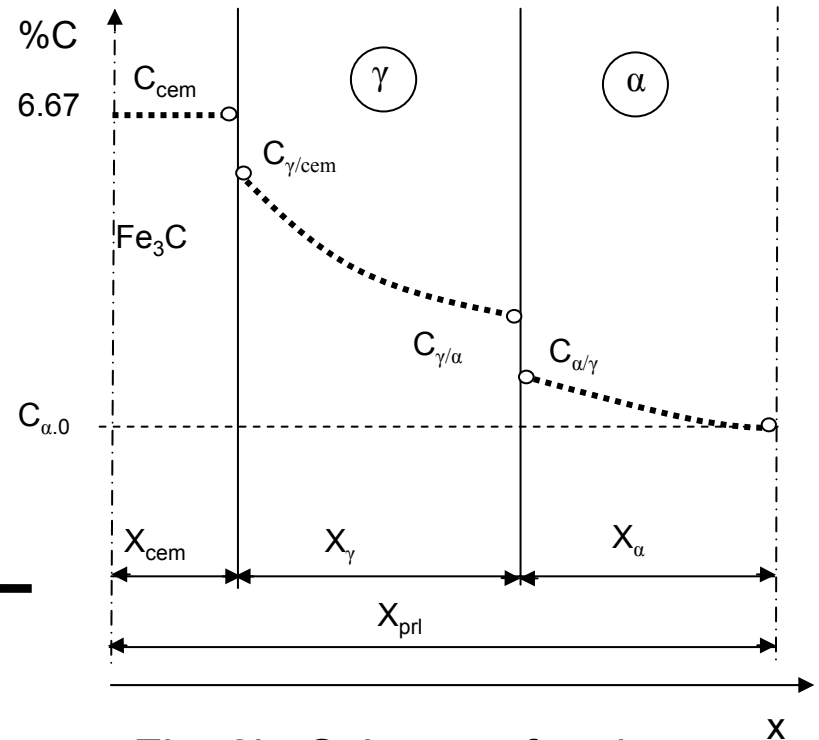


Fig. 2b. Scheme of carbon concentration in pearlite plate during austenitization.



Austenitization – profile of model (cont.)



The process is controlled by carbon diffusion coupled with temperature field. It is assumed that cementite, as a constituent of pearlite, has a constant carbon content (6,67% mass), while concentration gradients may occur in ferrite and in the growing austenite. For this case, a system of process equations can be written down as:

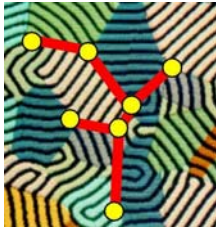
a diffusion-related equation
for phase α (ferrite):

$$\frac{\partial C_{\alpha}}{\partial \tau} = D_{\alpha} \frac{\partial^2 C}{\partial x^2}$$

and for phase γ (austenite):

$$\frac{\partial C_{\gamma}}{\partial \tau} = D_{\gamma} \frac{\partial^2 C}{\partial x^2}$$

where C , D , τ – concentration of carbon in Fe , diffusion coefficient and time



Austenitization – profile of model



Mass balance at the cementite – phase γ interface

$$u_{\gamma/cem} (C_{cem} \rho_{cem} - C_{\gamma/cem} \rho_{\gamma}) = D_{\gamma} \rho_{\gamma} \left. \frac{\partial C_{\gamma}}{\partial x} \right|_{x_{cem/\gamma}^+}$$

and at the phase α – phase γ interface

$$u_{\gamma/\alpha} (C_{\gamma/\alpha} \rho_{\gamma} - C_{\alpha/\gamma} \rho_{\alpha}) = -D_{\gamma} \rho_{\gamma} \left. \frac{\partial C_{\gamma}}{\partial x} \right|_{x_{\gamma/\alpha}^+} + D_{\alpha} \rho_{\alpha} \left. \frac{\partial C_{\alpha}}{\partial x} \right|_{x_{\gamma/\alpha}^-}$$

Condition at the pearlite lamella interface:

$$\left. \frac{\partial C_{\alpha}}{\partial x} \right|_{x=X_{prl}} = 0$$



Austenitization – profile of model



Heat conduction for casting:

$$\frac{\partial T}{\partial \tau} = a \nabla^2 T + \frac{L_p}{c} \frac{d\xi_\gamma}{d\tau}$$

where L_p – heat of ferrite – austenite transformation, J/g

c – specific heat of cast iron, J/(g K)

ξ_γ - fraction of austenite layer thickness

with boundary conditions of the 3rd type.



Austenitization – profile of model



A temperature relationship of carbon diffusion coefficient in austenite and ferrite according to Fig. 3 was adopted:

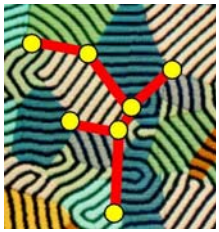
$$D_{\alpha} = 7.90 \cdot 10^{-3} \exp\left(-\frac{7.58 \cdot 10^4}{R \cdot T}\right) \quad D_{\gamma} = 1.67 \cdot 10^{-2} \exp\left(-\frac{1.20 \cdot 10^5}{R \cdot T}\right) \quad \text{cm}^2/\text{s}$$

as well as a relationship of equilibrium concentration limits according to an Fe-Fe₃C system:

$$C_{\alpha/\gamma} = -\frac{T - 912}{9249.96} \quad C_{\gamma/\alpha} = -\frac{T - 912}{240.26} \quad C_{\gamma/cem} = \frac{T - 485.08}{314.18}$$

By means of a *Thermocalc* program, the concentration limits were determined for an Fe-C system containing 2% Si and 0.8% Mn:

$$C_{\alpha/\gamma} = \frac{991.73 - T}{15498} \quad C_{\gamma/\alpha} = \frac{976.3 - T}{372.3} \quad C_{\gamma/cem} = \frac{T - 491.27}{365.95}$$



Austenitization – profile of model (cont.)

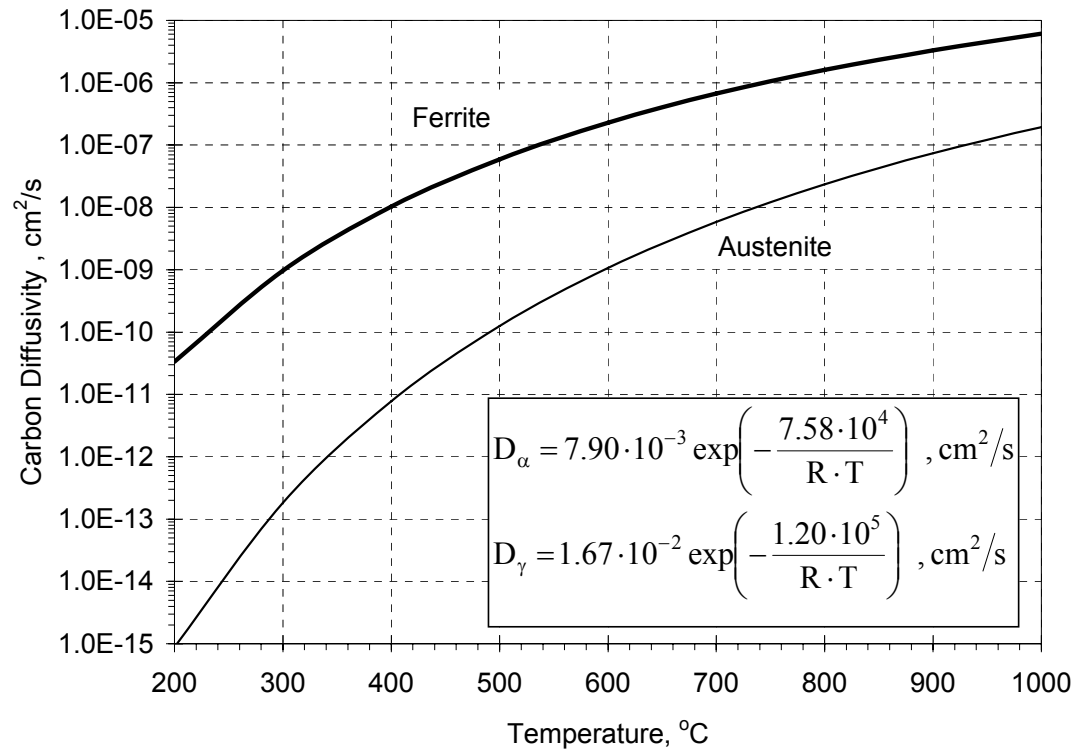
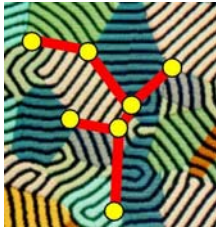


Fig. 3: Coefficient of carbon diffusion in austenite and ferrite

Remark: very strong relationship of the temperature (logarithmic scale), very high difference between carbon diffusivity in austenite and ferrite!



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To solve the system of equations, the methods of finite difference and of variable mesh were used (Appendix and Lecture III)



Kolmogorov model

According to [A.N. Kolmogorov, 1937], the content of transformation products can be determined from the following equation:

$$f_s = 1 - \exp(-\Omega(t))$$

For an arbitrary nucleation rate α and for an arbitrary growth rate u

$$\Omega(t) = \frac{4\pi}{3} c^3 \int_0^t \alpha(t') \left(\int_{t'}^t u(\tau) d\tau \right)^3 dt'$$

where c is the shape factor (for spherical grains $c = 1$), and t' is the nucleation time of particular grains.

Function $\Omega(t)$ determines the, so called, "Extended Volume" of the grains in transformation product. This is the total relative volume that all the crystals taken together might have occupied, if they had had the chance to grow free, and if their overlapping with the neighboring crystals in the space and blocking of each other had been neglected.



Kolmogorov model

In the adopted model, all the cases of the growth rate depending on overheating

$$u = \mu(\Delta T)^n$$

for $n = 0.5, 1$ and 2 and the instantaneous nucleation and continuous nucleation (the quantity of grains proportional to the second power of overheating) were checked.

In the case of instantaneous nucleation, the value of function α will equal zero over the entire time interval, the only exception being an infinitely small interval δt at the very beginning of the process. Within this interval $\alpha \rightarrow \infty$ while product $\alpha\delta = N$ and the function is confined and determines the number of grains in a unit volume.

Then the extended volume:

$$\Omega(t) = \frac{4\pi}{3} N \left(\int_{t'}^t u(\tau) d\tau \right)^3$$



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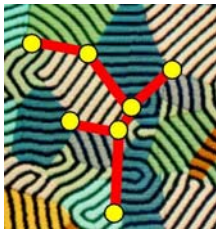


Results of experiments and computations

The results of computations were compared with the results of measurements of the temperature field in a sample of ductile iron (C- 3.5%, Si – 2.0%, Mn – 0.8%) of a pearlitic matrix and dimensions 6x10x15 mm.

The sample was placed in salt bath in a silite furnace with temperature control unit. The temperature was measured in the geometrical centre of the sample by means of an Ni-CrNi thermocouple of 0.2 mm thickness; the temperature of the salt bath was measured as well.

The run of temperature changes in the centre of the sample (for a series of four measurements) does not indicate the occurrence of any transformation related with thermal effects. An effect of this type is visible only when a temperature derivative is computed from the taken measurements and is plotted in the form of an arrest on the derivative curves within the time interval from about 65 to 100 seconds, counted from the beginning of sample preheating – Fig. 4.



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Results of experiments and computations

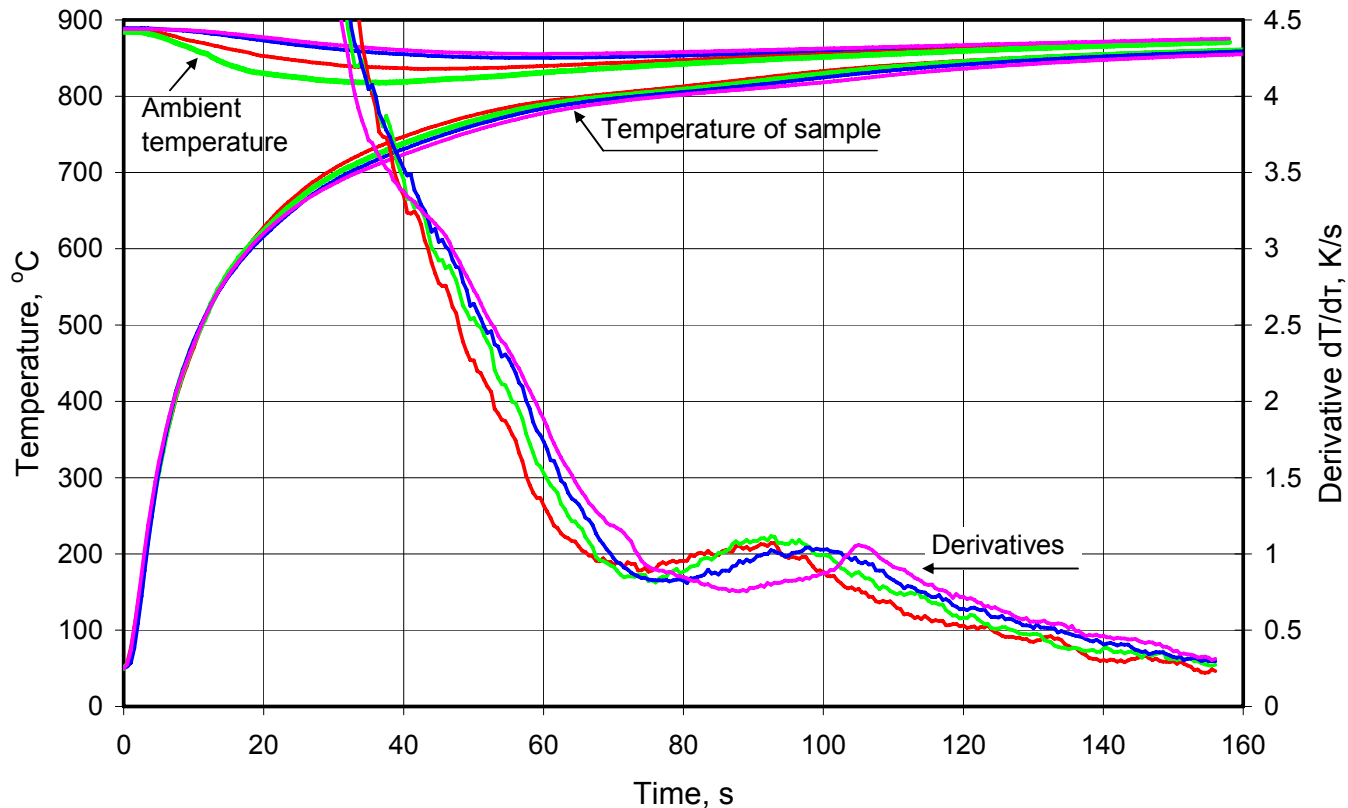


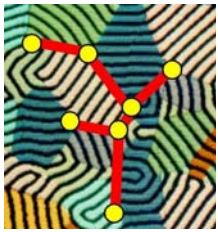
Fig. 4. The run of sample preheating curves for four measurements, the corresponding derivatives, and the temperature of salt bath (sample environment).



AUSTENITIZATION

Results of experiments and computations

An inflexion point on the temperature derivative curves plotted from the measurements, caused by the thermal effect of pearlite-austenite transformation, was used to estimate a value of this effect. In this case, the method of thermal analysis proposed by Chen and Stefanescu [1984] was applied, and using four preheating curves, a value of the heat of pearlite-austenite transformation was obtained (endothermic effect) $L_{prl}/\gamma = 12.8 \text{ J/g}$ (with standard deviation $\sigma = 1.8$).



AUSTENITIZATION



Results of computations

An example of modeled distribution of temperature, fractions of austenite and cementite across the casting section is shown in Fig. 5 and in Fig. 6 (screen printout, also with ferrite fraction). Differences in all the examined values across the casting section are visible.

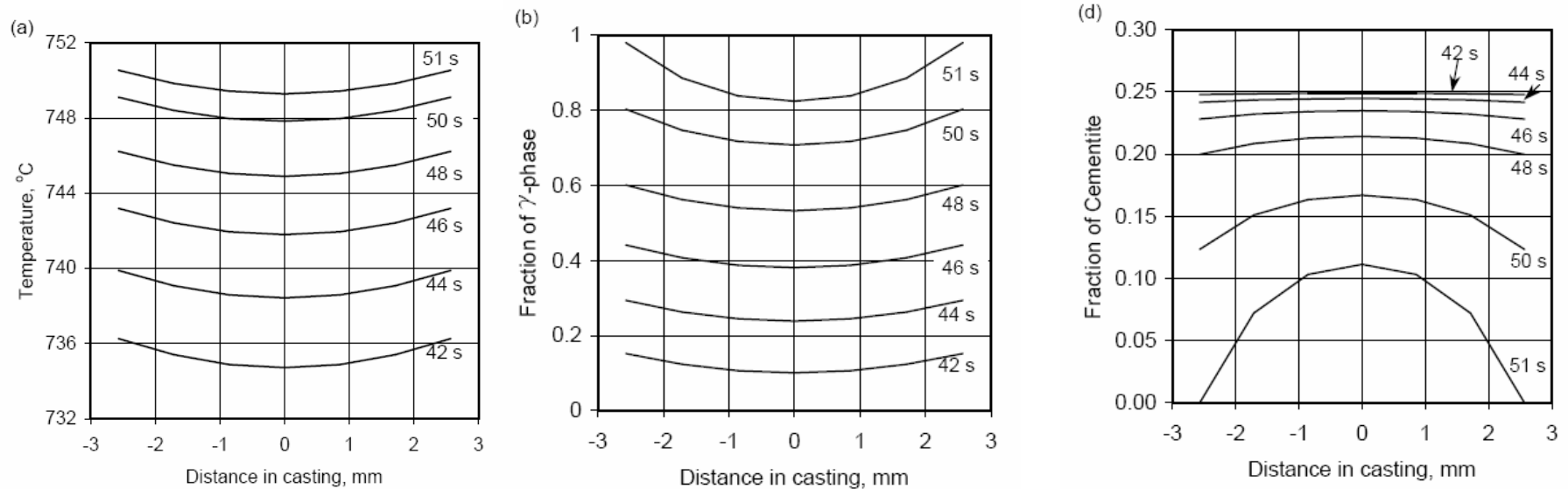
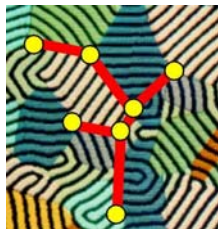


Fig. 5. Distribution of temperature (a), fraction of austenite (b), and cementite (d) across the casting section (modeling).



Results of computations



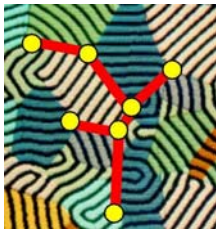
Time = 48.0 s; Temperature						
744.1	743.3	742.9	742.7	742.9	743.3	744.1
744.1	743.4	742.9	742.8	742.9	743.4	744.1
744.2	743.5	743.0	742.9	743.0	743.5	744.2
744.4	743.6	743.2	743.0	743.2	743.6	744.4
744.5	743.8	743.3	743.2	743.3	743.8	744.5
744.8	744.0	743.6	743.4	743.6	744.0	744.8
745.1	744.3	743.9	743.7	743.9	744.3	745.1
745.4	744.7	744.2	744.1	744.2	744.7	745.4
745.8	745.0	744.6	744.5	744.6	745.0	745.8
746.2	745.5	745.1	744.9	745.1	745.5	746.2
746.7	746.0	745.6	745.4	745.6	746.0	746.7
747.3	746.6	746.1	746.0	746.1	746.6	747.3
747.9	747.2	746.8	746.6	746.8	747.2	747.9
748.6	747.9	747.5	747.3	747.5	747.9	748.6
749.4	748.7	748.3	748.1	748.3	748.7	749.4
750.2	749.5	749.1	749.0	749.1	749.5	750.2
751.1	750.4	750.0	749.9	750.0	750.4	751.1

Austenite						
0.505	0.469	0.447	0.440	0.447	0.469	0.505
0.507	0.471	0.449	0.442	0.449	0.471	0.507
0.511	0.474	0.453	0.446	0.453	0.474	0.511
0.517	0.480	0.459	0.451	0.459	0.480	0.517
0.524	0.488	0.466	0.459	0.466	0.488	0.524
0.534	0.498	0.476	0.469	0.476	0.498	0.534
0.547	0.510	0.488	0.481	0.488	0.510	0.547
0.562	0.524	0.503	0.495	0.503	0.524	0.562
0.580	0.542	0.520	0.512	0.520	0.542	0.580
0.601	0.562	0.540	0.533	0.540	0.562	0.601
0.626	0.586	0.563	0.556	0.563	0.586	0.626
0.655	0.614	0.591	0.583	0.591	0.614	0.655
0.689	0.647	0.623	0.615	0.623	0.647	0.689
0.731	0.686	0.660	0.652	0.660	0.686	0.731
0.784	0.733	0.705	0.696	0.705	0.733	0.784
0.856	0.792	0.760	0.750	0.760	0.792	0.856
0.980	0.878	0.834	0.821	0.834	0.878	0.980

Ferrite						
0.276	0.307	0.325	0.331	0.325	0.307	0.276
0.274	0.305	0.324	0.330	0.324	0.305	0.274
0.271	0.302	0.320	0.327	0.320	0.302	0.271
0.266	0.297	0.315	0.322	0.315	0.297	0.266
0.260	0.290	0.309	0.315	0.309	0.290	0.260
0.252	0.282	0.300	0.307	0.300	0.282	0.252
0.242	0.272	0.290	0.296	0.290	0.272	0.242
0.230	0.260	0.278	0.284	0.278	0.260	0.230
0.216	0.246	0.264	0.270	0.264	0.246	0.216
0.199	0.229	0.247	0.253	0.247	0.229	0.199
0.181	0.211	0.228	0.234	0.228	0.211	0.181
0.160	0.189	0.207	0.213	0.207	0.189	0.160
0.137	0.166	0.183	0.189	0.183	0.166	0.137
0.111	0.139	0.157	0.162	0.157	0.139	0.111
0.083	0.110	0.127	0.133	0.127	0.110	0.083
0.052	0.079	0.095	0.100	0.095	0.079	0.052
0.020	0.044	0.060	0.065	0.060	0.044	0.020

Cementite						
0.219	0.225	0.227	0.228	0.227	0.225	0.219
0.219	0.224	0.227	0.228	0.227	0.224	0.219
0.218	0.224	0.227	0.228	0.227	0.224	0.218
0.217	0.223	0.226	0.227	0.226	0.223	0.217
0.216	0.222	0.225	0.226	0.225	0.222	0.216
0.214	0.220	0.224	0.225	0.224	0.220	0.214
0.212	0.218	0.222	0.223	0.222	0.218	0.212
0.209	0.216	0.219	0.221	0.219	0.216	0.209
0.205	0.213	0.217	0.218	0.217	0.213	0.205
0.200	0.208	0.213	0.214	0.213	0.208	0.200
0.193	0.203	0.208	0.210	0.208	0.203	0.193
0.185	0.196	0.202	0.204	0.202	0.196	0.185
0.174	0.187	0.194	0.196	0.194	0.187	0.174
0.158	0.175	0.183	0.186	0.183	0.175	0.158
0.134	0.157	0.168	0.171	0.168	0.157	0.134
0.092	0.129	0.145	0.150	0.145	0.129	0.092
-0.000	0.078	0.106	0.113	0.106	0.078	-0.000

Fig. 6. Screen printout of the modeled temperature field, values of the fraction of austenite, ferrite and cementite.



AUSTENITIZATION

Results of experiments and computations

Figure 7 shows experimental temperature curves and their respective derivatives, compared to the results of computations performed by means of the Kolmogorov model.

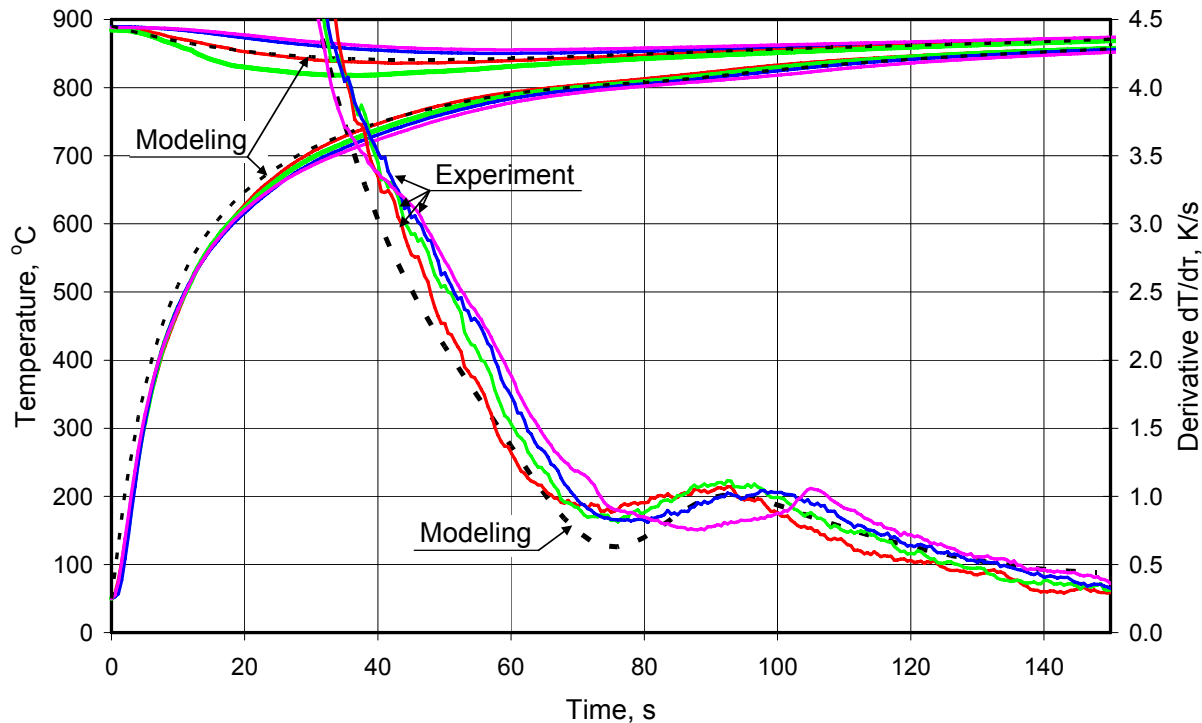


Fig. 7. A compilation of data from measurements (solid lines) and computations (dashed lines).



AUSTENITIZATION



Results of experiments and computations

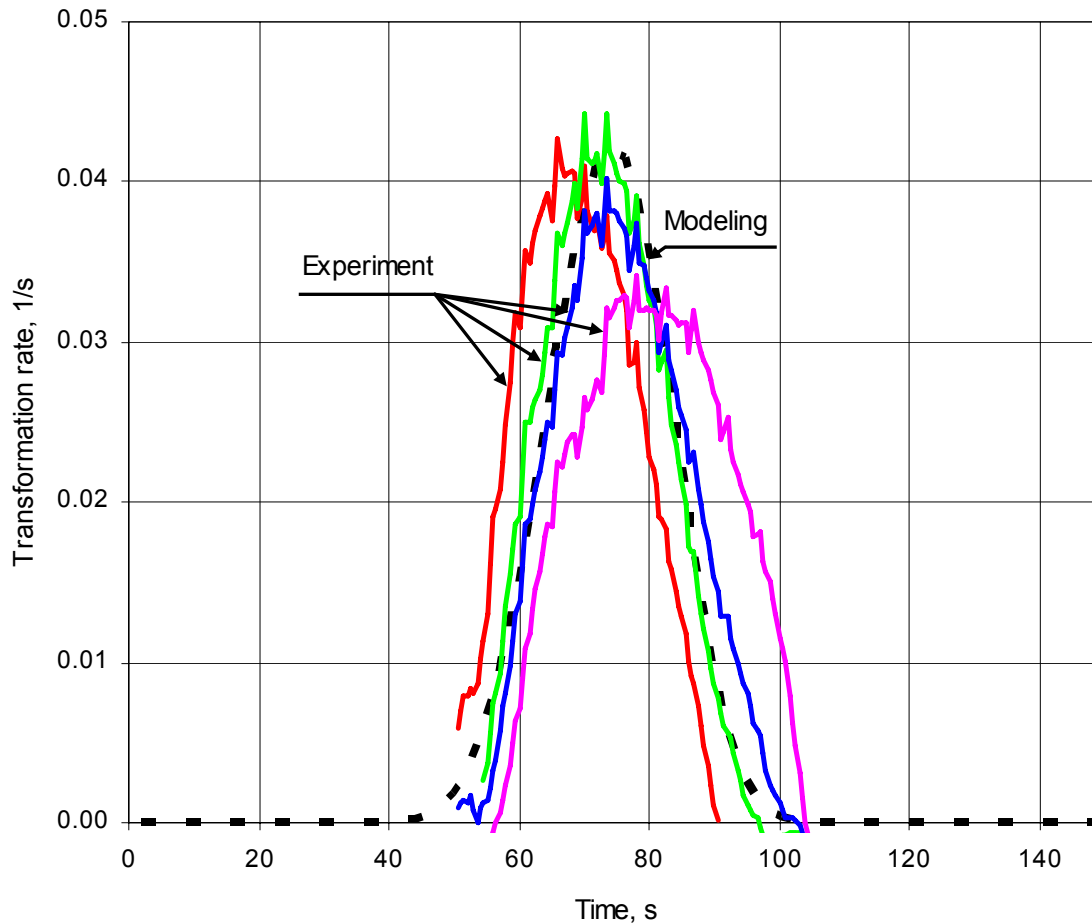
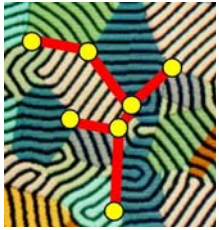


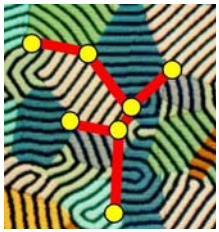
Fig. 8. Kinetics of phase transformation computed by an analysis of the derivatives from measurements (solid lines) and modeling (dashed line).



AUSTENITIZATION

SUMMARY

1. The diffusion model of austenite growth from pearlite (i.e. from the ferrite and cementite lamellae) enables quantitative calculation of the kinetics of austenite growth with determination of the kinetics of carbon concentration and temperature field across the casting.
2. Application of Kolmogorov equation with constant number of nuclei and variable rate of growth in function of overheating gave the values of the kinetics of transformation similar to the experimental ones.
3. In the process of austenitization an important role is played by the kinetics of sample (casting) heating. The time of preheating, even in the case of a high-rate preheating (e.g. in salt bath), considerably exceeds the time of the austenitizing process itself.



AUSTENITIZATION - APPENDIX



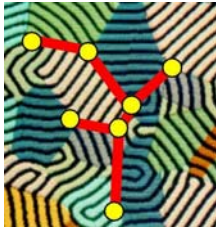
A numerical scheme to calculate „extended volume”

It is assumed that the grains are of a spherical shape, and the number of grains in a unit volume as well as the linear rate of their growth are the well known functions of undercooling: $N(\Delta T)$ and $u(\Delta T)$.

Let us introduce symbols R_i and S_i for the grain radius and surface area i , respectively.

Let us introduce the following symbols for the sum of extended volumes of all the grains (Ω) whose centers of nucleation are located within the area of a unit volume, for total area of external surfaces of the extended volumes of the examined grains (S_Ω), and for the sum of their radii (R_Ω):

$$\Omega = \frac{4}{3} \pi \sum_{i=1}^{N(\Delta T)} R_i^3 \quad S_\Omega = 4\pi \sum_{i=1}^{N(\Delta T)} R_i^2 \quad R_\Omega = \sum_{i=1}^{N(\Delta T)} R_i \quad (1)$$



AUSTENITIZATION – APPENDIX

– cont.



Since it has been assumed that at a given time instant all grains are growing with the same linear velocity, the derivatives Ω , S_Ω and R_Ω after the time τ are:

$$\frac{d\Omega}{d\tau} = u(\Delta T) \cdot 4\pi \sum_{i=1}^{N(\Delta T)} R_i^2 \quad \frac{dS_\Omega}{d\tau} = u(\Delta T) \cdot 8\pi \sum_{i=1}^{N(\Delta T)} R_i \quad \frac{dR_\Omega}{d\tau} = \sum_{i=1}^{N(\Delta T)} u(\Delta T) \quad (2)$$

or, allowing for (1):

$$\frac{d\Omega}{d\tau} = u(\Delta T) \cdot S_\Omega \quad \frac{dS_\Omega}{d\tau} = u(\Delta T) \cdot 8\pi R_\Omega \quad \frac{dR_\Omega}{d\tau} = u(\Delta T) \cdot N(\Delta T) \quad (3)$$



AUSTENITIZATION – APPENDIX – cont.



After transformation of differentials (3) to a difference form, the following difference model can be proposed for computation of extended volume for any arbitrary temperature dependence between the grains number and their growth rate:

$$R_{\Omega,k+1} = R_{\Omega,k} + u(\Delta T) N(\Delta T) \Delta \tau \quad (4)$$

$$S_{\Omega,k+1} = S_{\Omega,k} + u(\Delta T) 8\pi R_{\Omega,k} \Delta \tau \quad (5)$$

$$\Omega_{k+1} = \Omega_k + u(\Delta T) S_{\Omega,k} \Delta \tau \quad (6)$$