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# Chapter 7

# ALLOTRIOMORPHIC FERRITE FORMATION
# IN A HETEROGENEOUS STEEL

## 7.1 Introduction

Allotriomorphic ferrite is the first phase to form by the reconstructive trans-
formation of austenite in low alloy steels, when the austenite is cooled below the
$A_{e3}$ temperature[1,2]. It nucleates at the austenite grain boundaries and in low al-
loy steels can eventually form continuous polycrystalline layers decorating the grain
surfaces. Subsequent growth then essentially involves the one dimensional thickening
of these layers into the remaining austenite. During the growth of the ferrite, the car-
bon partitions into the residual austenite ahead of austenite/ferrite interface so that
the driving force for $\gamma \rightarrow \alpha$ transformation is decreased. Eventually, when the equi-
librium volume fraction is achieved, the driving force is reduced to zero and interface
motion ceases. The fundamental aspects of allotriomorphic ferrite have recently been
reviewed[3].

Variations in alloy content lead to differences in the driving force for transforma-
tion, which may have a strong effect on nucleation and the subsequent growth of allotri-
omorphic ferrite. This has important consequences in the prediction of microstructure.
The work presented here is an investigation of the paraequilibrium formation of ferrite
in a heterogeneous alloy of average composition Fe-0.2C-1.37Mn-0.35Si wt. %.

## 7.2 Theoretical Analysis

The lever rule suggests that the maximum volume fraction of ferrite that can form
at any given temperature should vary linearly with the average carbon content of the
steel concerned. However, it has been reported[4] that this relation does not hold for
chemically heterogeneous steels. Bhadeshia[5] presented a model for ferrite formation
in heterogeneous dual-phase steels which explained these data, and suggested that the
effect of segregation should vary with undercooling. This model was discussed in terms
of a ternary alloy, *e.g.,* Fe-Mn-C, of average Mn concentration $\overline{\text{Mn}}$, but with local
variations ranging between the limits $\text{Mn}_{min}$ and $\text{Mn}_{max}$. In his simplified model, the
transformation was considered to take place by the motion of a planar $\gamma/\alpha$ interface

is normal to the isoconcentration planes, as illustrated in Fig. 7.1. The position of this interface, with respect to Z, at any instant thus defines the volume fraction V of ferrite, *i.e.*, V≡Z, reaching its maximum value of unity when the interface reaches the position where $Mn = Mn_{max}$.

At relatively high temperatures (above the $A_{e3}$ of the homogeneous alloy), the interface is expected to stop at a point where $Mn < \overline{Mn}$ as shown in Fig. 7.2a. There will then be some transformation in the heterogeneous sample but none in the homogeneous alloy. This situation will continue until the interface reaches a stage where $Mn = \overline{Mn}$ (Fig. 7.2b) *i.e.*, the temperature falls to below the $A_{e3}$ temperature of the homogeneous alloy. The model then suggests that transformation will occur to an identical extent, in both the heterogeneous and homogeneous samples. Beyond this point (Figs. 7.2c and 7.2d) it is expected that there should be more transformation in the homogeneous sample relative to that in the segregated sample.

### 7.2.1 Computer Simulation of the Published Model[5]

As will be seen later, circumstances may arise where the transformation front does not necessarily advance in a direction normal to the isoconcentration surfaces. The problem is here investigated by developing a computer model, whose performance is first checked against Bhadeshia's analytical approach.

The computer program was designed to simulate the development of ferrite formation in chemically heterogeneous steels. In this model, consistent with the previous work[5], the substitutional solute was assumed to vary linearly with distance as illustrated in Fig. 7.3 although the program is able to adopt any arbitrary composition profiles. The heterogeneous steel was represented as a composite of $N$ slices of equal thickness (Fig. 7.4). Each slice, identified by a subscript $i$, was assigned a different chemical composition within the range of experimental measurements of the minimum and maximum alloy content (Fig. 7.5). Microanalysis experiments were carried out using energy dispersive X-ray analysis (interaction volume approximately 4.5 $\mu m^3$) on a scanning electron microscope. The composition within each slice was set to be uniform. The mean composition of all the slices was set to be identical to the mean composition of the as-received steel.

The calculation begins with the complete transformation of the first slice in the solute-depleted region (*i.e.*, i=1), given that its $A_{e3}$ temperature ($T^i_{A_{e3}}$) is higher than

the isothermal transformation temperature $T$ and at the same time $x_\gamma = \overline{x}$ is also less than its $x_{A_{e3}}$, which is the maximum carbon that can be tolerated by the austenite transforming under paraequilibrium conditions. $x_\gamma$ and $\overline{x}$ are the carbon concentrations of the residual austenite and of the average carbon content of the alloy respectively. This transformation changes the carbon concentration of the residual austenite $x_\gamma$ according to the following simple mass balance equation.

$$x_\gamma = \overline{x} + \frac{\frac{i}{N}(\overline{x} - x_\alpha)}{(1 - \frac{i}{N})} \qquad (7.1)$$

Where, $\frac{i}{N} = V$ is the total volume fraction of ferrite when $i$ number of slices are able to transform. $x_\alpha$ is the amount of carbon which is left in the ferrite assumed to be 0.03 wt. %.

The growth of allotriomorphic ferrite in dilute steels generally occurs without the bulk partitioning of substitutional alloying elements[6], especially when the growth rates involved are large[7]. Only carbon then partitions during growth. In such circumstances, ferrite growth can occur at a rate controlled by the diffusion of carbon in the austenite ahead of the interface. In these calculations it was, therefore, assumed that $\alpha$ growth occurs by a carbon diffusion paraequilibrium[8−12] mechanism so that substitutional alloying elements do not partition at all between the phases; carbon then partitions to an extent which allows its chemical potential to be identical in all phases.

Hence, transformation is only allowed to continue in the next slice $i$ if for that slice $x_\gamma < x^i_{A_{e3}}$. The calculation is stopped at a slice $i$ when $x_\gamma = x^i_{A_{e3}}$ as illustrated in Fig. 7.4.

*7.2.2 Results and Discussion*

The results obtained from the simulation of the Bhadeshia model[5] are shown in Fig. 7.6. At low undercoolings a greater volume fraction of ferrite was obtained in the heterogeneous alloy compared with the homogeneous alloy. Both volume fractions increased on decreasing temperature but their difference decreased until a crossover point after which the situation is reversed. It can be seen from Fig. 7.7 that the number of transforming slices decreased with an increase in the isothermal transformation temperature. During the course of transformation at any specified temperature, the amount of carbon that can be tolerated by the austenite decreases while at the same

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time, the carbon content of the residual austenite goes on increasing. The point where these two curves meet gives the limiting volume fraction of ferrite. These results are in good agreement with the predictions forwarded by Bhadeshia[5].

Although the model is a good representation of transformation in a heterogeneous sample during continuous cooling, it might not be applicable under isothermal transformation conditions. If the driving force for transformation is large, the initial nucleation and growth of ferrite may not be restricted to the solute-depleted region. The nucleation and growth of ferrite can start at more than one place in case of isothermal transformation at large undercoolings. In these circumstances it is no longer reasonable to expect the transformation front to proceed from the solute-depleted to the solute-enriched regions, but reaction may occur everywhere.

To study this, the computer model was arranged to permit the motion of the $\gamma/\alpha$ interface to occur parallel to the isoconcentration planes as shown in Fig. 7.8. The calculation was carried out in incremental stages (Fig. 7.9), with each stage identified by the subscript $j$. It should be noted that each incremental step of transformation now happens in a direction normal to the isoconcentration planes, so that several slices could be reacting at any instant. The computation begins with all the slices being fully austenitic. For the first step ($j = 1$) $A_{e3}$ temperatures are calculated for all the slices. If for any slice, $T^i_{A_{e3}} < T$ then that slice remains untransformed throughout the experiment. For slices which are below their $T^i_{A_{e3}}$ temperatures, a small amount of ferrite is permitted to form, giving a volume fraction increment of $\Delta V$. This increment of transformation changes the carbon concentration in the unreacted regions of the slices according to a simple mass balance equation

$$x^{ij}_\gamma = \overline{x} + \frac{V_{ij}(\overline{x} - x_\alpha)}{(1 - V_{ij})} \tag{7.2}$$

where $V_{ij}$ and $x^{ij}_\gamma$ are, respectively, the total volume fraction of ferrite, and the total carbon concentration of the residual austenite in slice $i$ at stage $j$ of the calculation.

Hence, for $j > 1$, an increment of transformation is only allowed in any given slice if for that slice $x^{ij}_\gamma < x^i_{A_{e3}}$. $x_{A_{e3}}$ is the carbon that can be tolerated by the austenite transforming under paraequilibrium conditions. The mean volume fraction of transformation in the alloy as a whole at stage $j$ is given by:

$$\overline{V}_j = \sum_i V_{ij}/N. \tag{7.3}$$

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The calculation is stopped when all slices cease to transform; $x_\gamma^{ij} = x_{A_{e3}}^i$ for all $i$.

We consider first the case where the slices transform independently of each other, *i.e.*, without any homogenisation of carbon between the slices. The results thus obtained are shown in Fig. 7.10 which illustrate that as long as the alloy is transformed below the $A_{e3}$ temperature of the homogeneous alloy, there is no difference of volume fractions between the homogeneous and heterogeneous samples. This might be due to the fact that the composition variations detected here are not large eneough to produce a remarkable difference in volume fractions of allotriomorphic ferrite in homogeneous and heterogeneous samples. Moreover, due to the small slope of the $A_{e3}$ curve, the effect of chemical heterogeneity in shifting the $A_{e3}$ temperature is less as compared to that on $B_s$ while considering the slope of $T_0$ curve.

On the other hand, if transformation was induced at temperatures above the $A_{e3}$ temperature of the homogeneous alloy, ferrite formation obviously does not occur in the homogeneous sample, but some slices are able to transform in the heterogeneous sample.

At higher undercoolings, the nucleation and growth of ferrite is restricted to the solute depleted regions of the heterogeneous alloy, with relatively rapid reaction in those regions compared with the homogeneous alloy. The reaction in the segregated alloy will always be faster than the homogenised alloy. Limited transformation in the solute-enriched regions appears to be compensated by the ease of transformation in the solute-depleted regions.

At still higher undercoolings, nucleation and growth becomes possible everywhere in both the homogeneous and heterogeneous samples, *i.e.*, at these temperatures all the slices are able to transform to ferrite to a greater or lesser extent. Growth is then expected to be limited by the carbon enrichment of the residual austenite. For the case consisderd here, where it is assumed that excess carbon cannot redistribute between slices, the untransformed regions of the heterogeneous sample which are rich in substitutional alloy content, are unable to act as sinks for the excess carbon, so as to allow further transformation in the substitutional solute-depleted regions. When compared with bainite, the allotriomorphic ferrite carbon diffusion field in the austenite will be relatively large partly due to the higher transformation temperatures involved and partly because of the large size and less convoluted morphology of the growing

phase. The significance of this effect can be examined theoretically using the computer model with the additional condition that after every increment $\Delta V$ of transformation, the carbon is allowed to redistribute and homogenise between the slices. This should permit the solute-enriched regions to act as sinks for any excess carbon, thereby facilitating further transformation in the solute-depleted regions. The results (Fig. 7.10) show that if carbon is permitted to homogenise in the residual austenite after every increment of transformation, the volume fraction of transformation in the heterogeneous samples should always exceed that in the homogenised samples. The difference between the two cases decreases with an increase in undercooling.

## 7.3 Dilatometry

Dilatometric experiments were carried out to compare the experimental results with the predictions made by the models described above. The specimens were austenitised at 1000 °C for 10 minutes before helium gas quenching to a variety of isothermal transformation temperatures within the range where the reconstructive growth of ferrite alone is expected. The length change during the isothermal reaction was measured and the corresponding relative length change versus time data plotted as in Fig. 7.11. The optical micrographs in Fig. 7.12 give a comparison of the extent of transformation in the homogeneous and heterogeneous samples. The relative length change corresponding to a volume fraction of ferrite transformed $V_b$ is given by:

$$\frac{\Delta l}{l} = \frac{2V_b a_\alpha^3 + (1 - V_b)a_\gamma^3 - \bar{a}_\gamma^3}{3\bar{a}_\gamma^3} \tag{7.4}$$

where $a_\alpha$ is the lattice parameter of ferrite at the transformation temperature, given by:

$$a_\alpha = a_\alpha^o[1 + e_\alpha(T - 25)] \tag{7.5}$$

and $\bar{a}_\gamma$, which is the lattice parameter of austenite of the alloy composition at the transformation temperature, is give by:

$$\bar{a}_\gamma = (a_o^\gamma + \Sigma c_i x_i)[1 + e_\gamma(T - 25)]. \tag{7.6}$$

In these equations, $e_\alpha$ and $e_\gamma$ represent the linear thermal expansivities of ferrite and austenite respectively, $a_o$ is the lattice parameter of austenite in pure iron at 25 °C, $x_i$

is the concentration of alloying element $i$ and $c_i x_i$ represents the change in $a_o$ due to the addition of the alloying elements to pure iron. $T$ is the temperature in °C.

The ferrite linear expansion coefficient was determined by first tempering a specimen at 600 °C for 10 minutes to decompose any retained austenite and then recording the length change during very slow cooling. The measurements do not therefore account for the presence of any carbide, whose volume fraction is in any case expected to be negligibly small for the present purposes.

The graph of relative length versus temperature is plotted in Fig. 7.13, from which the linear expansion coefficient of ferrite was found to be $e_\alpha = 9.847 \times 10^{-6}$ K$^{-1}$. The expansion coefficient of austenite was measured while specimen was in the single-phase field, as shown in Fig. 7.14 ($e_\gamma = 2.122 \times 10^{-5}$K$^{-1}$). The ferrite lattice parameter $(a_\alpha^o)$ at ambient temperature was measured using a Debye-Scherrer technique. The test specimen was annealed at 600 °C for half an hour, and then machined to the form of 0.5mm × 0.5mm × 15mm wire. It was then immersed in an aqueous solution made up of 5% HF and 45% $H_2O_2$ (by volume) for two minutes to remove the deformation layer before testing. The specimens were irradiated with Mo K$_\alpha$ radiations using a standard Debye-Scherrer camera. A value of lattice parameter was calculated for each reflection from the resulting photograph and plotted against the Nelson-Riley function[13] of Bragg angle $\theta$. Linear regression technique was used to extrapolate a best-fit line back to $\theta = 90°$, to find the intercept and the standard error in the intercept (Fig. 7.15). The resulting value of lattice parameter was found to be as $2.8675 \pm 0.0015$ $\mathring{A}$ which is in good agreement with the value calculated to be 2.8667 $\mathring{A}$ using data from Leslie[14]. With these measured values and making the appropriate substitutions in equation 7.4, the volume fractions of ferrite transformed could be deduced using a computer program.

*7.3.1 Results and Discussion*

The carbon content of residual austenite when isothermal transformation ceases is very useful in understanding the transformation mechanism. The maximum relative length change was converted into the volume fraction of ferrite transformed, from which the carbon content of the residual austenite can be calculated using equation 7.1. It should be noted that no carbide precipitation was observed even at the lowest isothermal transformation temperature considered here which is 700 °C. That is evident from the transmission electron micrograph shown in Fig. 7.16 of the sample isothermally

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transformed at 700 °C. Isothermal transformation experiments were carried out over the temperature range 700-760 °C. The data thus obtained are plotted on a phase diagram as shown in Fig. 7.17. It is clear that for the short time heat treatments studied here, the reaction becomes imperceptibly slow before the austenite reaches its equilibrium composition. Hence, the assumption involved in the slice model, that the growth of $\alpha$ occurs under paraequilibrium conditions, seems reasonable.

The experimental data provided in Fig. 7.17 are not sufficiently extensive to confirm how the volume fraction of ferrite in a heterogeneous alloy should differ from a homogeneous alloy but the comparison available at two temperatures (i.e., 700 and 740 °C) shows that more transformation is obtained in heterogeneous sample. This is supported by the results obtained from the slice model, provided the carbon is allowed to homogenise among the slices. The data obtained at 730 °C are not consistent with the rest of the experiments as it shows lesser transformation than that observed at 740 °C. No obvious reasons could be found for this discrepancy, which is tentatively assigned to experimental error.

## 7.4 Conclusions

Allotriomorphic ferrite formation in a heterogeneous alloy has been modelled for situations equivalent to "continuous cooling" and isothermal transformation. In the first case, the $\gamma/\alpha$ transformation front was considered to move normal to the iso-concentration planes, i.e., from solute-depleted region to solute-enriched region. The results support the published predictions[5] that below the volume fraction of 0.5, there will be more transformation in a heterogeneous alloy than the homogeneous alloy while above the volume fraction of 0.5 the situation is reversed.

For isothermal transformation, the motion of $\gamma/\alpha$ transformation front was considered to be parallel to the isoconcentration planes. At any undercooling below $A_{e3}$ temperature of the homogeneous alloy, limited nucleation (in the areas whose alloy content is either equal or below the average alloy content) in the heterogeneous alloy can be compansated by the faster growth in the solute depleted regions. Moreover, due to higher transformation temperatures involved, carbon can distribute evenly throughout the residual austenite to facilitate still more transformation. It is found that the extent

of transformation is always larger for the heterogeneous samples when compared with the homogenised samples.

The model is based on the hypothesis that the growth of $\alpha$ occurs under paraequilibrium conditions. The experimental results presented here support this hypothesis, and provide a new way of deducing the paraequilibrium mode of transformation.
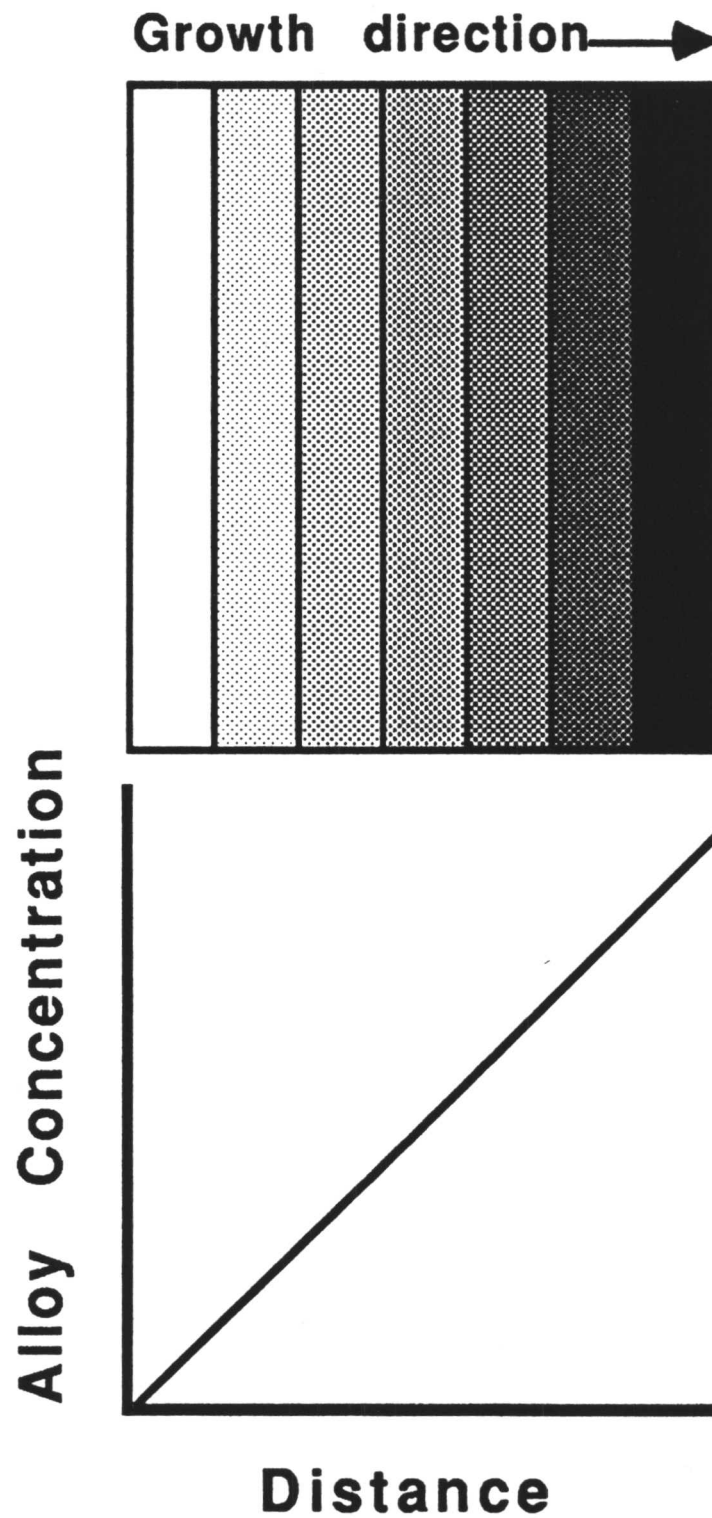
**Fig. 7.1:** *In the model for allotriomorphic ferrite in heterogeneous steels[5], the growth direction of the ferrite is considered to be normal to the isoconcentration planes.*
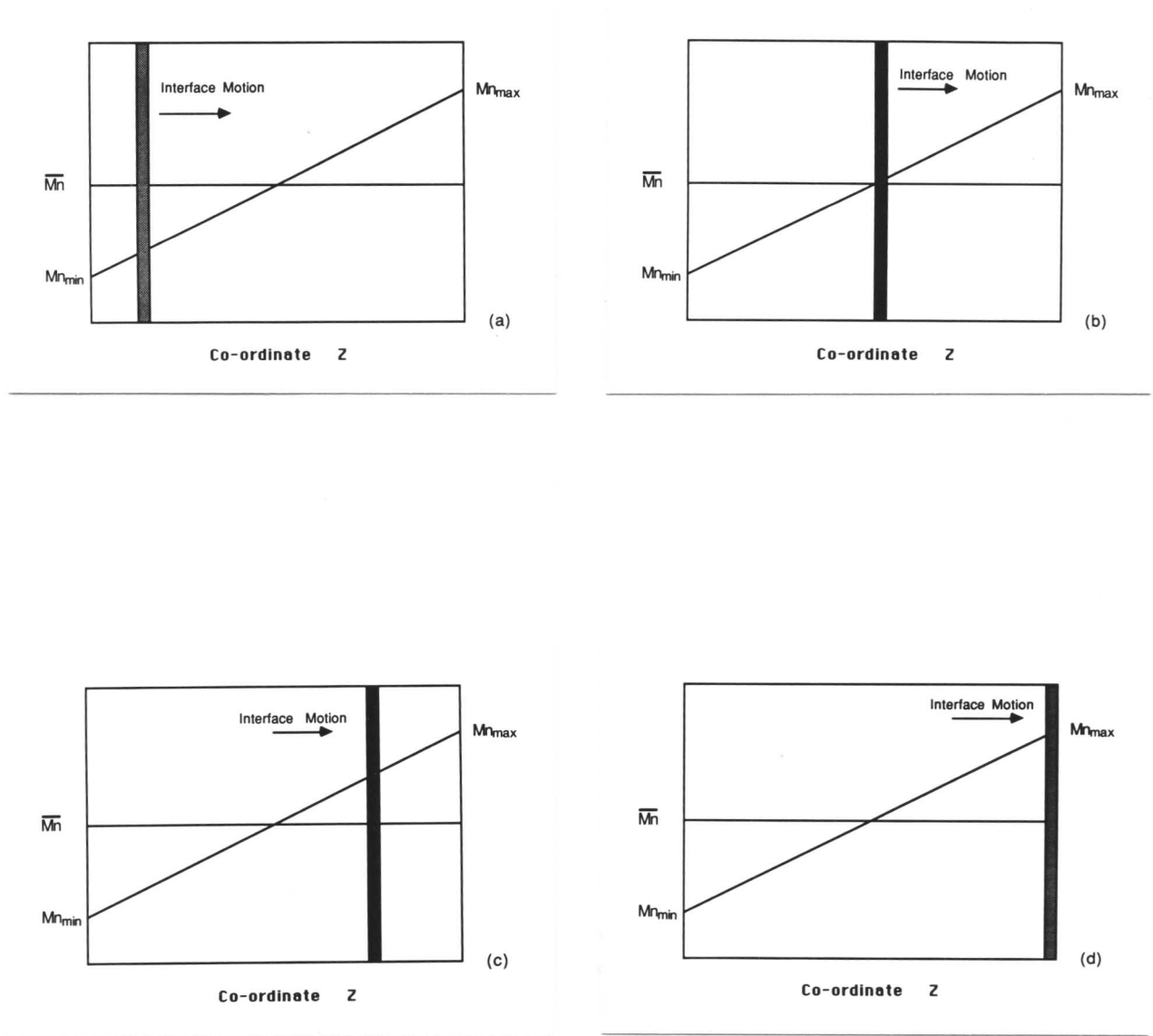
**Fig. 7.2:** *Schematic representation of the position of the $\gamma/\alpha$ interface in a heterogeneous alloy. The coordinate 'Z' is defined to be normal to the planes of constant composition and is normalised with respect to the specimen length in the Z-direction. Four different positions of the interface are shown:*

*(a) when $Mn < \overline{Mn}$,*

*(b) when $Mn = \overline{Mn}$,*

*(c) when $Mn > \overline{Mn}$,*
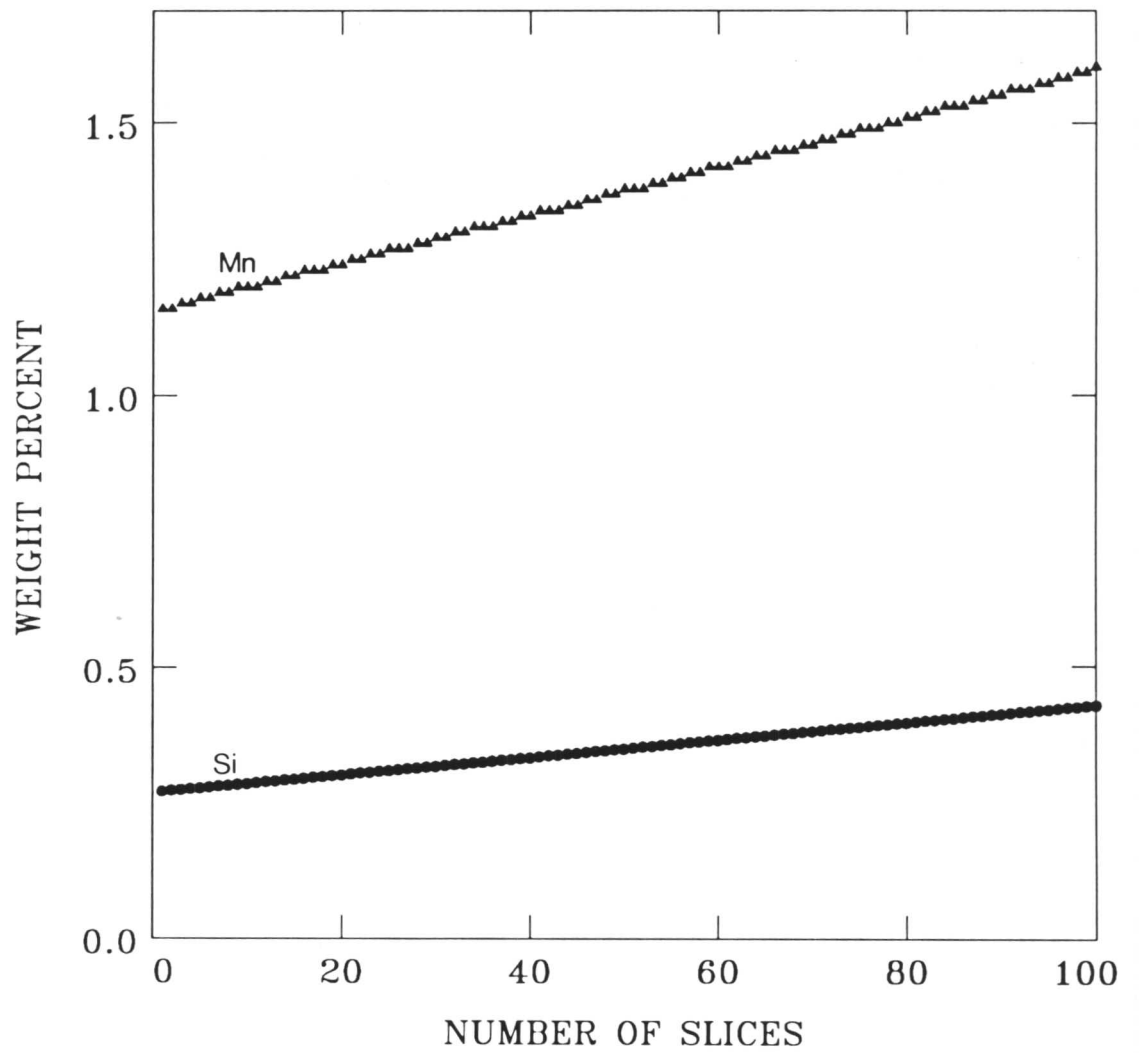
*(d) when $Mn = Mn_{max}$.*

**Fig. 7.3:** *Graph showing the linear variation of Mn and Si concentrations as a function of distance (slice number) as utilised in the slice model presented in the text.*
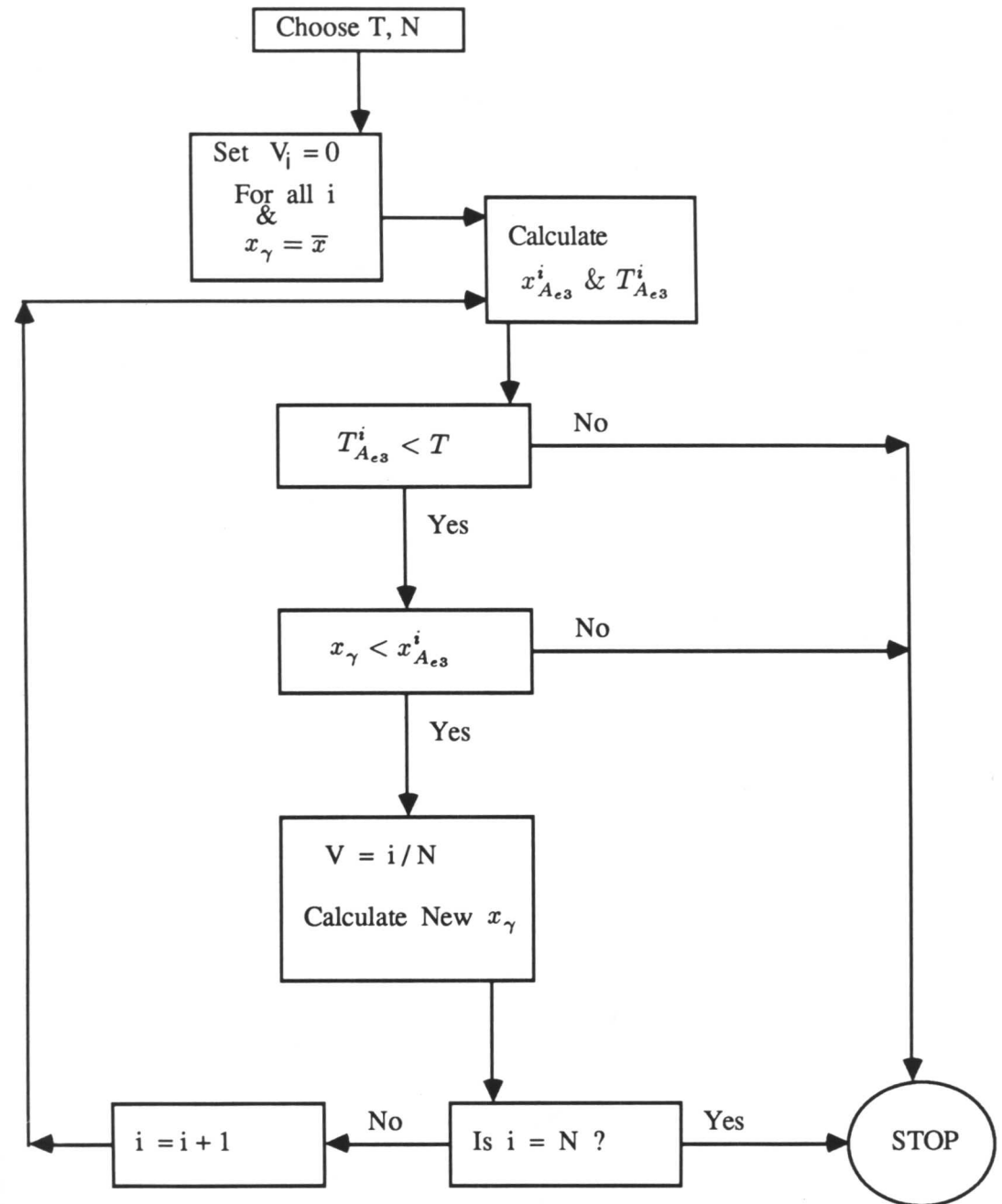
**Fig. 7.4:** *Flow chart illustrating the calculation procedure used to simulate the development of transformation in a heterogeneous steel while the $\gamma/\alpha$ interface moves normal to the isoconcentration planes in accordance with the Bhadeshia model*[5].
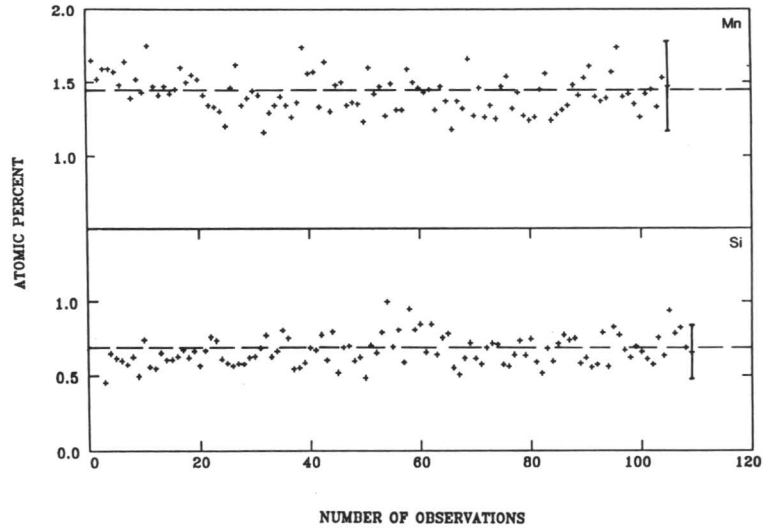
**Fig. 7.5:** *Microanalysis data from heterogeneous sample of Fe-0.17C-0.35Si-1.38Mn wt. % steel which was austenitised at 1000 °C and then transformed isothermally at 700 °C for 60 minutes. The error bars indicate the typical 95% confidence statistical error and the average composition is in each case indicated by the dashed horizontal line.*
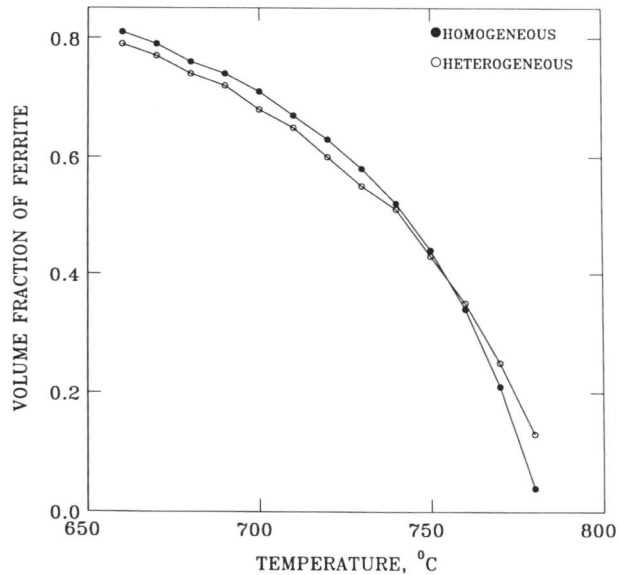


**Fig. 7.6:** *Calculated ferrite volume fraction as a function of isothermal transformation temperature in a heterogeneous alloy as the growth direction of the $\gamma/\alpha$ interface was considered to be normal to the isoconcentration planes.*

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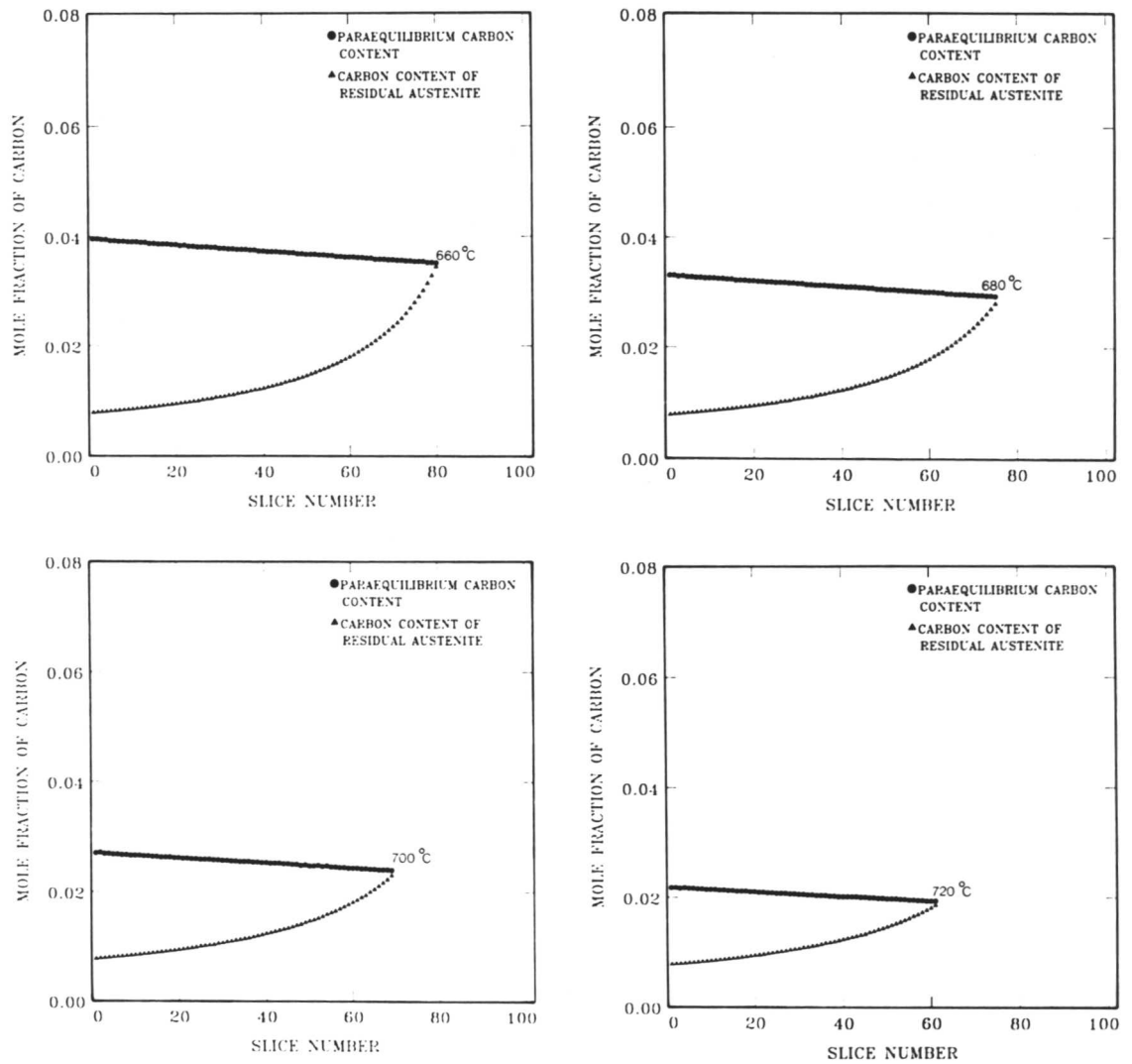**Fig. 7.7:** *Illustration of how the paraequilibrium carbon concentration and the actual carbon concentration of the residual austenite converge as the transformation front advances into solute-enriched regions.*
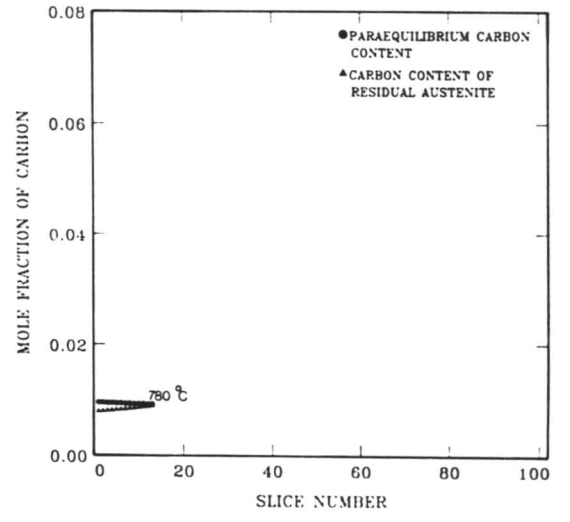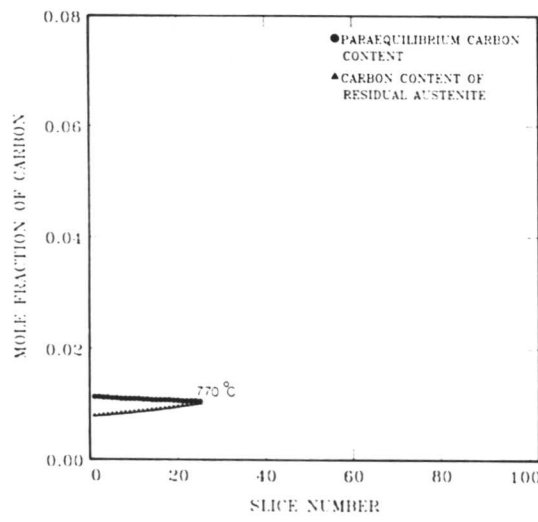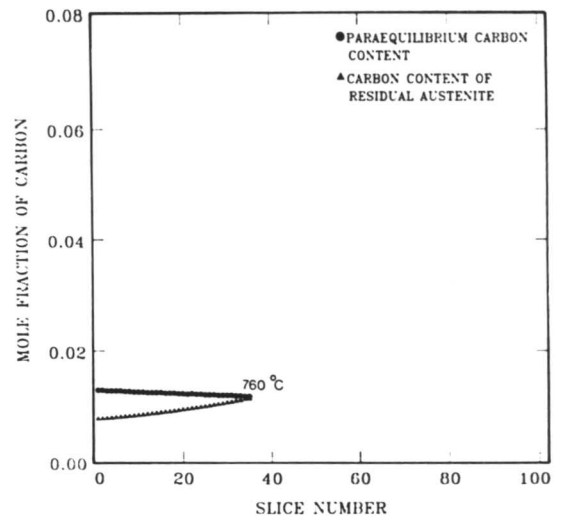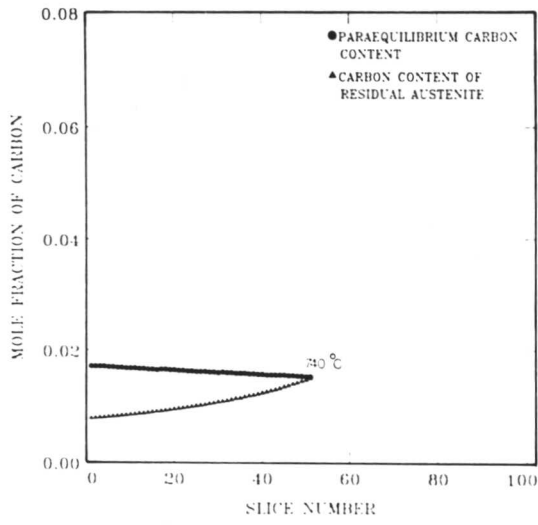
Fig. 7.7: ( continued ..... )
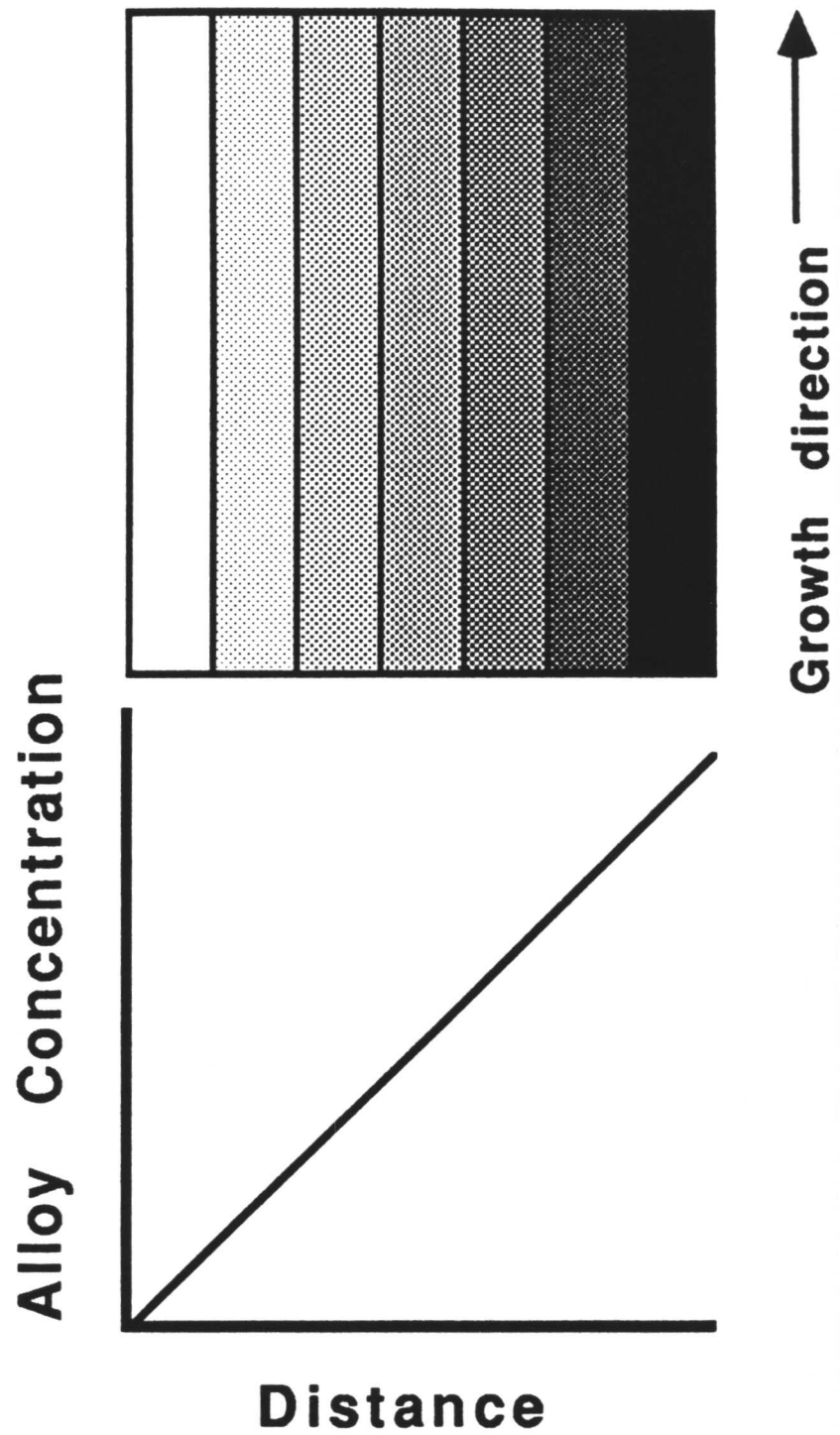
**Fig. 7.8:** *In another model for allotriomorphic ferrite in heterogeneous steels, the growth direction of the ferrite can be considered to be parallel to the isoconcentration planes.*
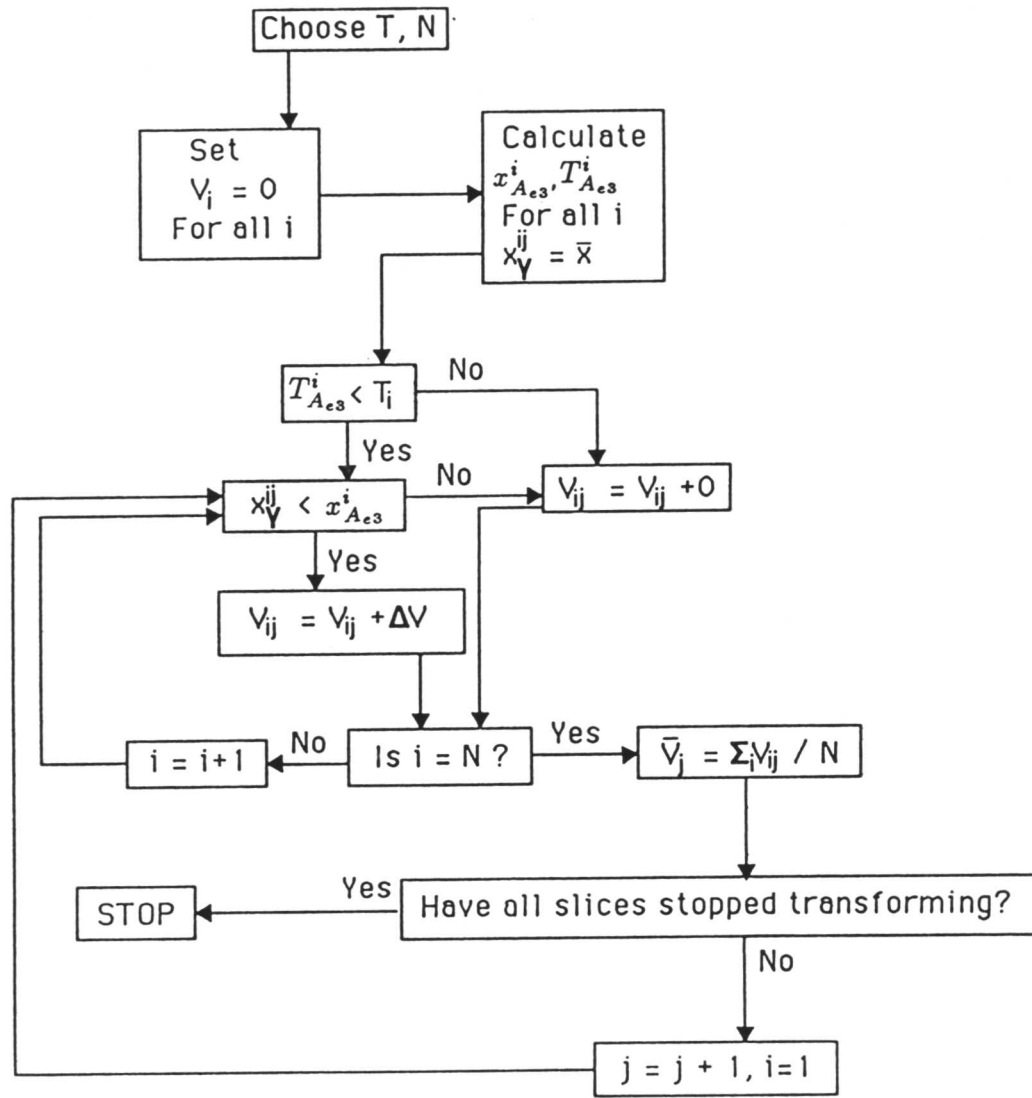
**Fig. 7.9:** *Flow chart illustrating the calculation procedure used to simulate the development of transformation in a heterogeneous steel. $T_i$ represents the isothermal transformation temperature and the subscript $i$ identifies the slice number and composition; the total number of slices is $N$ The calculation is carried out in stages, with each stage identified by the subscript $j$. For each value of $j$ (i.e., at each stage of the calculation), the volume fraction $V_{ij}$ of ferrite in each slice is incremented by a small fraction $\Delta V$ if transformation is feasible in that slice. The total volume fraction of ferrite at stage $j$ is thus given by $\Sigma_i V_{ij}/N$.*
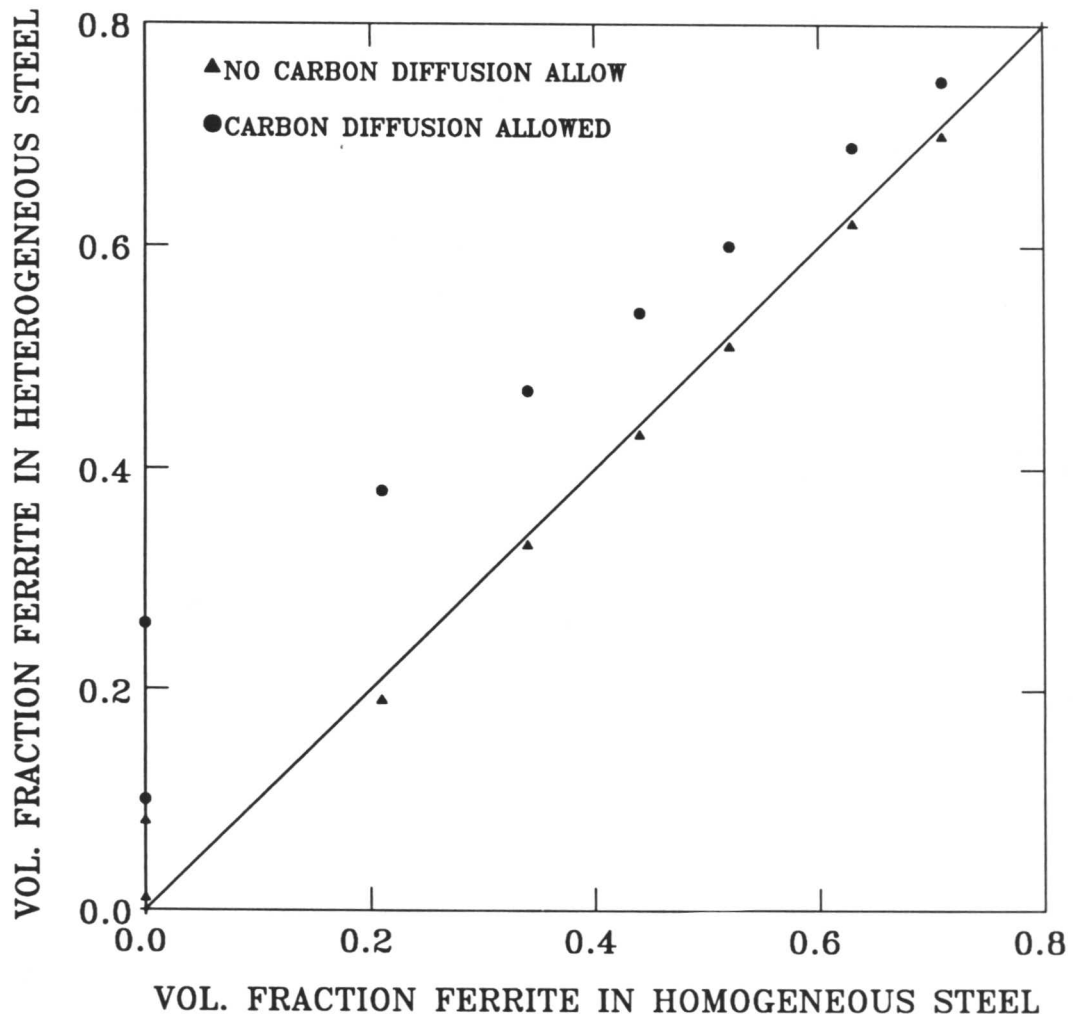
**Fig. 7.10:** *Comparison of maximum volume fraction transformed in homogeneous and heterogeneous samples as calculated by the slice model in which $\gamma/\alpha$ interface was assumed to move in a direction parallel to the isoconcentration planes. The line has a slope of unity, and serves to show that except above the $A_{e3}$ of the homogeneous sample (where the degree of transformation is larger in case of heterogeneous sample) there is no significant difference between the two, provided the slices are allowed to transform independent of each other. But if an opportunity is provided for carbon to distribute evenly throughout the residual austenite, the extent of transformation is always larger in the heterogeneous samples.*
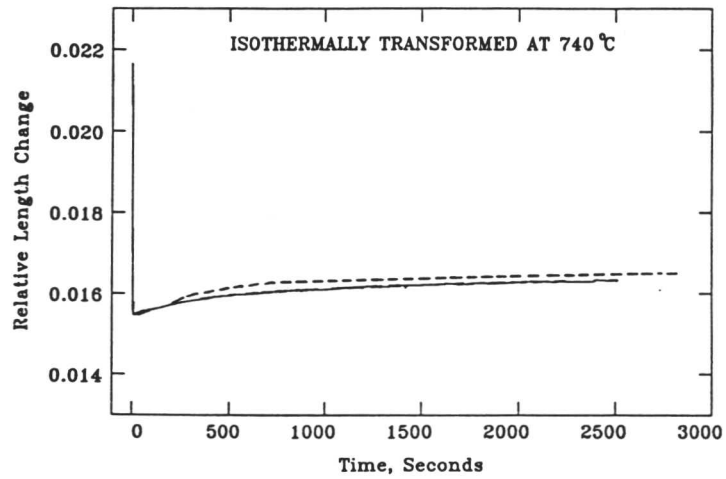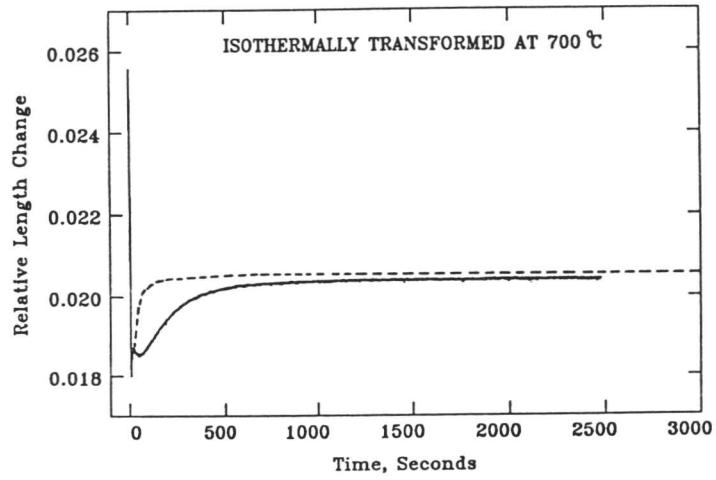
**Fig. 7.11a:** *Dilatometric curves for Fe-0.17C-0.35Si-1.38Mn wt.% steel isothermally transformed at the temperatures indicated. The continuous curves are for the homogenised samples and the dashed curves for the heterogeneous samples.*
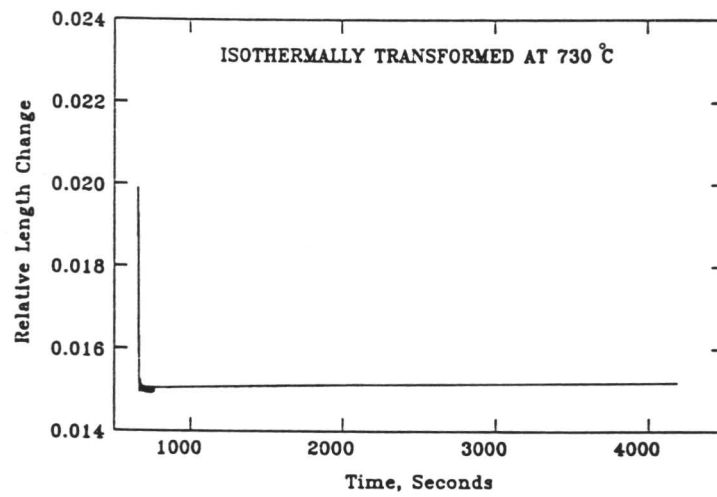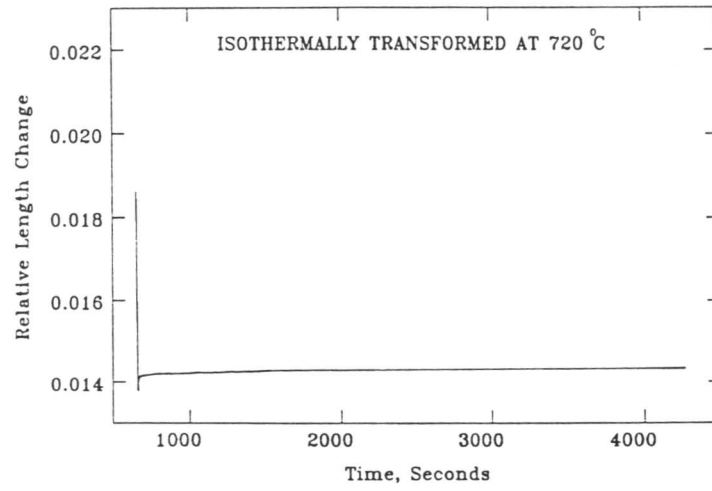
**Fig. 7.11b:** *Dilatometric curves for the homogenised Fe-0.17C-0.35Si-1.38Mn wt. % steel isothermally transformed at the temperatures indicated.*
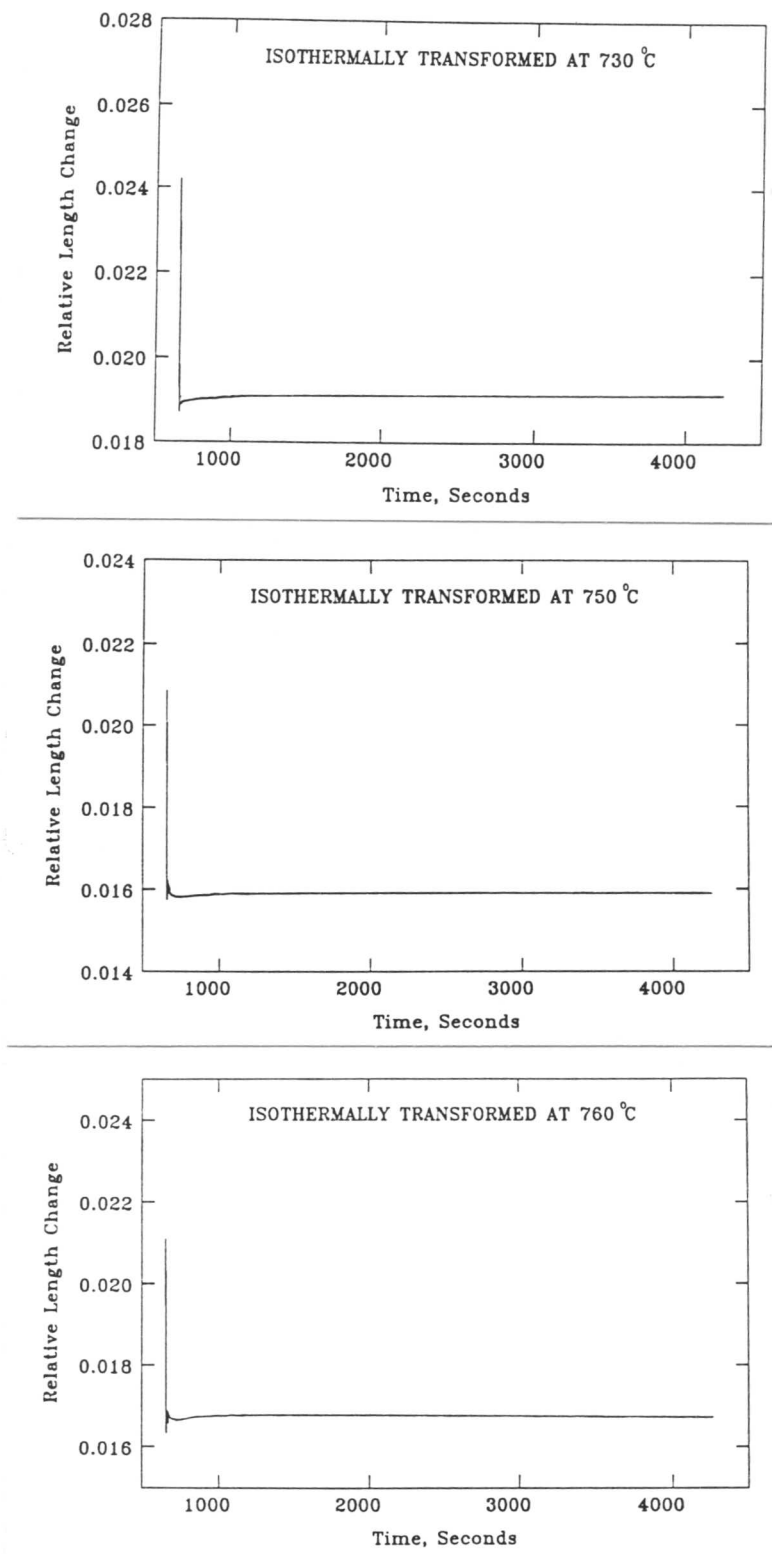
**Fig. 7.11c:** *Dilatometric curves for the heterogeneous Fe-0.17C-0.35Si-1.38Mn wt. % steel isothermally transformed at the temperatures indicated.*

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a



b
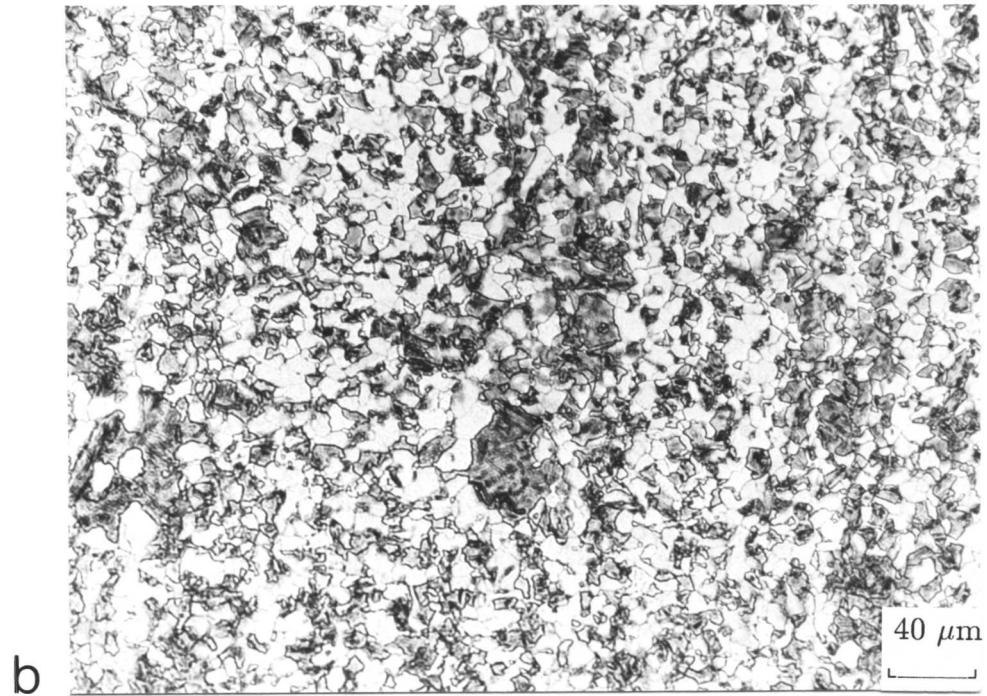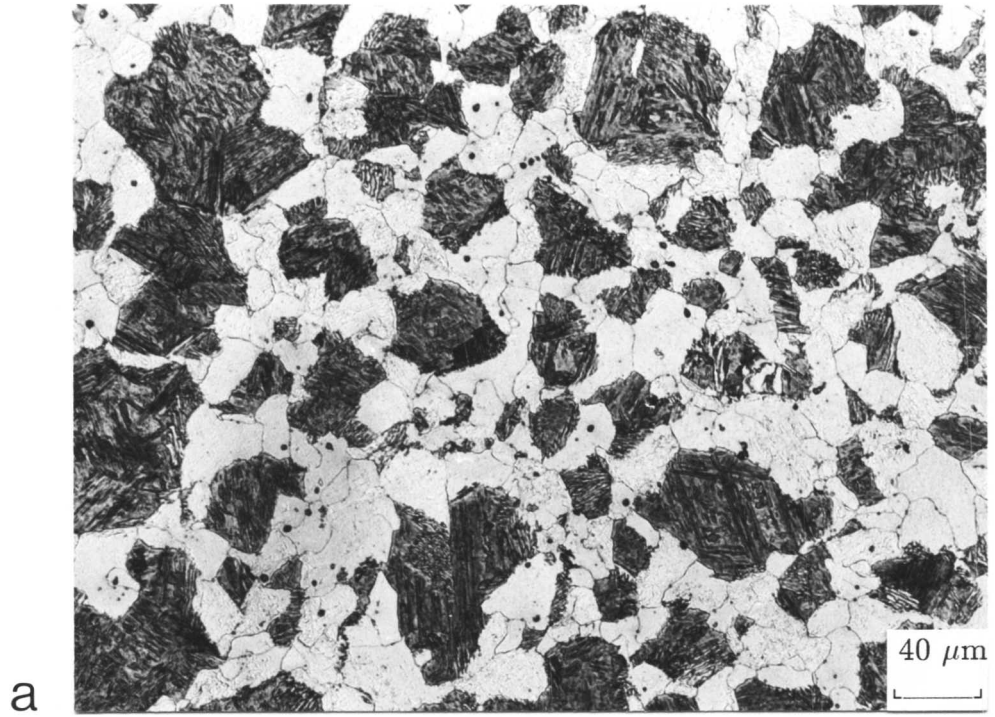
**Fig. 7.12:** *Metallographic confirmation of the curves shown in Fig. 7.9a.*

*(a) Optical micrograph of the homogeneous specimen isothermally transformed at 700 °C.*

*(b) Optical micrograph of the heterogeneous specimen isothermally transformed at 700 °C.*

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c

40 μm



d

40 μm
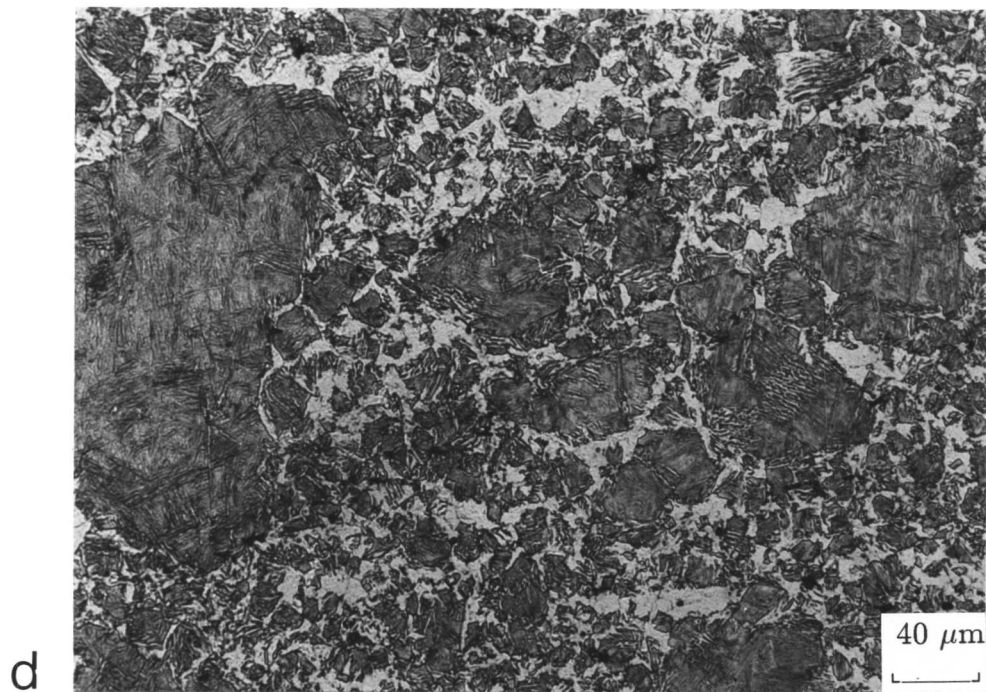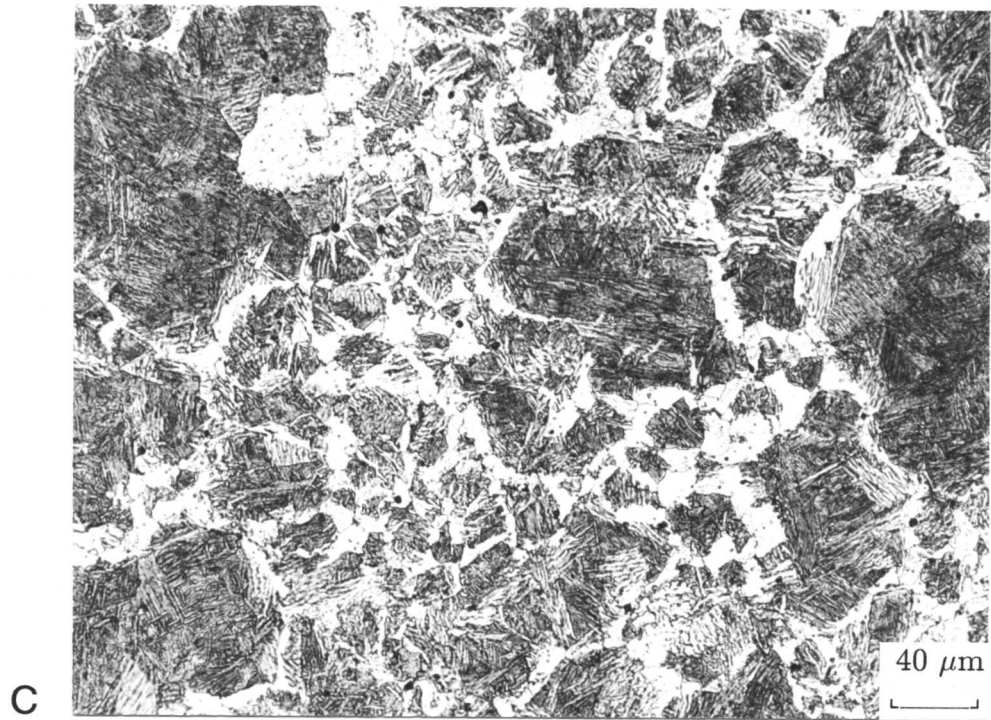
Fig. 7.12: ( continued ..... )

(c) Optical micrograph of the homogeneous specimen isothermally transformed at 740 °C.

(d) Optical micrograph of the heterogeneous specimen isothermally transformed at 740 °C.

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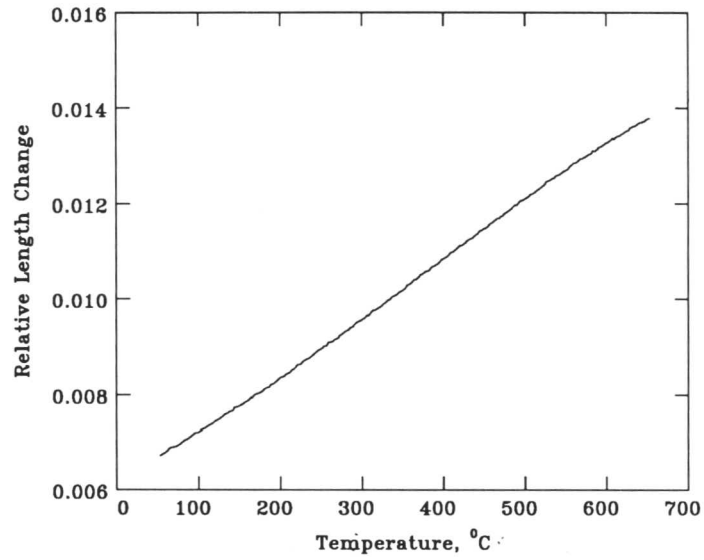
**Fig. 7.13:** *Graph of relative length change versus temperature, from which the linear expansion coefficient of ferrite is obtained.*
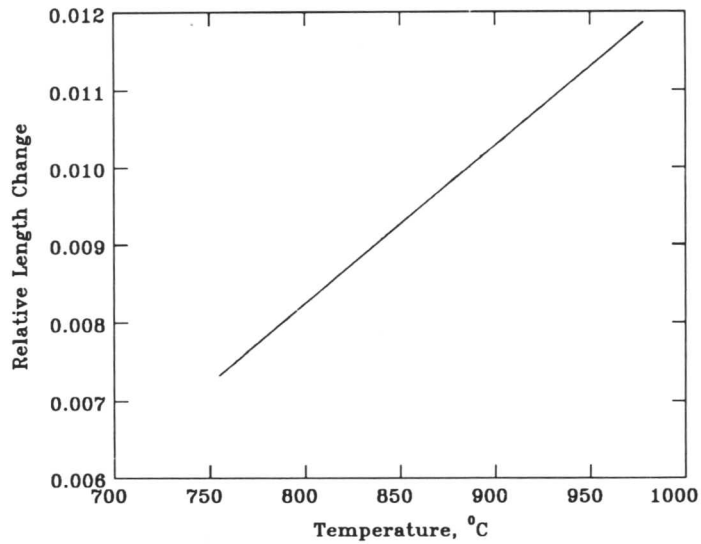


**Fig. 7.14:** *Graph of relative length change versus temperature, from which the linear expansion coefficient of austenite is obtained.*
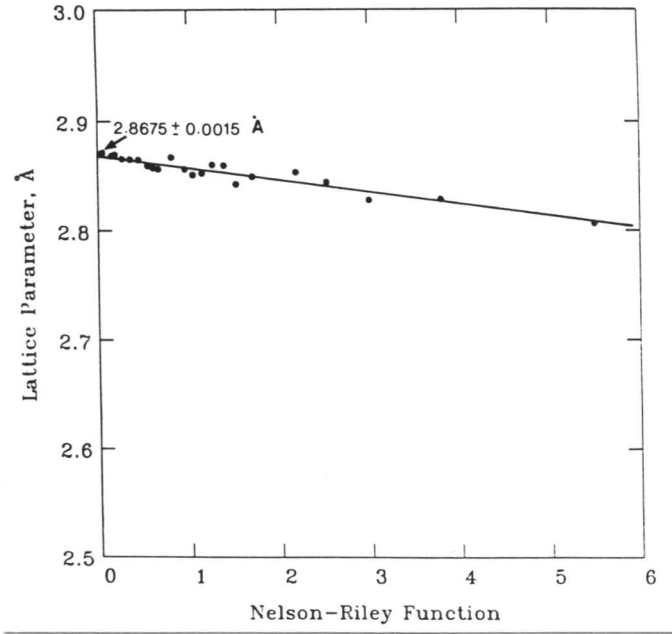
**Fig. 7.15:** *Extrapolation of measured lattice parameter against Nelson-Riley function (i.e., $\frac{cos^2\theta}{sin\theta} + \frac{cos^2\theta}{\theta}$). $\theta$ is the diffraction angle.*



**Fig. 7.16:** *Bright field transmission electron micrograph from a heterogeneous sample of Fe-0.17C-0.35Si-1.38Mn wt. % steel, transformed isothermally to allotriomorphic ferrite at 700 °C for 60 minutes before quenching to ambient temperature. Shows allotriomorphic ferrite and residual austenite.*

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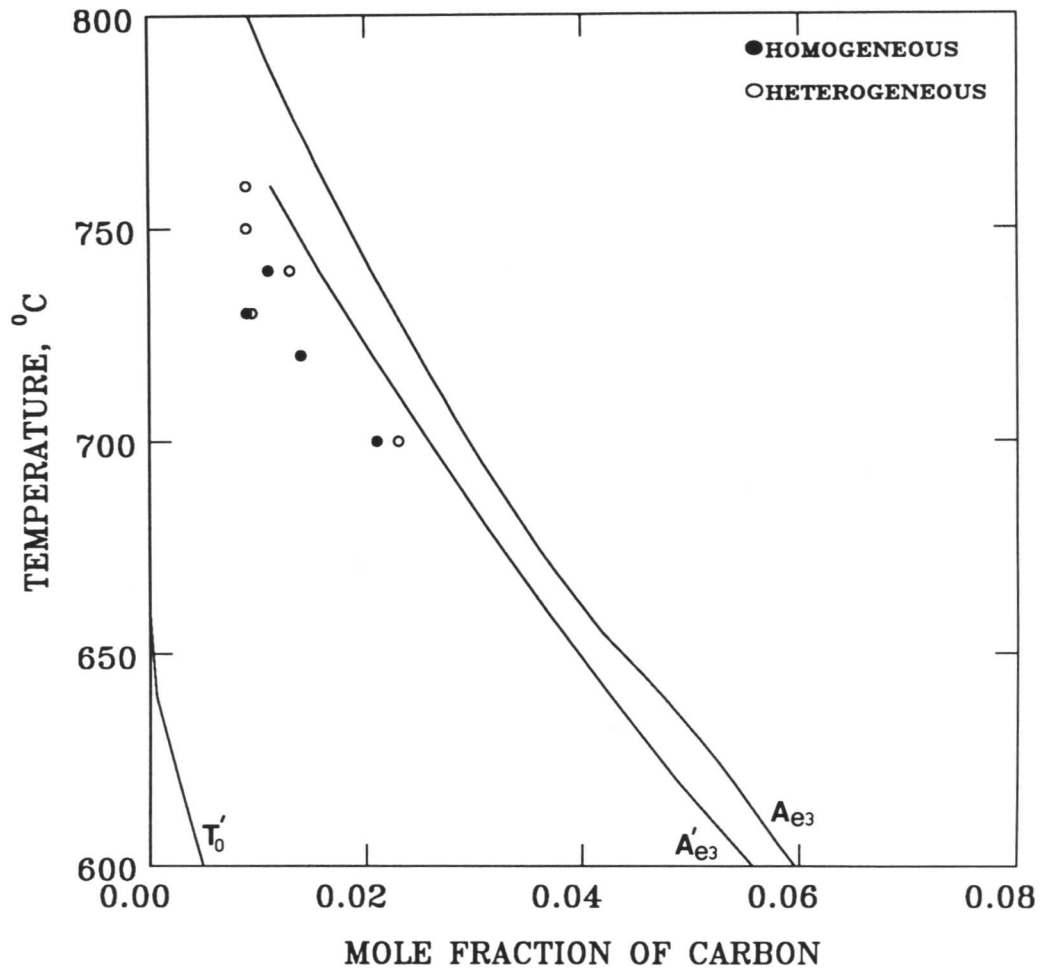
**Fig. 7.17:** *Calculated $T_0'$, $A_{e3}'$ and $A_{e3}$ phase boundaries for Fe-0.17C-0.35Si-1.38Mn wt. % steel. The experimental data are for samples transformed isothermally to allotriomorphic ferrite.*

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# Chapter 8

# COMPLETE CALCULATION OF MICROSTRUCTURAL EVOLUTION IN HETEROGENEOUS AUTOMOBILE STEELS

## 8.1 Introduction

In the previous chapters, various aspects of the transformation of austenite to allotriomorphic ferrite, bainite and martensite in a heterogeneous alloy were discussed. Moreover, some models were presented to help predict the volume fractions and other characteristics of these transformation products both for homogeneous and for chemically segregated steels. The purpose of the work presented in this chapter was to use to apply the models to some new steels which are being developed at Inland Steel (USA) for automobile crash reinforcement bars. The steels are at an early stage of development and could benefit from fundamental alloy design. Cars manufactured in the old days had door panels which were very thick ( ~20 cm), and consequently could be reinforced against sidewise impact using relatively low strength steel in the form of zig-zag concertina type rectangular rods incorporated within the doors. Modern cars however have thinner panels which are reinforced by high-strengh steel bar (the present steels are candidate alloys) running across the panels, in a way which transmits any impact into the structural frame, thereby ensuring the passenger safety. The steels 'US83' and 'US24' are of average compositions Fe-0.20C-0.63Si-2.80Mn-0.04Ni-0.01Mo-1.10Cr wt.% and Fe-0.18C-0.75Si-1.98Mn-0.02Ni-0.01Mo-1.33Cr wt.% respectively. The interesting feature of the alloys is their relatively high silicon concentration, and their bainite microstructure, of the type discussed earlier.

## 8.2 Dilatometry

Dilatometry was used to study the development of transformation. The specimens were austenitised at 1000 °C for 10 minutes before helium gas quenching to a variety of isothermal transformation temperatures within the bainite transformation range (Fig. 8.1). The length change during the isothermal reaction was measured and the corresponding relative length change versus time data plotted as in Figs. 8.2 and 8.3. The interesting feature of these sigmoidal curves is once again, that the maximum

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extent of transformation (i.e., the maximum value of relative length change) at any temperature decreases with increasing isothermal transformation temperature and this is expected from the slope of the $T_0$ curve as discussed earlier. These results are supported by optical microscopy as seen in Figs. 8.4 and 8.5 which also gives a visual comparison of the extent of reaction in the homogeneous and heterogeneous samples. Banding is always apparent in the as-received alloy, although it seems to become less obvious at high degrees of transformation (i.e., at low transformation temperatures).

Figure 8.6 shows a typical dilatometric curve of the relative length change as a function of temperature for the two steels during cooling from the austenitising temperature to the lowest isothermal transformation temperature used in the present experiments. The linearity of the plot proves the absence of any transformation during the quench to the isothermal transformation temperature, so that the equipment used is clearly capable of permitting isothermal transformation experiments.

To reveal further information from the dilatometric experiments, the data were analysed as in previous chapters. The relative length change corresponding to a volume fraction of bainitic ferrite $V_b$ that grows from austenite, is given by:

$$\frac{\Delta l}{l} = \frac{2V_b a_\alpha^3 + (1 - V_b)a_\gamma^3 - \bar{a}_\gamma^3}{3\bar{a}_\gamma^3} \tag{8.1}$$

where $a_\alpha$ is the lattice parameter of ferrite at the transformation temperature, given by:

$$a_\alpha = a_\alpha^o[1 + e_\alpha(T - 25)] \tag{8.2}$$

and $\bar{a}_\gamma$, which is the lattice parameter of austenite of the alloy composition at the transformation temperature, is give by:

$$\bar{a}_\gamma = (a_o^\gamma + \Sigma c_i x_i)[1 + e_\gamma(T - 25)]. \tag{8.3}$$

In these equations, $e_\alpha$ and $e_\gamma$ represent the linear thermal expansivities of ferrite and austenite respectively, $a_o$ is the lattice parameter of austenite in pure iron at 25 °C, $x_i$ is the concentration of alloying element $i$ and $c_i x_i$ represents the change in $a_o$ due to the addition of the alloying element to pure iron. $T$ is the temperature in °C. The ferrite linear expansion coefficient was determined by first tempering a specimen at 600 °C for 10 minutes to decompose any retained austenite and then recording the length

change during very slow cooling. The measurements do not therefore account for the presence of any carbide whose volume fraction is in any case expected to be negligibly small for the present purposes. The graphs of relative length versus temperature are plotted in Fig. 8.7, from which the linear expansion coefficients of ferrite were obtained for the two steels ($e_\alpha = 1.022 \times 10^{-5} K^{-1}$ and $e_\alpha = 1.430 \times 10^{-5} K^{-1}$ for 'US83' and 'US24' steels respectively). The expansion coefficients of austenite were measured while specimens were in the single-phase field, as shown in Fig. 8.8 ($e_\gamma = 2.030 \times 10^{-5} K^{-1}$ and $e_\gamma = 2.230 \times 10^{-5} K^{-1}$ for 'US83' and 'US24' steels respectively).

The ferrite lattice parameter ($a_\alpha^o$) at ambient temperature was measured using a Debye-Scherrer technique. The test specimen was annealed at 600 °C for half an hour, and then machined in the form of 0.5mm × 0.5mm × 15mm wire. Finally the specimen was immersed in an aqueous solution made up of 5% HF and 45% $H_2O_2$ (by volume) for two minutes to remove the deformation layer before testing. The specimens were irradiated with Mo $K_\alpha$ radiations using a standard Debye-Scherrer camera. A value of lattice parameter was calculated for each reflection from the resulting photograph and plotted against the Nelson-Riley function[1] of Bragg angle $\theta$. The linear regression technique was used to extrapolate a best-fit line back to $\theta = 90°$, to find the intercept and the standard error in the intercept (Fig. 8.9). The resulting values of lattice parameter came out as $2.8692 \pm 0.0012$ Å for 'US83' and $2.8670 \pm 0.002$ Å for 'US24' which are in agreement with the respective values calculated to be $2.8679$ Å and $2.8675$ Å using data from Leslie[2] but the steel has Mo, which is not included in the data from Leslie.

Using these measured values and making the appropriate substitutions in equation 8.1, the volume fractions of bainitic ferrite transformed were obtained using a computer program and the results thus obtained are shown in Figs. 8.10 and 8.11.

The range of concentration variation was found (Fig. 8.12 and 8.13) to be approximately 0.53-0.73Si,2.48-3.12Mn,1.03-1.17Cr wt. % for 'US83' steel and 0.60-0.90Si,1.65-2.31Mn,1.15-1.51Cr wt. % for 'US24' steel. Ni, Mo and V concentrations were too low to detect the corresponding small variations using microanalysis.

## 8.3 Transformation to Bainitic Ferrite

More transformation to bainite was observed in the homogenized samples as compared with the the heterogeneous sample, at high undercoolings below the $B_s$ temperature of the homogeneous sample (*i.e.*, 465 °C) for both 'US83' and 'US24' steels. At low undercoolings, the extent of isothermal transformation is found to be larger in the heterogeneous samples. Typical microstructures, as characterised using transmission electron microscopy are illustrated in figures 8.14 and 8.15. Carbide-free upper bainite was obtained even at the lowest temperatures shown in these figures. The carbon content of residual austenite was calculated using following mass balance equation[3].

$$x_\gamma = \bar{x} + \frac{V_b(\bar{x} - x_\alpha)}{(1 - V_b)} \tag{8.4}$$

where, $V_b$ is the volume fraction of bainitic ferrite. $x_\alpha$ is the amount of carbon which is left in the ferrite assumed to be 0.03 wt.%. $\bar{x}$ is the actual carbon content of the alloy.

In this way, the carbon concentration in the austenite at the point where isothermal transformation ceases can be calculated, and a comparison of such data for upper bainite, with the $T_0$, $T_0'$ and $A_{e3}'$ curves, calculated[3,4] from the chemical composition of the homogeneous alloy, is presented in Figs. 8.16 and 8.17. The experimental results are more consistent with the $T_0'$ curve relative to $T_0$ curve. It is evident from these figures that the experimental data support the conclusion that the growth of bainite is diffusionless, with the carbon being partitioned subsequently into the residual austenite. The results show that both of these steels accurately exhibit the incomplete reaction phenomenon, which can be used to estimate theoretically the degree of transformation expected as a function of isothermal transformation temperature or in terms of the alloy chemistry.

### 8.3.1 Theoretical Analysis

The transformation behaviour of these steels was also studied theoretically using the slice model fully described in chapter 4 and compared with the experimental data in figures 8.18 and 8.19. In these calculations, The heterogeneous steel was represented as a composite of many slices of equal thickness but of different chemical composition consistent with the experimentally measured composition range. The $\gamma/\alpha$ interface is

considered to move parallel to the isoconcentration planes as the microstructure shows banding.

In one case, the slices transform independently of each other, which is the more likely circumstance because of the sheaf morphology of bainite, where carbon trapped in the residual austenite remains isolated from one another.

The reasonable agreement is found in predicting the different behaviours of the as-received and homogenised samples. For most of the data, both theory and experiment show a higher degree of transformation in the homogenised samples, and both show a reversal of this trend as the transformation temperature approaches the $B_s$ temperature of the homogenised alloy. However, the difference in the calculated volume fraction of bainite in the homogeneous and heterogeneous "US24" steel samples was found to be negligible above the $B_s$ temperature of the homogeneous alloy. It should be noted that the "US24" steel not only has lower carbon content but Mn is also less than that in the "US83" steel which is affecting the transformation behaviour of the two steels. To make this point more clear, calculations were carried out for different compositions with varying average Mn content and also for different Mn variation ranges for the "US24" steel. In one case the average Mn content was varied keeping the Mn range constant as shown in Fig. 8.20a. The results were not very different as still the maximum Mn content considered (2.83 wt. %) was just the same as the average Mn concentration (2.80 wt. %) of the "US83" steel. So in another set of calculations the maximum Mn concentration of the heterogeneous "US24" steel was varied (up to 3.35 wt. %) while the minimum comcentration was kept constant (*i.e.,* 1.65 wt. %). Fig. 8.20b illustrates that as we increase the Mn content, the austenite can tolerate less and less carbon and the difference in the homogeneous and heterogeneous samples becomes more significant.

In another case of the slice model, carbon is allowed to distribute evenly throughout the residual austenite (*i.e.,* among the slices) during the development of bainitic microstructure. The fact that the carbon does not homogenise during transformation is emphasized by the results shown in Figs. 8.18 and 8.19, where the calculated data (assuming that carbon homogenises between the slices) are seen to overestimate the volume fraction of bainite.

## 8.4 Martensitic Transformation in 'US83' Steel

The dilatometric specimens from the 'US83' steel of average composition Fe-0.20C-0.63Si-2.80Mn-0.04Ni-0.01Mo-1.10Cr wt. % were quenched to ambient temperature after an appropriate time of isothermal holding at different temperatures ($T_b$) in the bainite range. Dilatometric curves of relative length change versus temperature are shown in Fig. 8.21. These data were converted into the volume fraction of martensite ($f$) using the following relationship:

$$f = \frac{3\Delta L a_\gamma^3}{V_\gamma L(2a_\alpha^2 c_\alpha - a_\gamma^3)} \tag{8.5}$$

where $a_\gamma$ is the lattice parameter of the the carbon–enriched residual austenite, $a_\alpha$ and $c_\alpha$ are the lattice parameters of tetragonal martensite, and $V_\gamma$ is the volume fraction of austenite present in the sample prior to martensitic transformation. The absolute volume fraction of martensite ($V_{\alpha'}$) can be obtained by multiplying the fraction of austenite transformed to martensite ($f$) with the actual volume fraction of austenite ($V_\gamma$) initially present at $T_B$, i.e.,

$$V_{\alpha'} = fV_\gamma \tag{8.6}$$

A computer program was written and used for these calculations which takes full account of the changes in lattice parameters as a function of alloy composition and temperature, as described elsewhere [5,6].

Another very useful information obtained from these dilatometric curves was the experimental measurement of the martensitic start temperature ($M_s$) as the point where the curve deviates from straight line during cooling. A good agreement between the calculated[7,8] and measured $M_s$ temperature of can be seen from the Fig. 8.22. All these data were further used in the theoretical study of the progress of the athermal martensitic transformation as described empirically by the following equation:

$$1 - f = \exp\{-C_1(M_S - T_Q)\} \tag{8.7}$$

where $f$ is the volume fraction of martensite divided by the volume fraction of austenite prior to the formation of martensite, $T_Q$ is a temperature to which the sample is cooled below $M_S$; $C_1$ is a constant obtained originally [9] by fitting to experimental data. The comparison of the experimental and calculated volume fraction of martensite using the

above equation is shown in Fig. 8.23. As mentioned previously in chapter 5, the above empirical equation cannot predict the kinetics of martensite formation at all stages of the reaction. A new model, as described in chapter 5, was then used to study the development of martensitic transformation as a function of undercooling below the $M_S$ temperature. This model includes the effects of autocatalysis[10−12] and can be described by the following equation:

$$-\frac{\ln\{1-f\}}{f} = 1 + \overline{V}C_6(M_S - T_Q) \tag{8.8}$$

or

$$-\frac{\ln\{1-f\}}{f} = 1 + C_7(M_S - T_Q) \tag{8.9}$$

where $C_7 = \overline{V}C_6$. $\overline{V}$ is the average volume per newly formed martensite plate assumed to be constant for the course of these calculations.

Figure 8.24 shows that the new model can better predict the kinetics of the martensite reaction at all stages.

## 8.5 Conclusions

All the experimental and theoretical work presented in the previous chapters was tried and tested for two more heterogeneous steels. Figure 8.25 shows the cumulative results of the complete calculation of microstructure in the homogeneous and heterogenous "US83" steel samples. As expected, more transformation to martensite was obtained with a decrease in the bainitic ferrite volume fraction. The results confirm that the models illustrated previously are valid for other steels also.
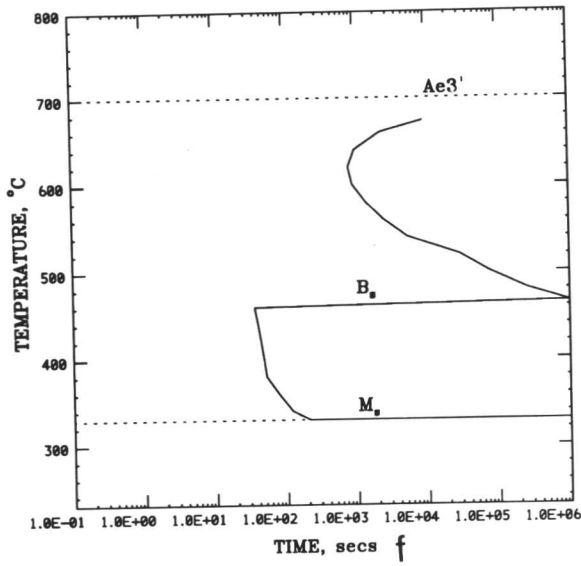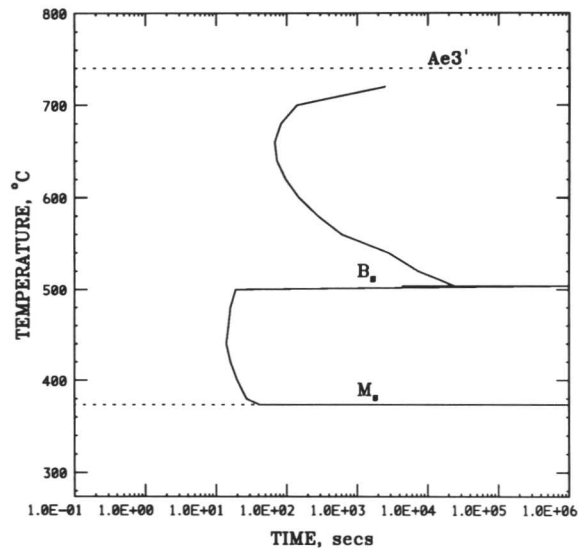
**Fig. 8.1:** *Calculated*[4,13] *time-temperature-transformation (TTT) diagrams.*
(a) "US83" steel of average composition Fe-0.20C-0.63Si-2.80Mn-0.04Ni-0.01Mo-1.10Cr wt. %.
(b) "US24" steel of average composition Fe-0.18C-0.75Si-1.98Mn-0.02Ni-0.01Mo-1.33Cr wt. %.
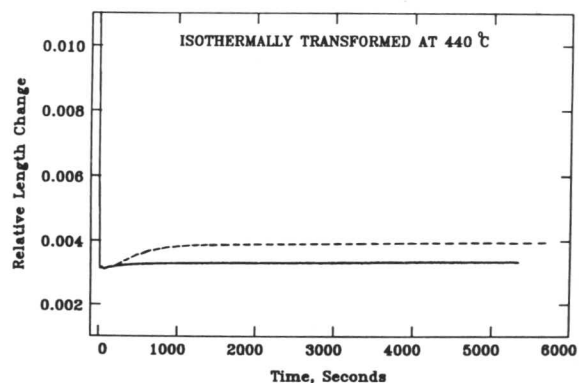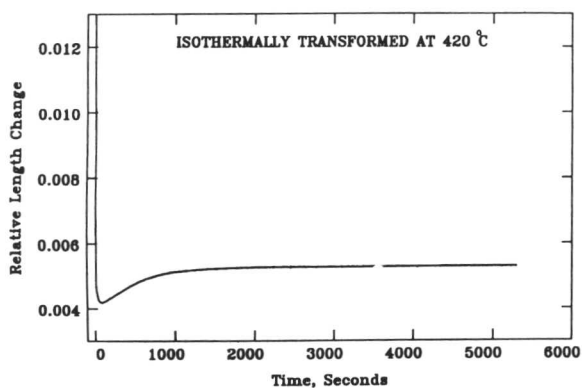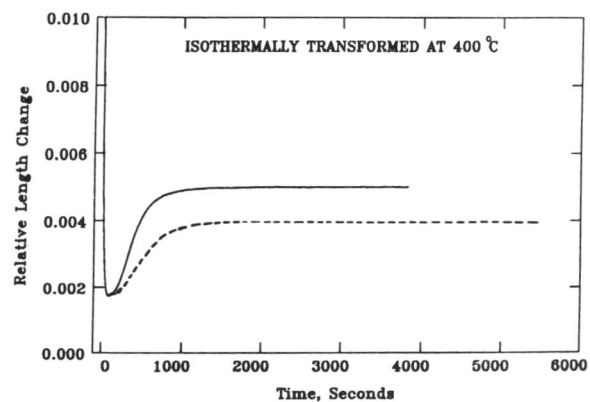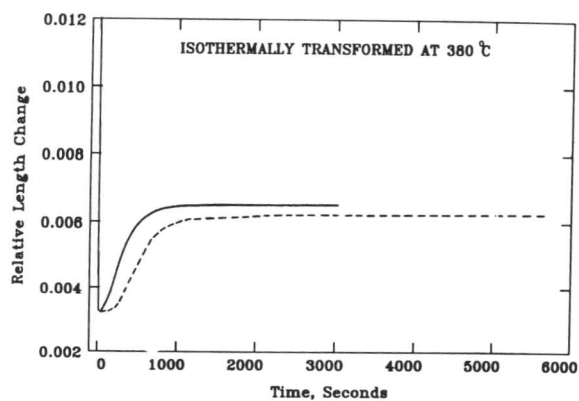
**Fig. 8.2:** *Dilatometric curves for samples of 'US83' steel isothermally transformed at the temperatures indicated. The continuous curves are for the homogenised samples and the dashed curves for the heterogeneous samples.*
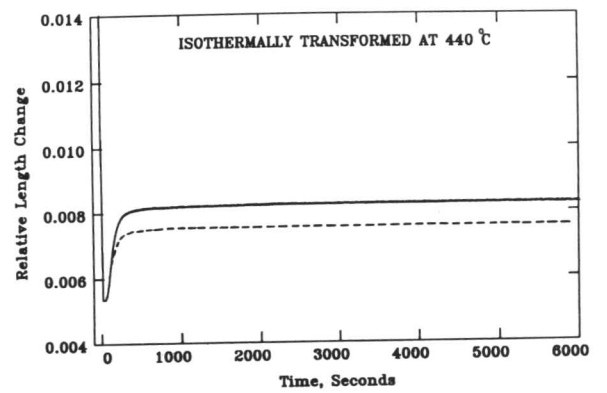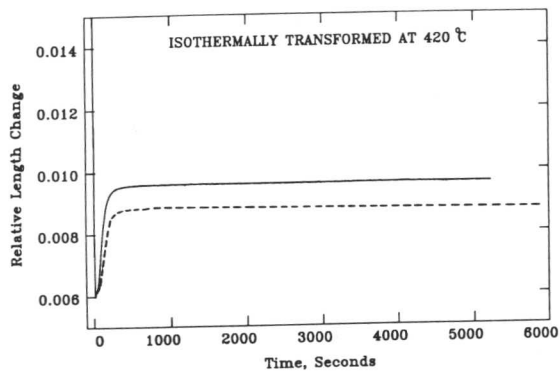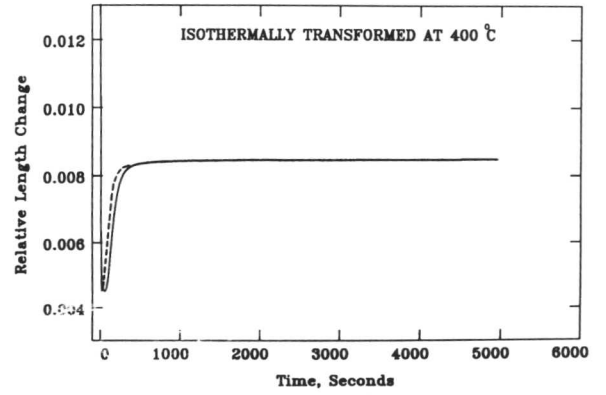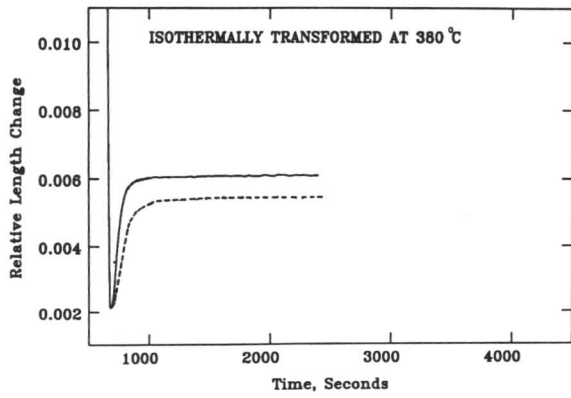
**Fig. 8.3:** *Dilatometric curves for samples of 'US24' steel isothermally transformed at the temperatures indicated. The continuous curves are for the homogenised samples and the dashed curves for the heterogeneous samples.*
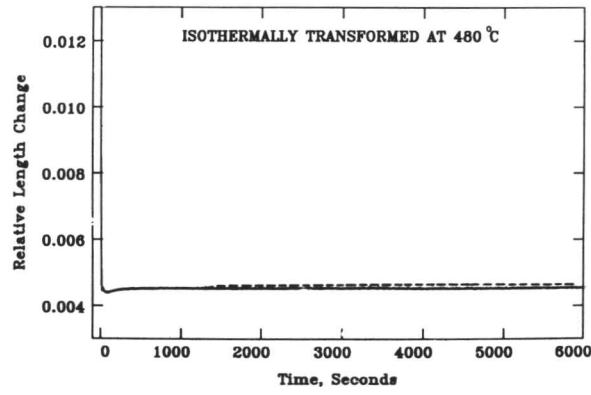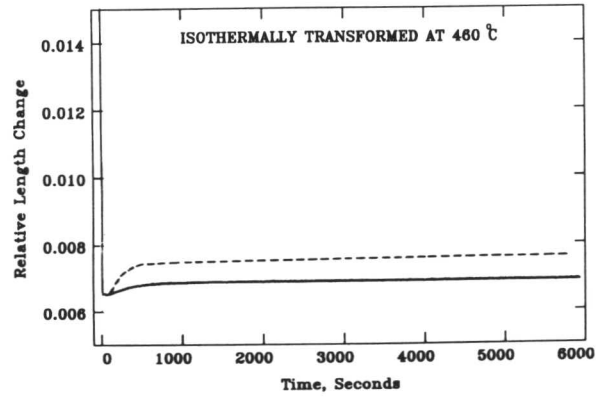
Fig. 8.3:( *continued .....* )
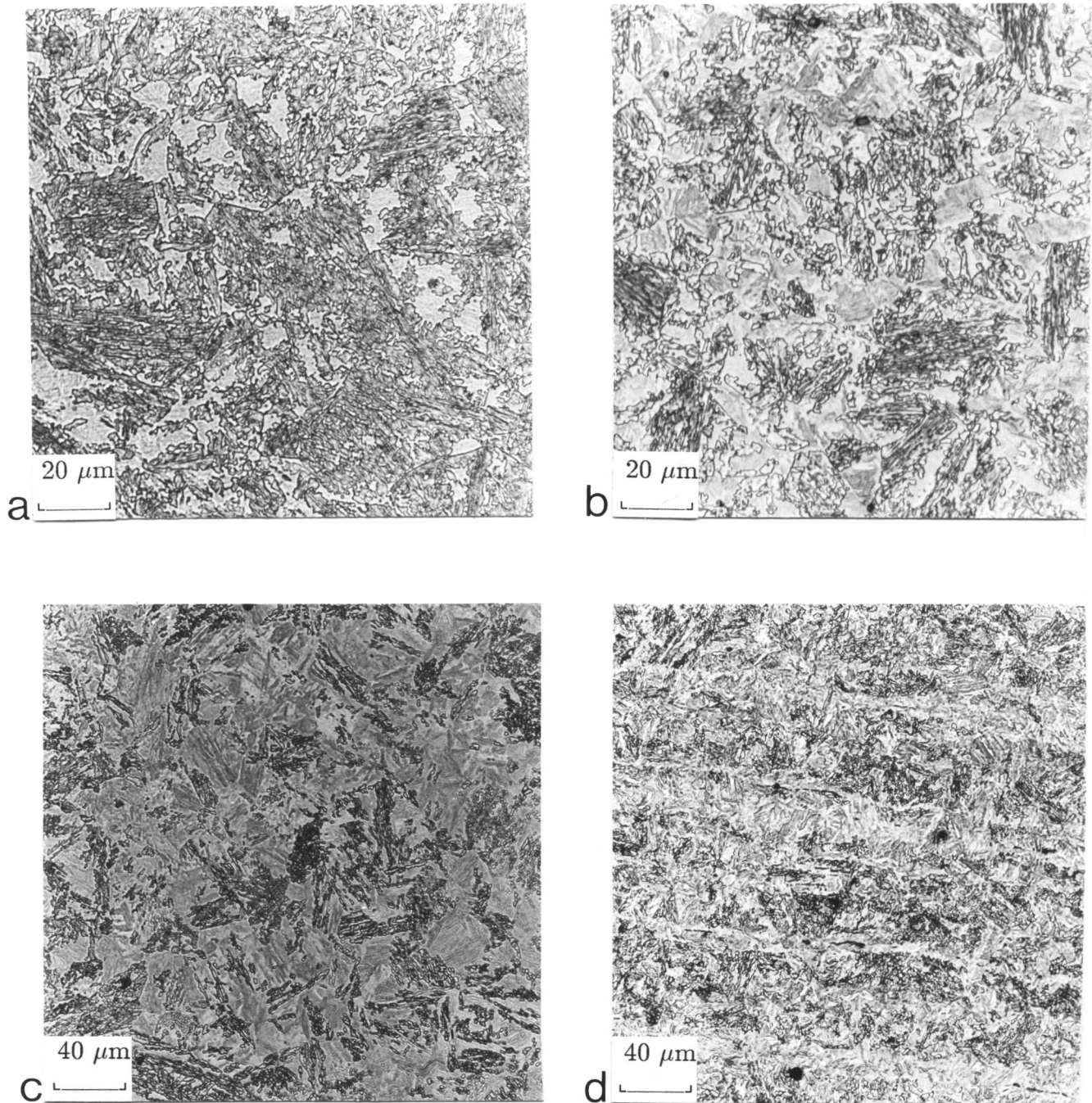
**Fig. 8.4:** *Metallographic confirmation of the curves shown in figure 8.1:*

*(a) Optical micrograph of the homogeneous specimen, from 'US83' steel, isothermally transformed at 400 °C.*

*(b) Optical micrograph of the heterogeneous specimen, from 'US83' steel, isothermally transformed at 400 °C.*

*(c) Optical micrograph of the homogeneous specimen, from 'US83' steel, isothermally transformed at 420 °C.*

*(d) Optical micrograph of the heterogeneous specimen, from 'US83' steel, isothermally transformed at 420 °C.*

20 μm

e



20 μm

f
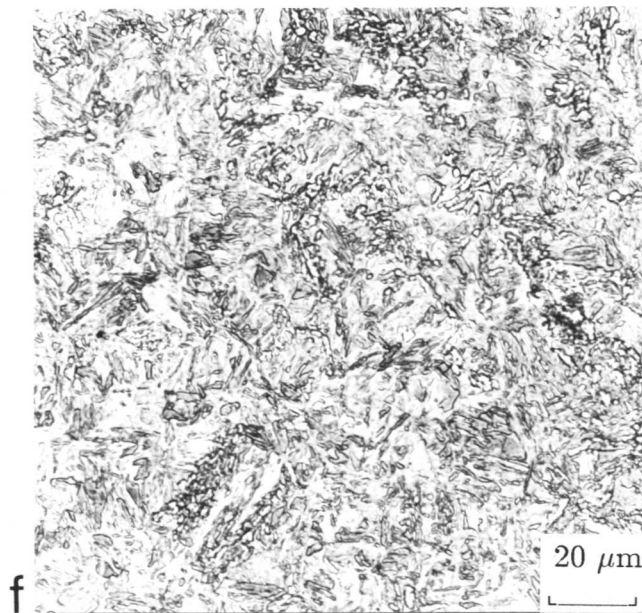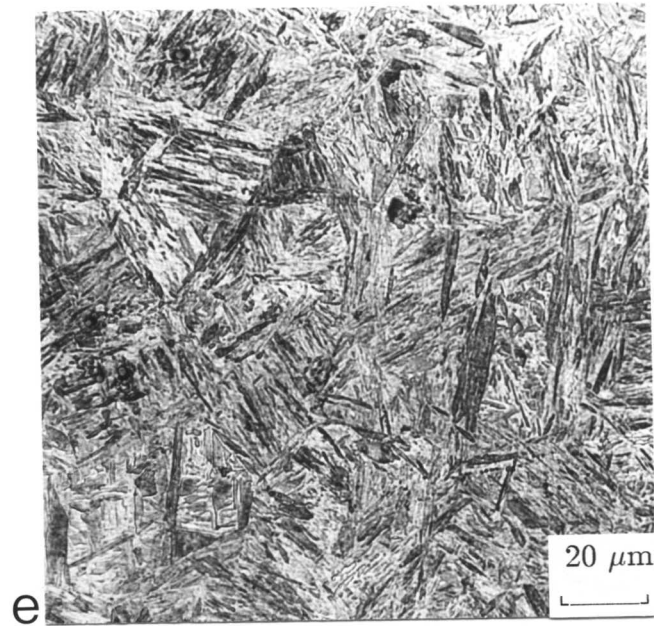
**Fig. 8.4:** *( continued ..... )*

    *(e) Optical micrograph of the homogeneous specimen, from 'US83' steel, isothermally transformed at 440 °C.*

    *(f) Optical micrograph of the heterogeneous specimen, from 'US83' steel, isothermally transformed at 440 °C.*

g



h

**Fig. 8.4:** *( continued ..... )*

(g) *Optical micrograph of the homogeneous specimen, from 'US83' steel, isothermally transformed at 460 °C.*

(h) *Optical micrograph of the heterogeneous specimen, from 'US83' steel, isothermally transformed at 460 °C.*
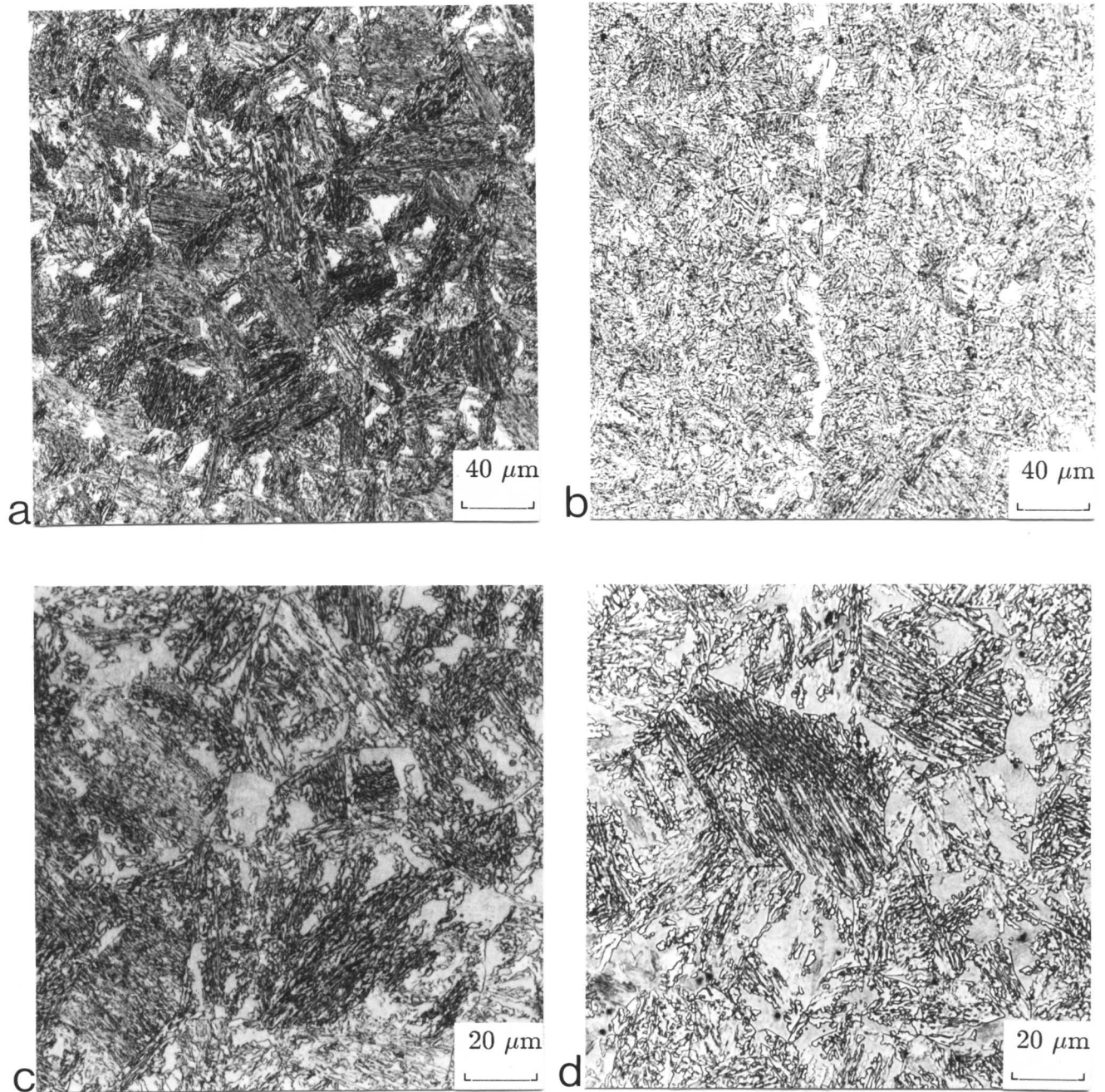
**Fig. 8.5:** *Metallographic confirmation of the curves shown in figure 8.1:*

*(a) Optical micrograph of the homogeneous specimen, from 'US24' steel, isothermally transformed at 400 °C.*

*(b) Optical micrograph of the heterogeneous specimen, from 'US24' steel, isothermally transformed at 400 °C.*

*(c) Optical micrograph of the homogeneous specimen, from 'US24' steel, isothermally transformed at 420 °C.*

*(d) Optical micrograph of the heterogeneous specimen, from 'US24' steel, isothermally transformed at 420 °C.*
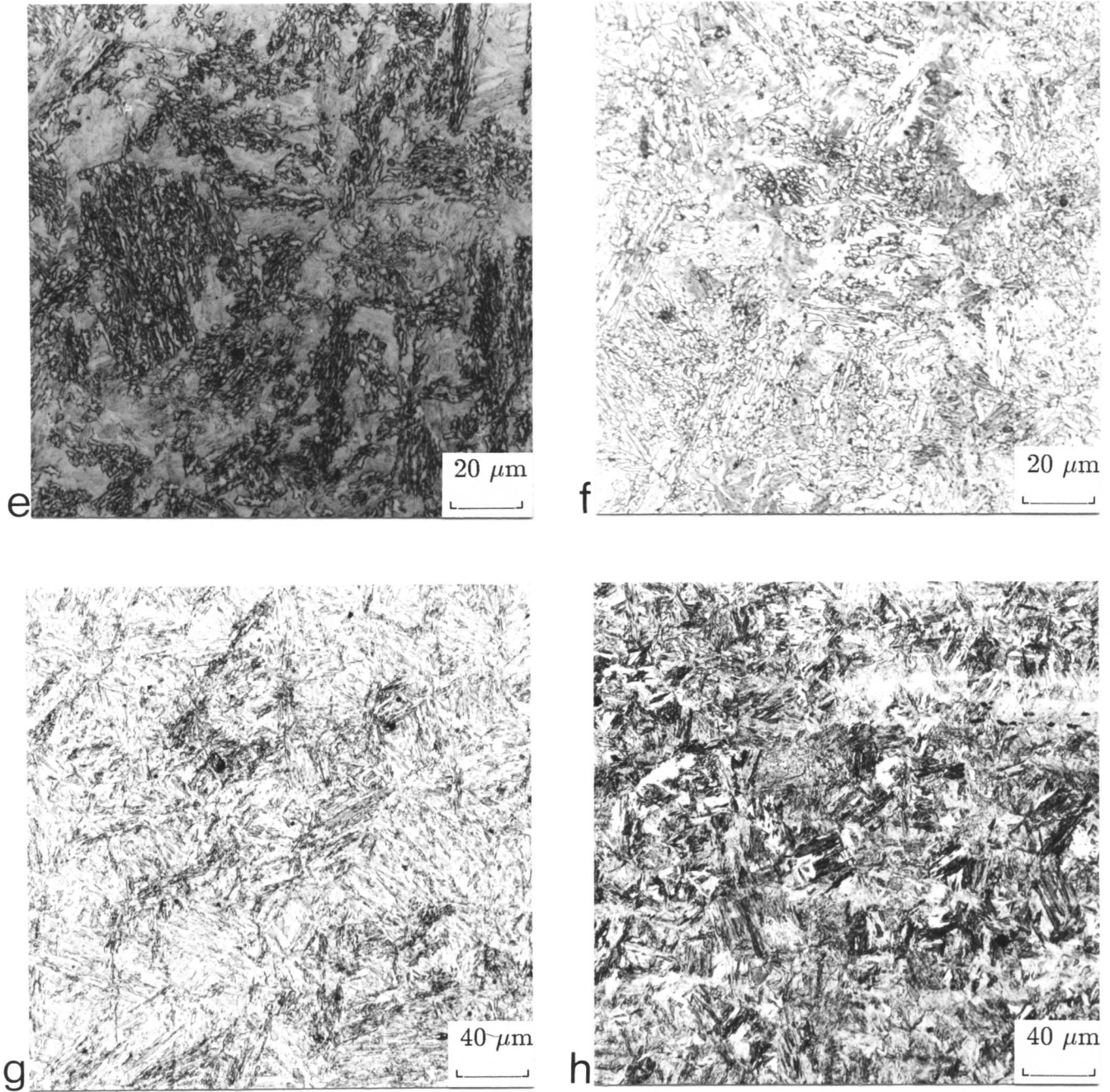
**Fig. 8.5:** *( continued ..... )*

*(e) Optical micrograph of the homogeneous specimen, from 'US24' steel, isothermally transformed at 440 °C.*

*(f) Optical micrograph of the heterogeneous specimen, from 'US24' steel, isothermally transformed at 440 °C.*

*(g) Optical micrograph of the homogeneous specimen, from 'US24' steel, isothermally transformed at 460 °C.*

*(h) Optical micrograph of the heterogeneous specimen, from 'US24' steel, isothermally transformed at 460 °C.*
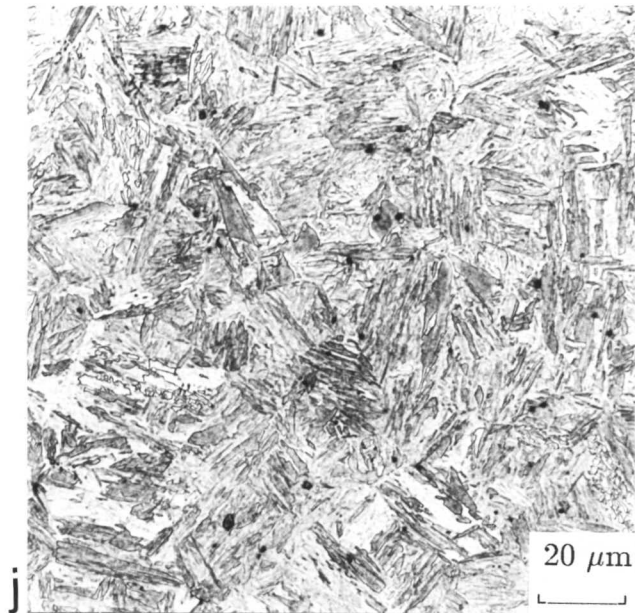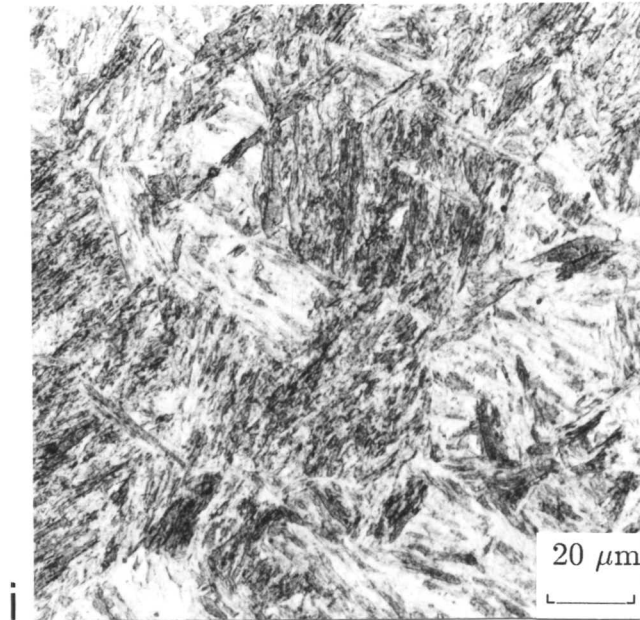
**Fig. 8.5:** *( continued ..... )*

(i) *Optical micrograph of the homogeneous specimen, from 'US24' steel, isothermally transformed at 480 °C.*

(j) *Optical micrograph of the heterogeneous specimen, from 'US24' steel, isothermally transformed at 480 °C.*
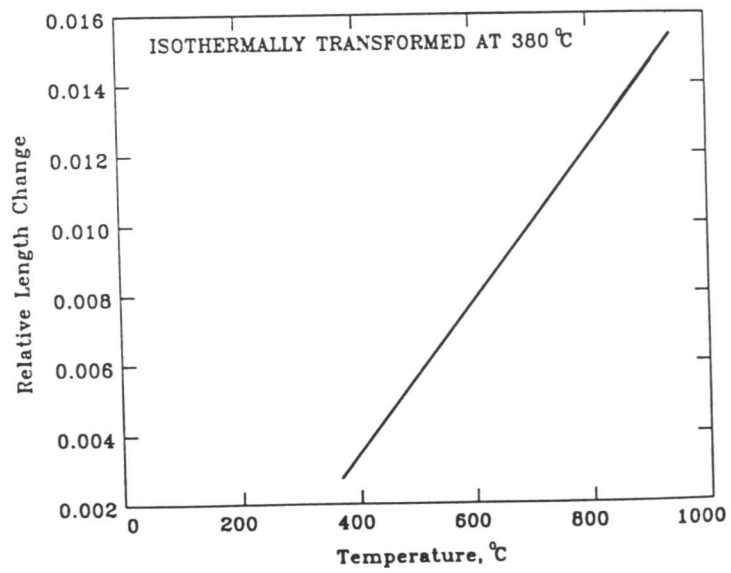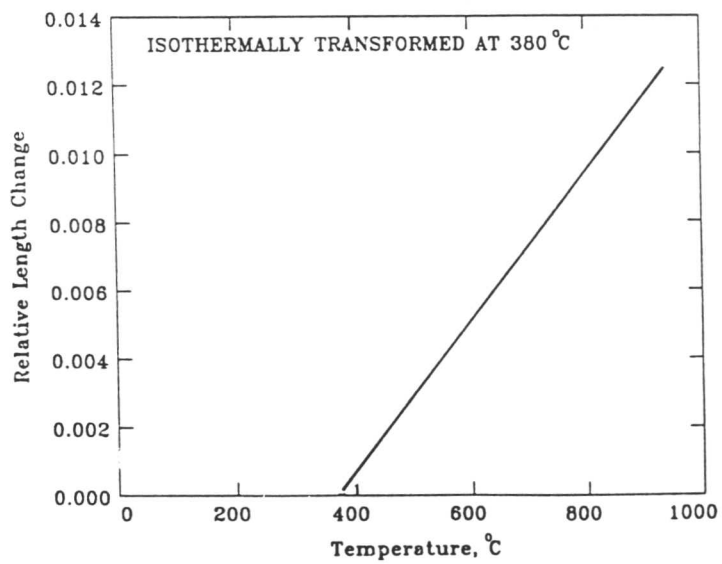
**Fig. 8.6:** *Dilatometric curves showing the linear variation of relative specimen length as a function of temperature during cooling from the austenitising temperature to the isothermal transformation temperature.*

*(a) Heterogencous 'US83' steel.*

*(b) Heterogeneous 'US24' steel.*
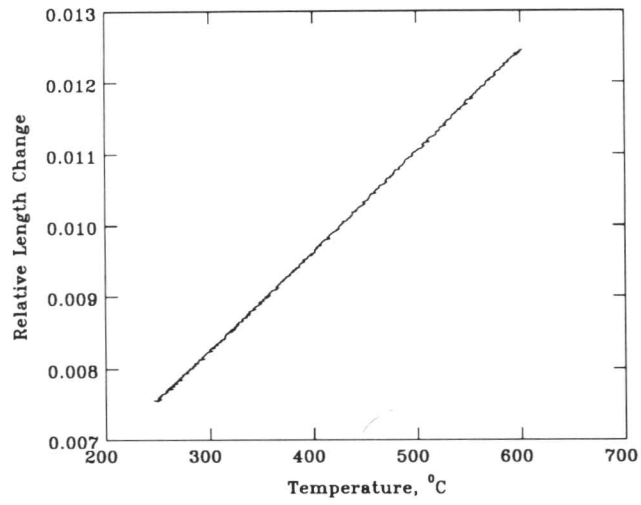
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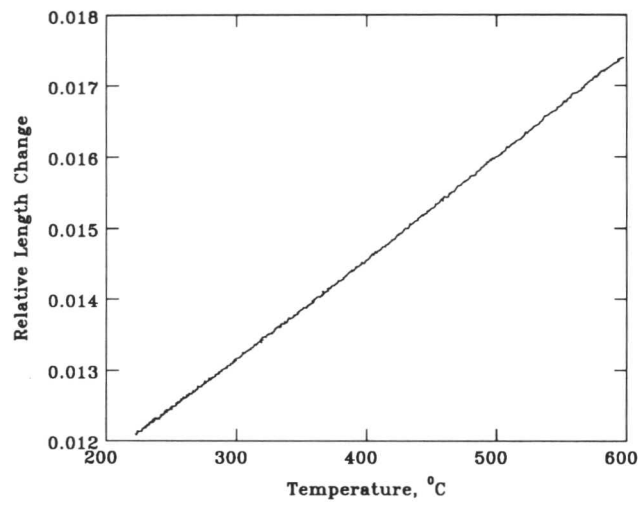


b

**Fig. 8.7:** *Graph of relative length change versus temperature, from which the linear expansion coefficient of ferrite is obtained.*

*(a) 'US83' steel.*
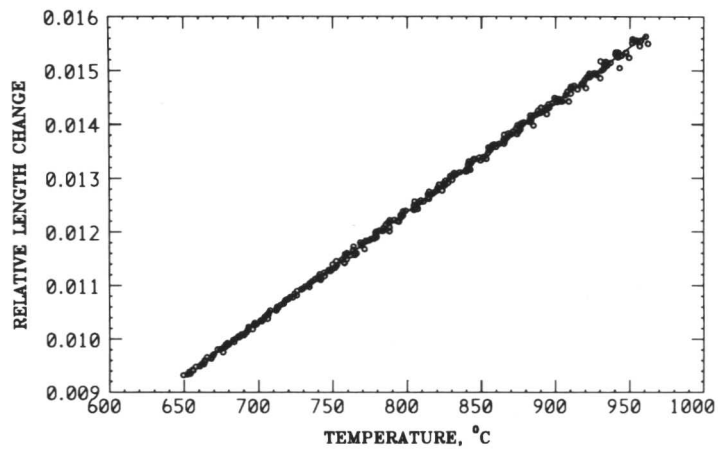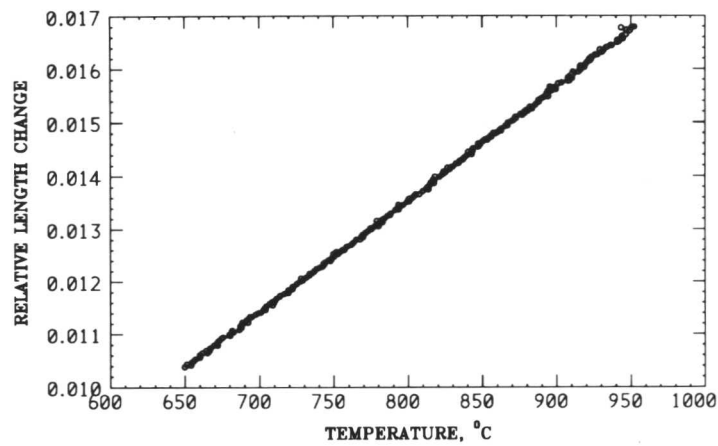
*(b) 'US24' steel.*

**Fig. 8.8:** *Graph of relative length change versus temperature, from which the linear expansion coefficient of austenite is obtained.*

*(a) 'US83' steel.*

*(b) 'US24' steel.*

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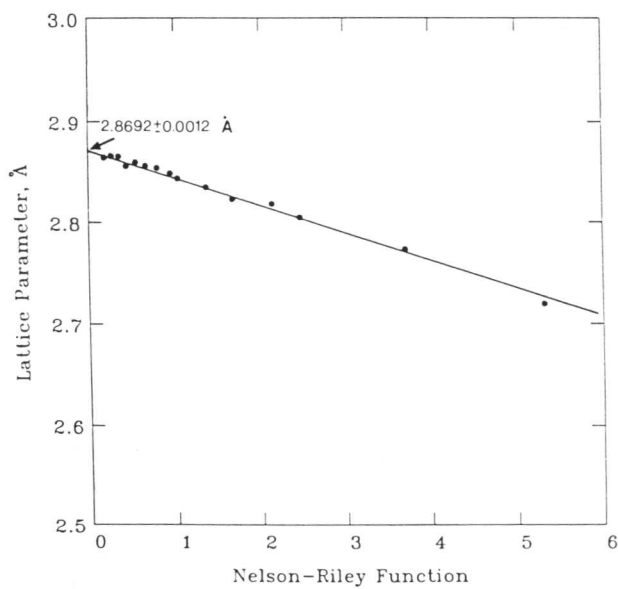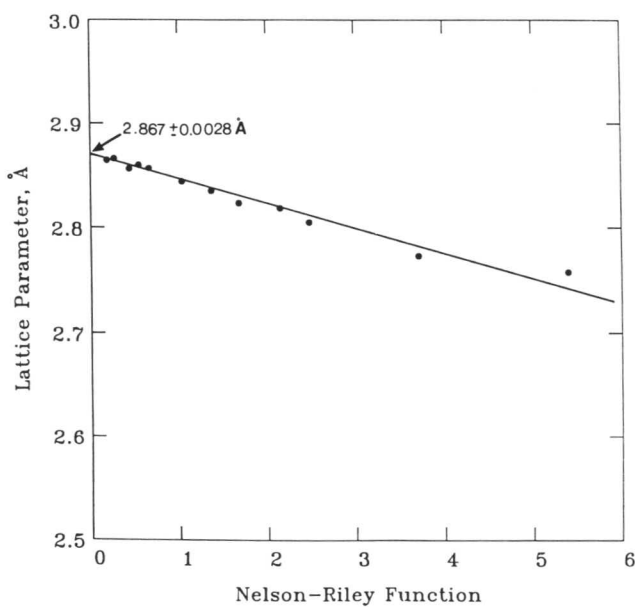
**Fig. 8.9:** *Extrapolation of measured lattice parameter against Nelson-Riley function (i.e., $\frac{cos^2\theta}{sin\theta} + \frac{cos^2\theta}{\theta}$). $\theta$ is the diffraction angle.*
*(a) 'US83' steel.*
*(b) 'US24' steel.*
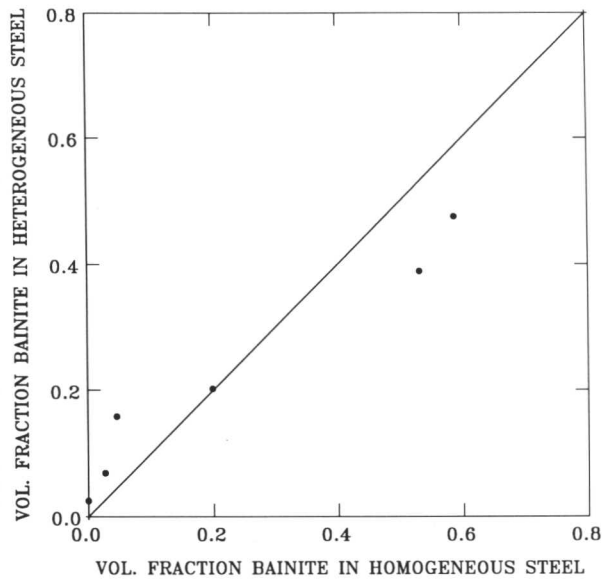
**Fig. 8.10:** *A plot of the maximum volume fraction of bainitic ferrite obtained in homogenised 'US83' steel, versus the corresponding volume fraction for as-received 'US83' steel. The line has a slope of unity and serves to illustrate that except at the transformation temperatures near $B_s$, the extent of transformation is larger in the homogenised samples.*
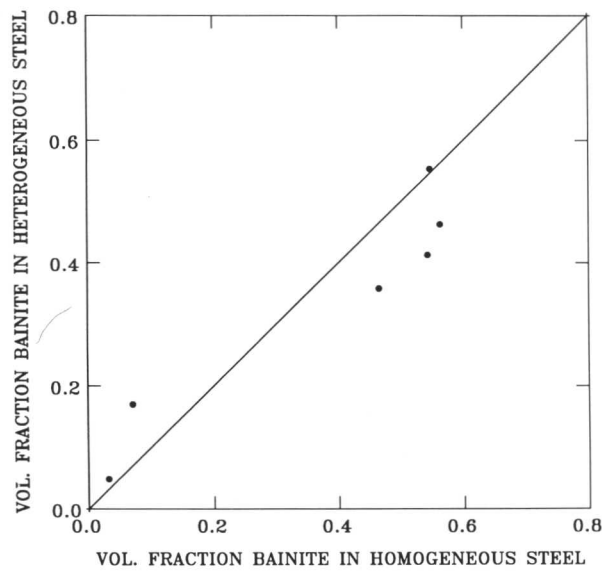


**Fig. 8.11:** *A plot of the maximum volume fraction of bainitic ferrite obtained in homogenised 'US24' steel, versus the corresponding volume fraction for as-received 'US24' steel. The line has a slope of unity and serves to illustrate that except at the transformation temperatures near $B_s$, the extent of transformation is larger in the homogenised samples.*

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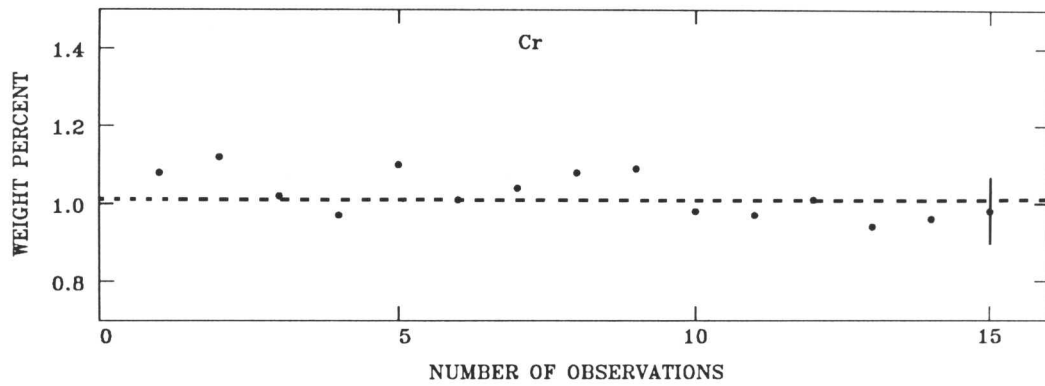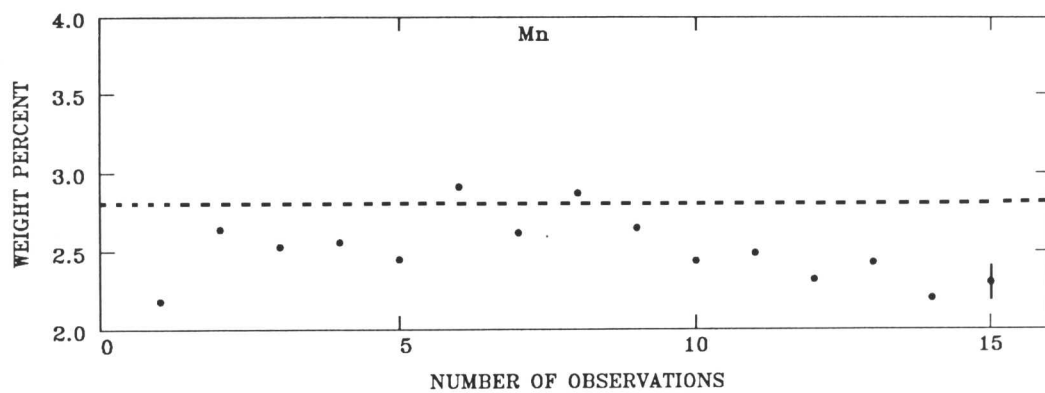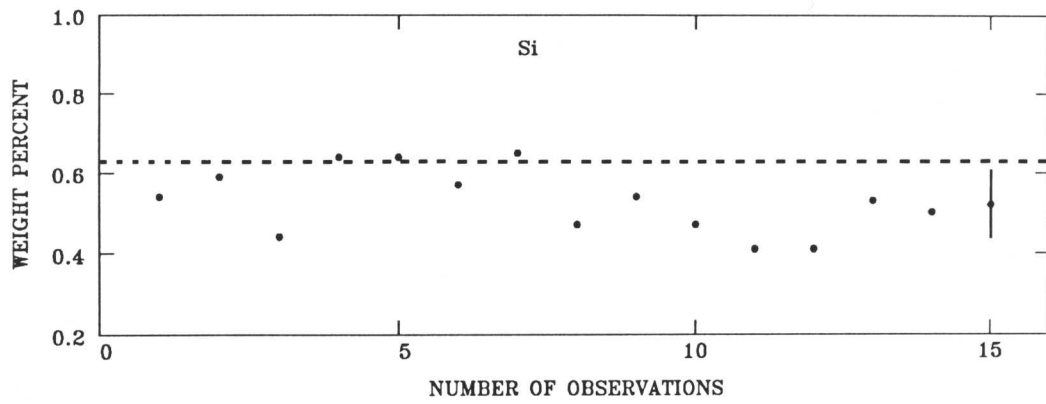
**Fig. 8.12a:** *Microanalysis data from the bainitic regions in a heterogeneous sample of 'US83' steel. The error bars indicate the typical 95% confidence statistical error and the average composition is in each case indicated by the dashed horizontal line.*
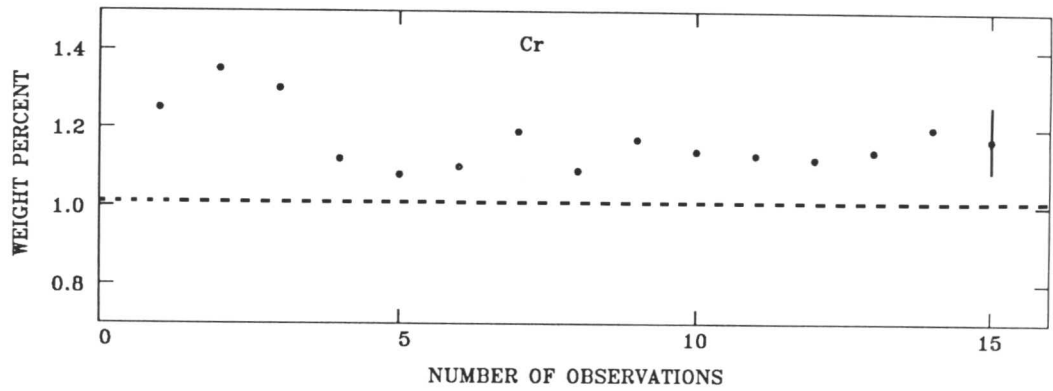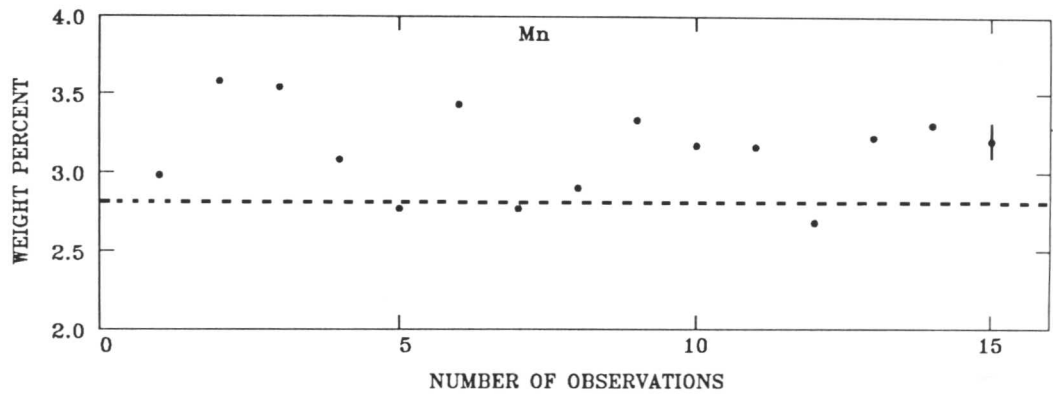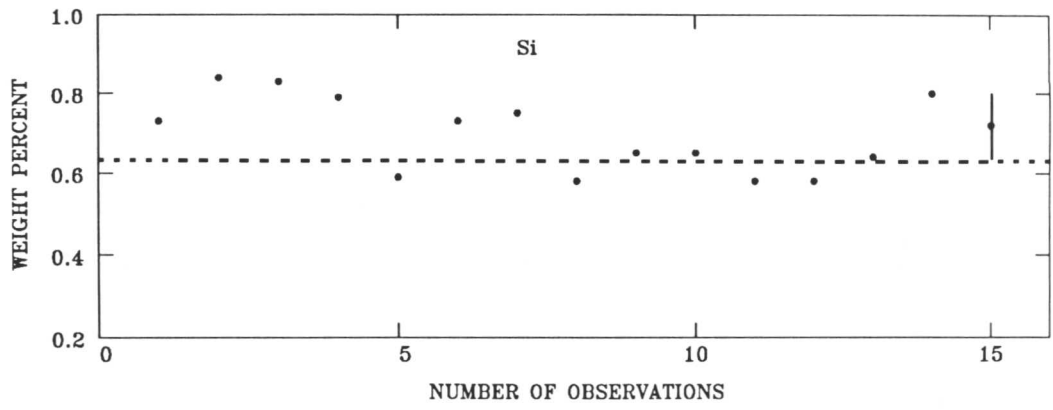
**Fig. 8.12b:** *Microanalysis data from the martensitic regions in a heterogeneous sample of 'US83' steel. The error bars indicate the typical 95% confidence statistical error and the average composition is in each case indicated by the dashed horizontal line.*

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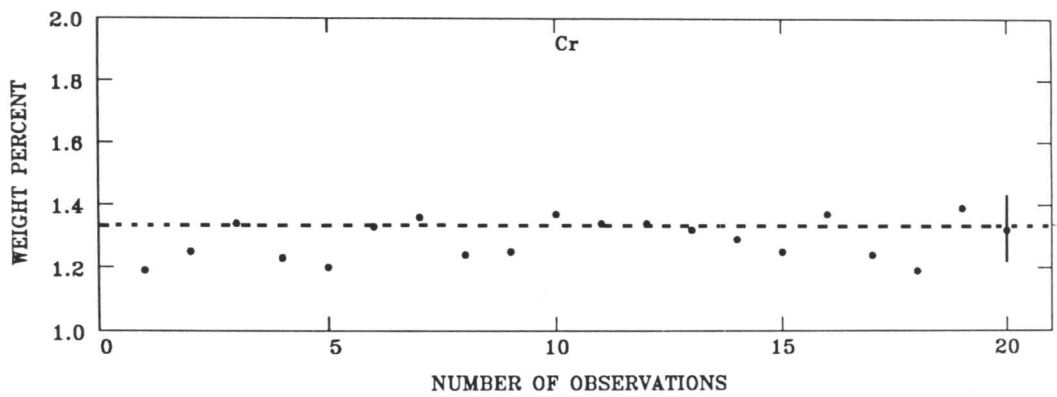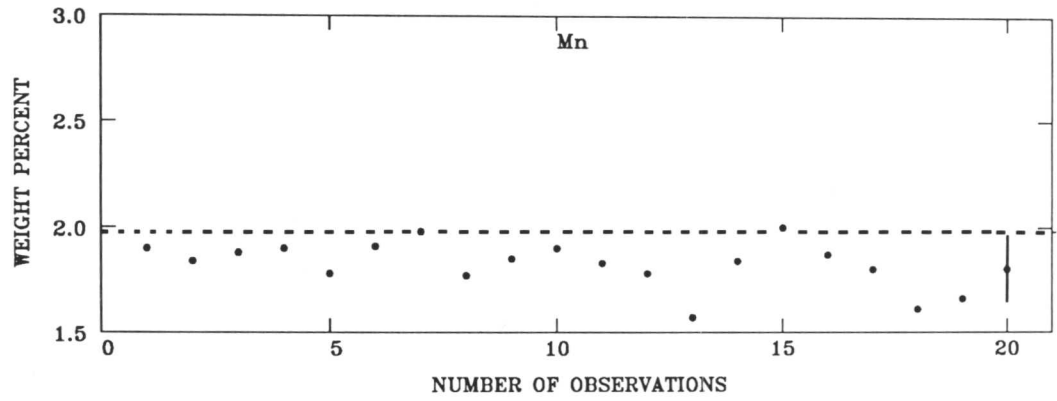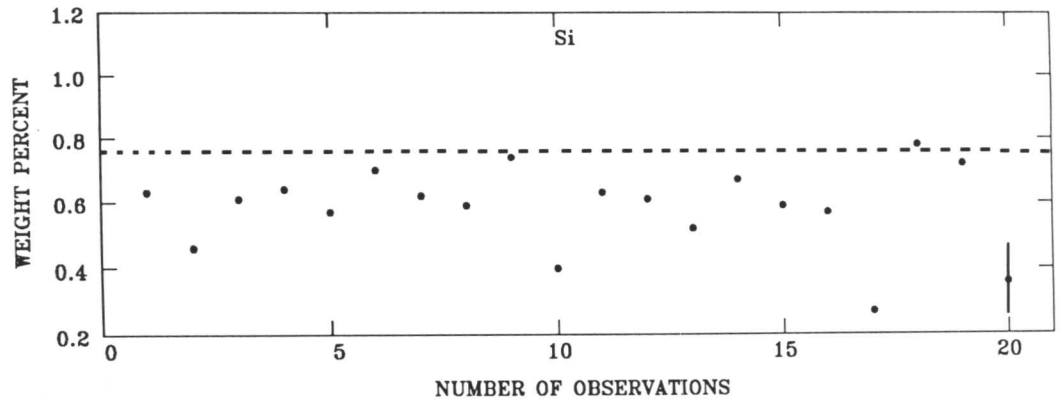
**Fig. 8.13a:** *Microanalysis data from the bainitic regions in a heterogeneous sample of 'US24' steel. The error bars indicate the typical 95% confidence statistical error and the average composition is in each case indicated by the dashed horizontal line.*
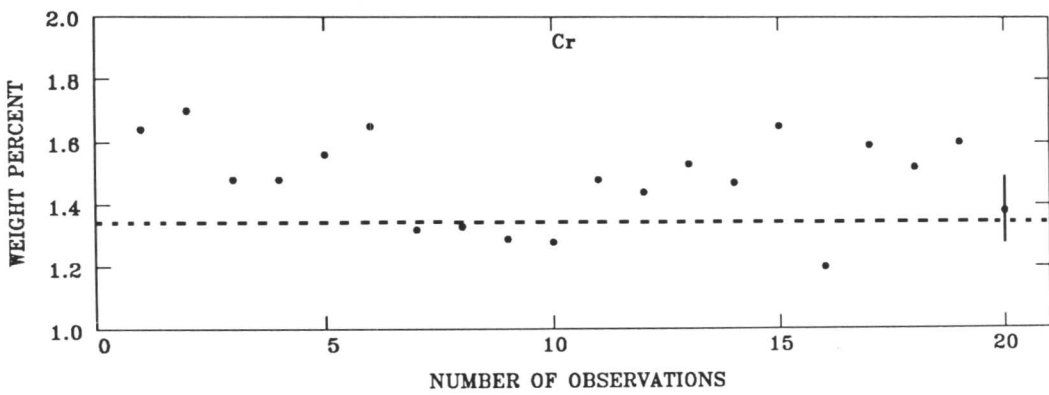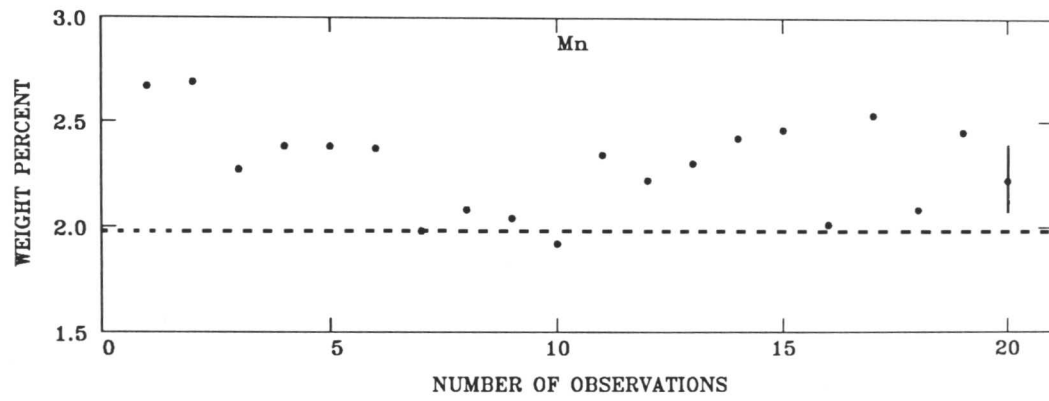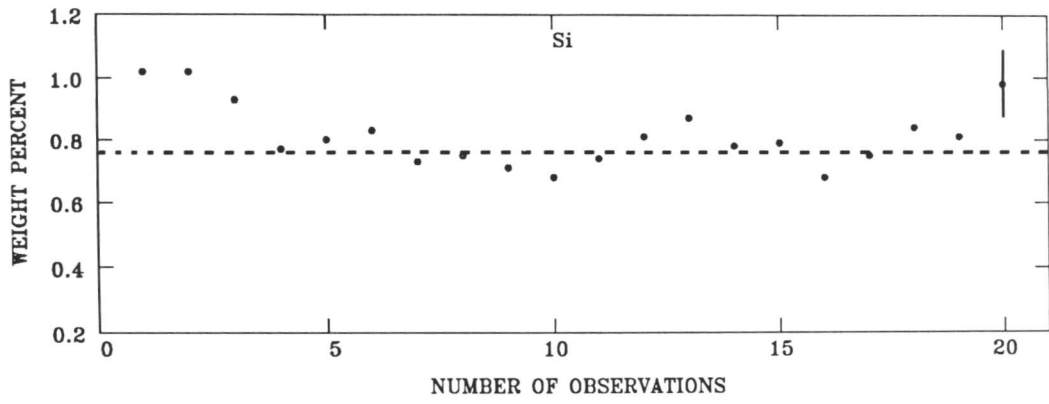
**Fig. 8.13b:** *Microanalysis data from the martensitic regions in a heterogeneous sample of 'US24' steel. The error bars indicate the typical 95% confidence statistical error and the average composition is in each case indicated by the dashed horizontal line.*
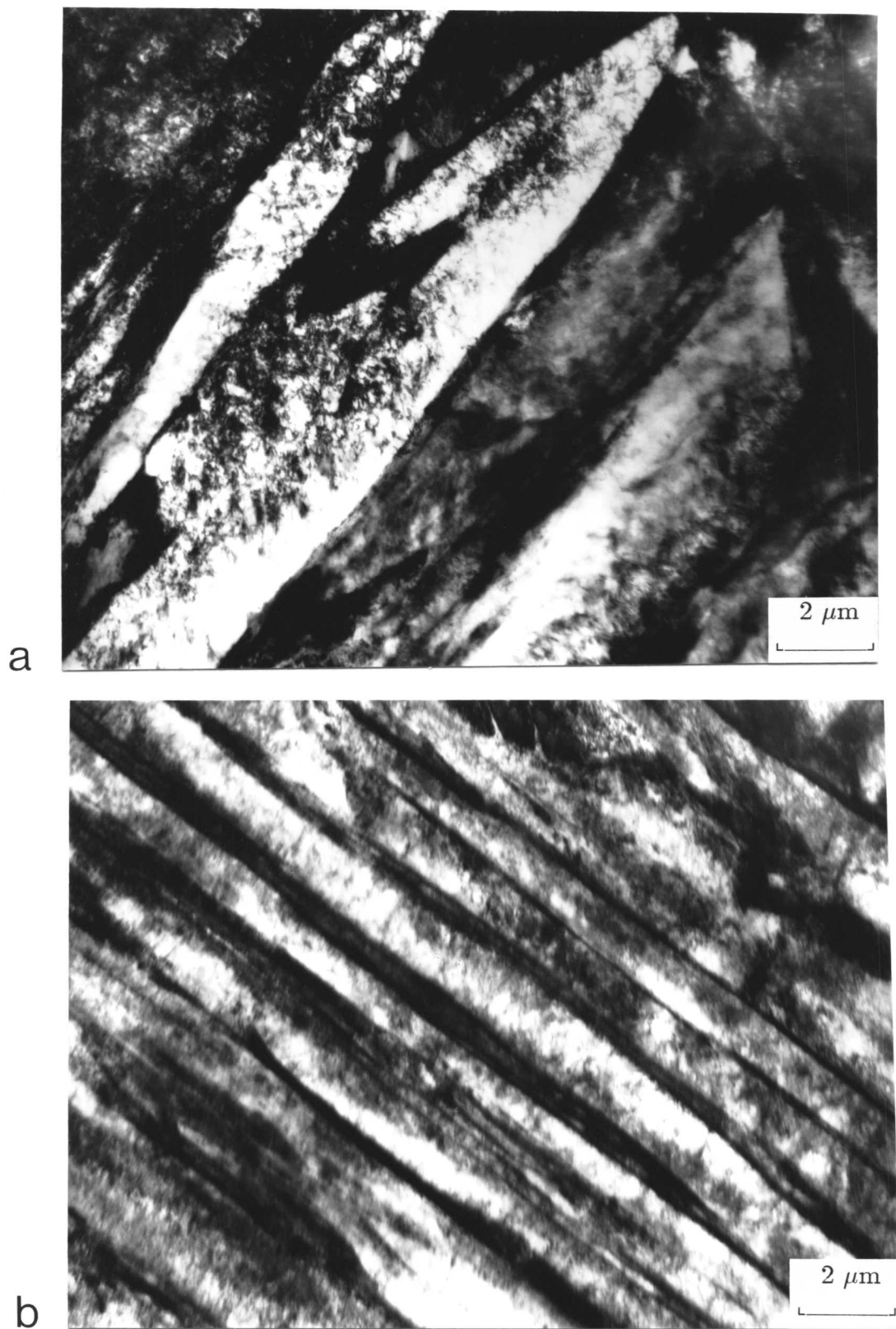
**Fig. 8.14:** *Bright field transmission electron micrograph showing upper bainite in a heterogeneous sample of 'US83' steel.*

*(a) Isothermally transformed to bainitic ferrite at 400 °C for approximately 90 minutes before quenching to ambient temperature.*

*(b) Isothermally transformed to bainitic ferrite at 420 °C for approximately 90 minutes before quenching to ambient temperature.*
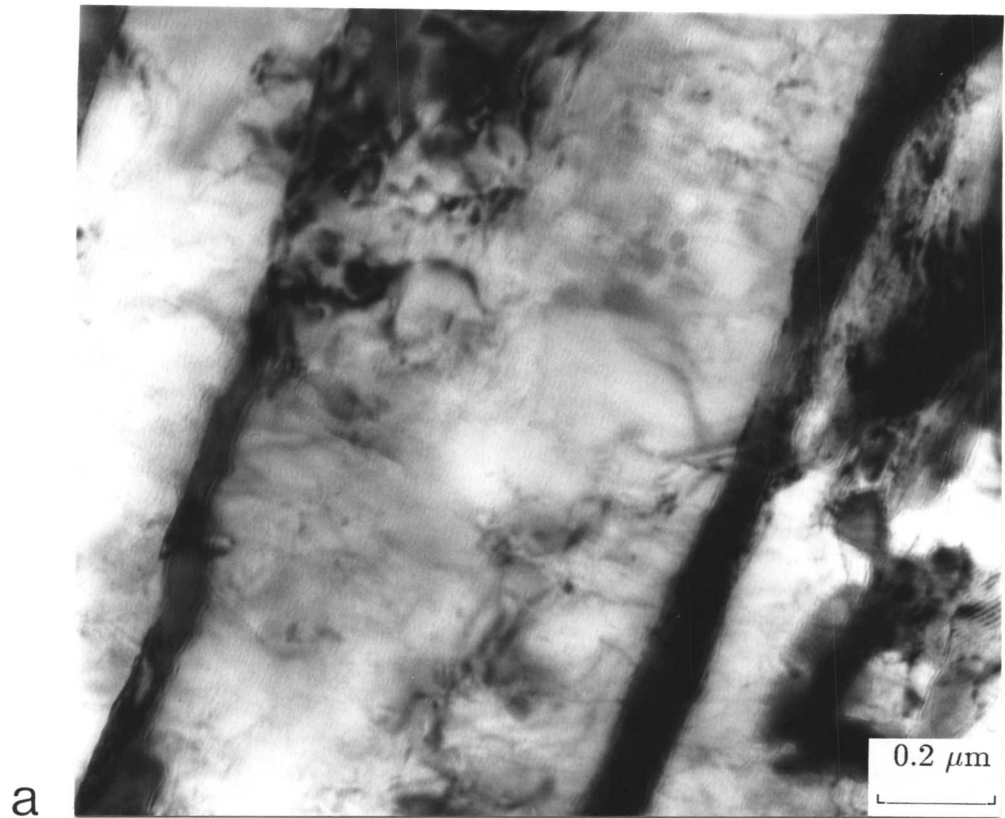
**Fig. 8.15:** *Bright field transmission electron micrograph showing upper bainite in a heterogeneous sample of 'US24' steel.*

*(a) Isothermally transformed to bainitic ferrite at 400 °C for approximately 90 minutes before quenching to ambient temperature.*

*(b) Isothermally transformed to bainitic ferrite at 420 °C for approximately 90 minutes before quenching to ambient temperature.*

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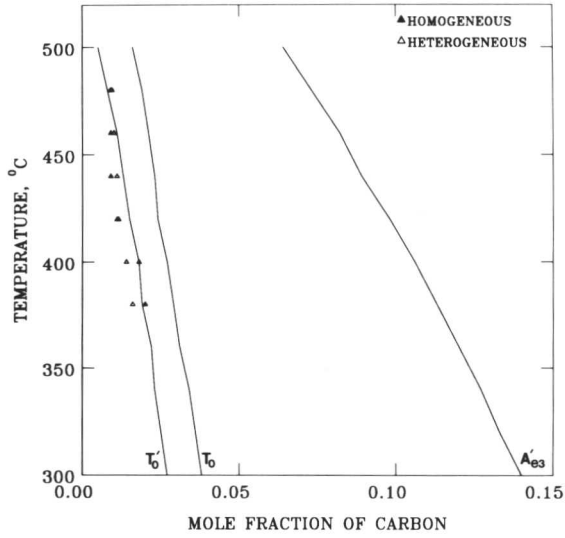
**Fig. 8.16:** *Calculated*[3,4] $T_0'$, $A_{e3}'$ *and* $A_{e3}$ *phase boundaries for 'US83' steel. The experimental data are for samples transformed isothermally to bainitic ferrite and carbon enriched residual austenite at a variety of temperatures.*
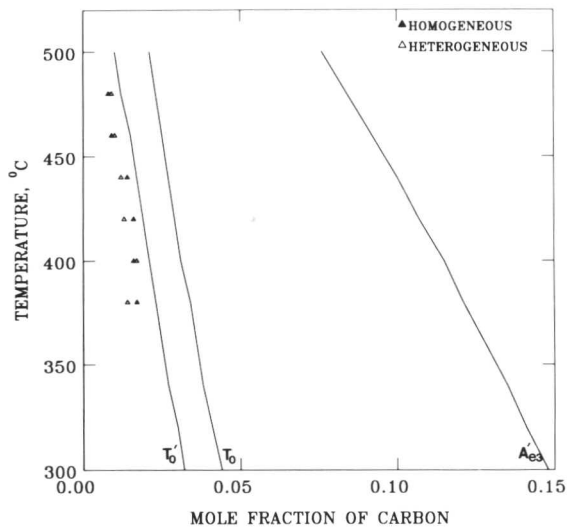


**Fig. 8.17:** *Calculated*[3,4] $T_0'$, $A_{e3}'$ *and* $A_{e3}$ *phase boundaries for 'US24' steel. The experimental data are for samples transformed isothermally to bainitic ferrite and carbon enriched residual austenite at a variety of temperatures.*

220
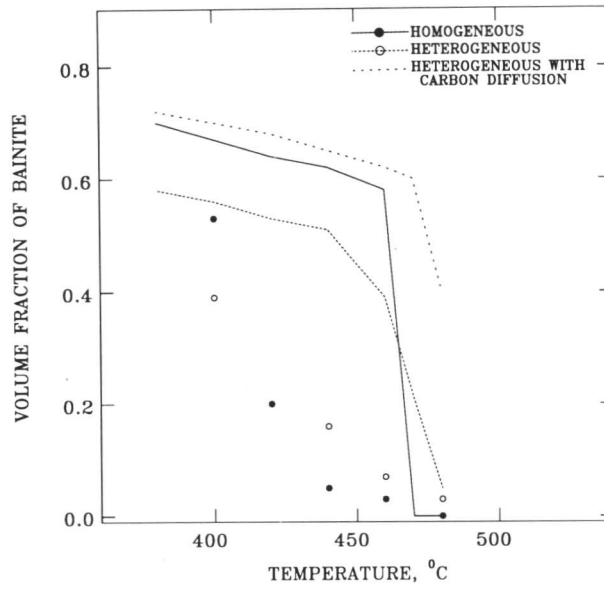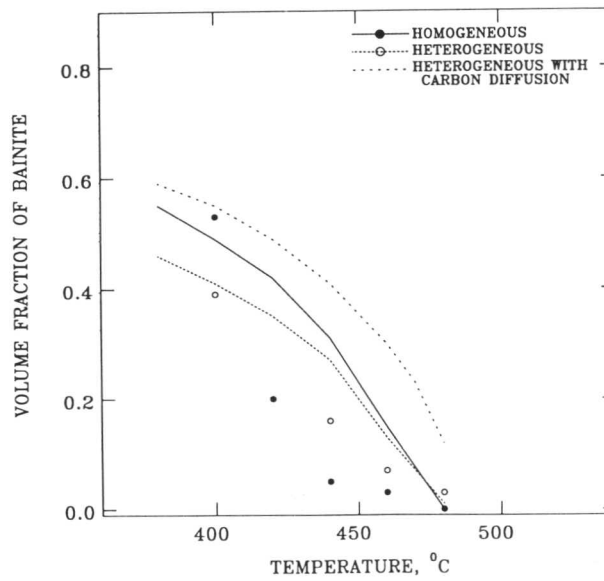
**Fig. 8.18:** *Results from the slice model calculations for as-received and homogenised samples of 'US83' steel. Points in the graph represent the experimental data.*

*(a) Calculations based on $T_0$ curve.*

*(b) Calculations based on $T_0'$ curve.*

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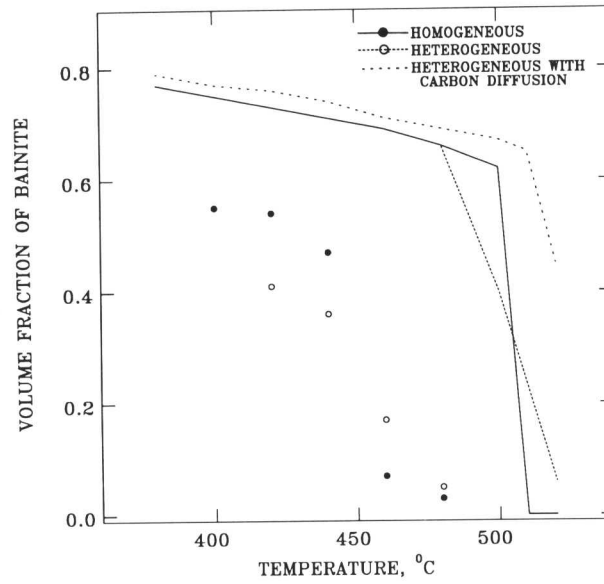
a
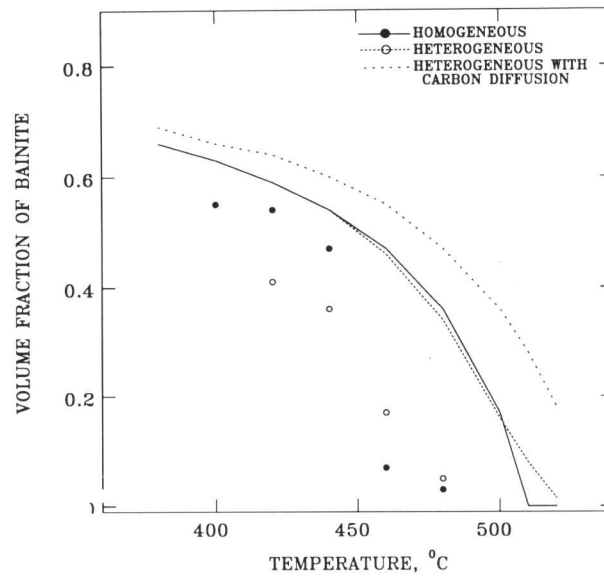


b

**Fig. 8.19:** *Results from the slice model calculations for as-received and homogenised samples of 'US24' steel. Points in the graph represent the experimental data.*

*(a) Calculations based on $T_0$ curve.*

*(b) Calculations based on $T'_0$ curve.*
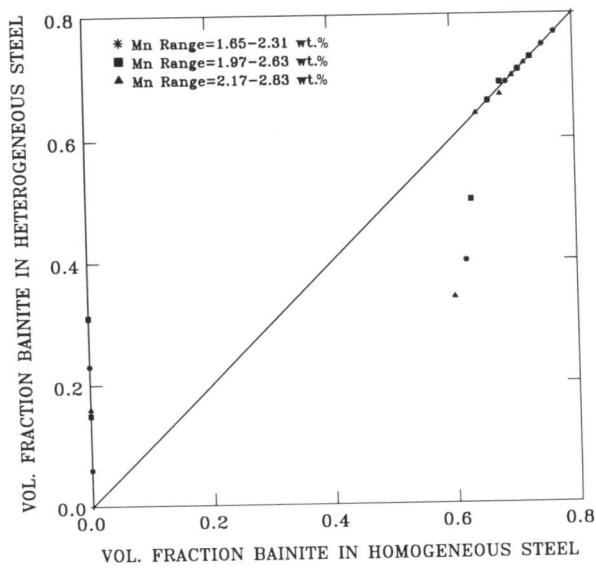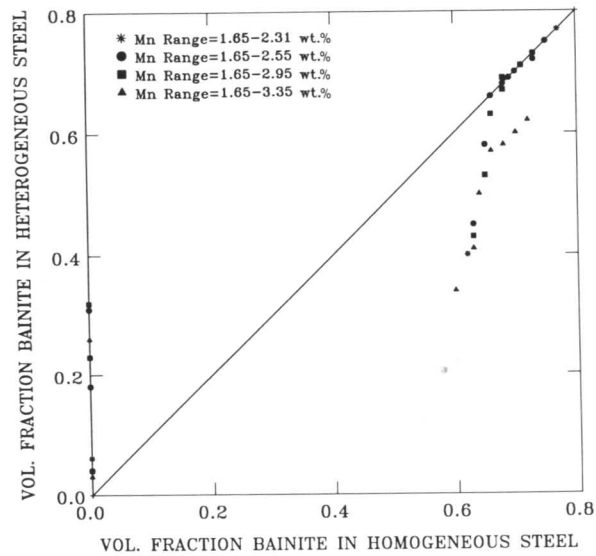
**Fig. 8.20:** *Graphs showing the differences in the volume fraction of bainite in the homogeneous and heterogeneous "US24" steel samples as a function of Mn concentration.*

*(a) The average Mn concentration was varied keeping the absolute range same.*

*(b) The Mn concentration range was varied keeping the minimum at a constant.*

a



b



c



d
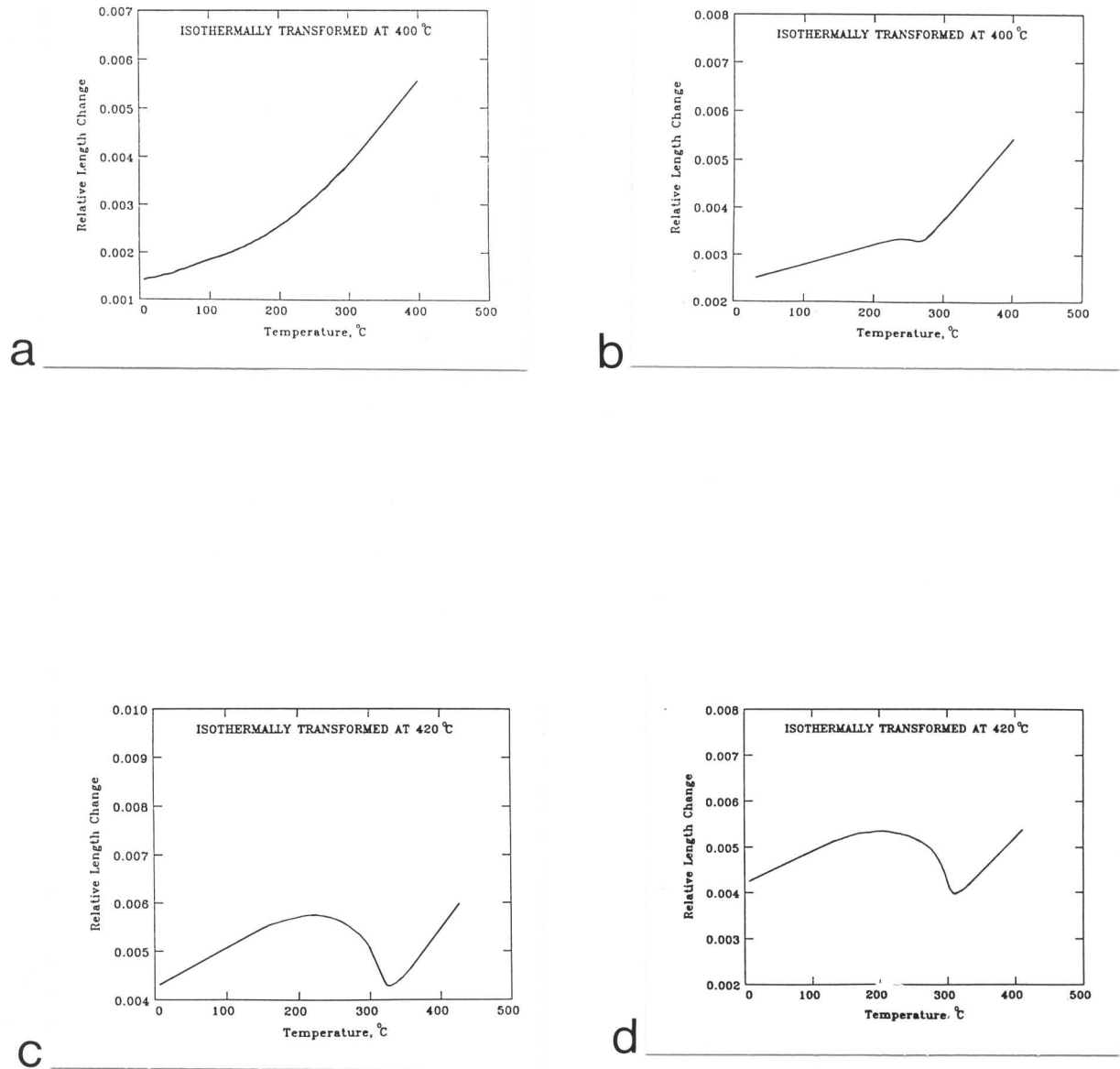
**Fig. 8.21:** *Dilatometric curves showing the transformation to martensite in heterogeneous and homogeneous 'US83' steels, after the specimens were isothermally transformed to bainite at different temperatures, with enough time at each isothermal transformation temperature to ensure that bainitic ferrite formation stopped. Graphs (a), (c), (e), (g) and (i) are for homogeneous samples and (b), (d), (f), (h) and (j) are from heterogeneous samples.*

e



f



g



h



i



j

**Fig. 8.21:** ( *continued ....* )

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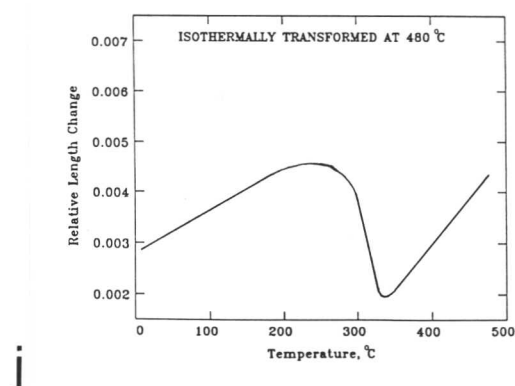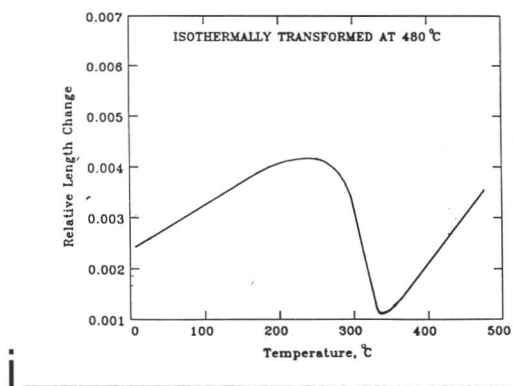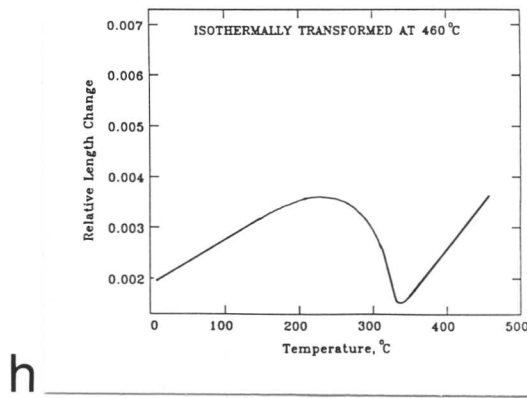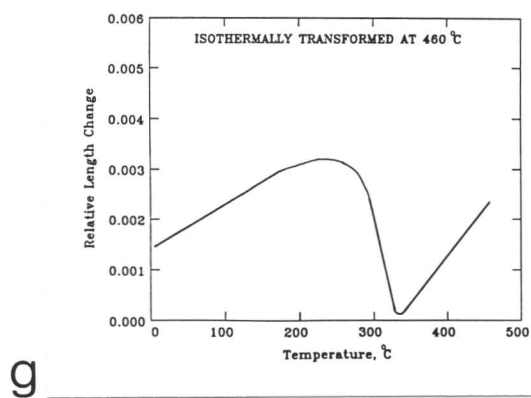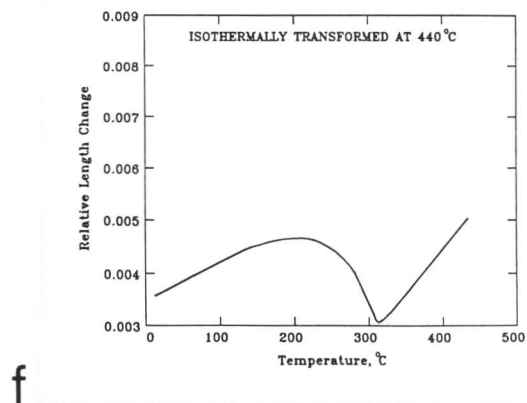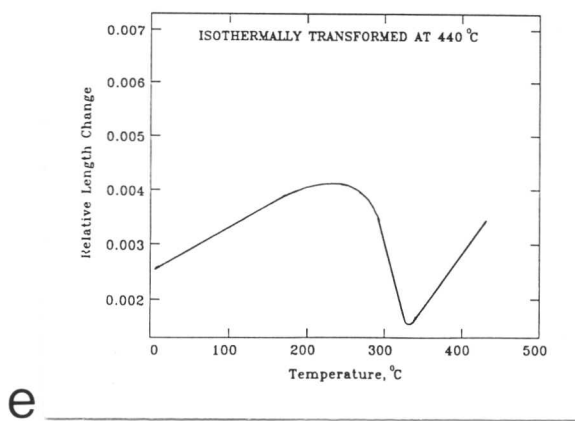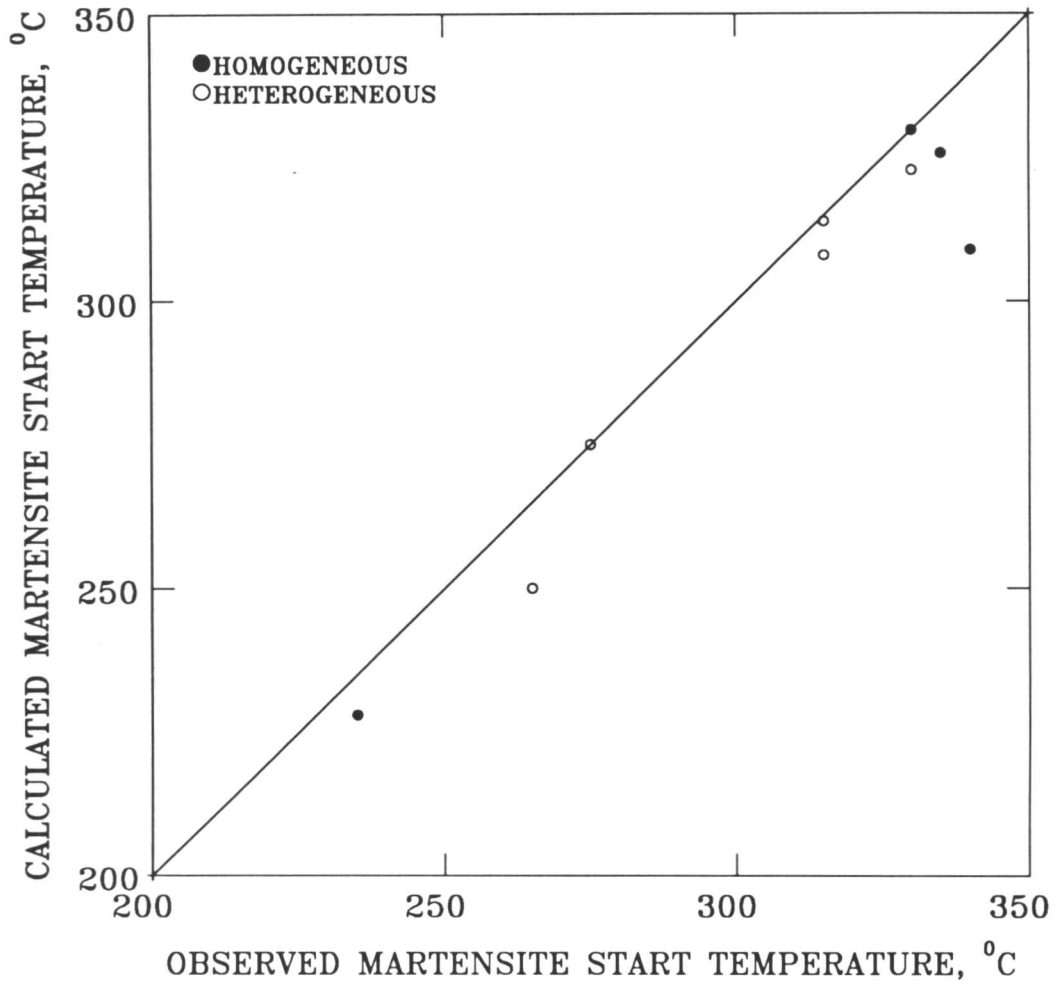
**Fig. 8.22:** *Thermodynamically calculated*[7,8] *and experimentally determined* $M_S$ *temperatures for homogenised and heterogeneous samples, after partial isothermal transformation to bainite.*
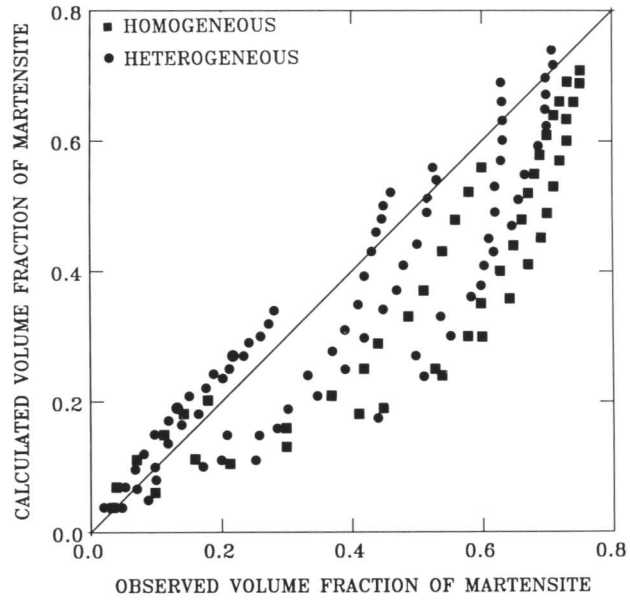
**Fig. 8.23:** *Comparison of the observed and calculated volume fractions of martensite. The calculations utilise the Koistinen and Marburger's equation[9]. A common value of 0.004 was assigned to $C_1$ for all these calculations.*
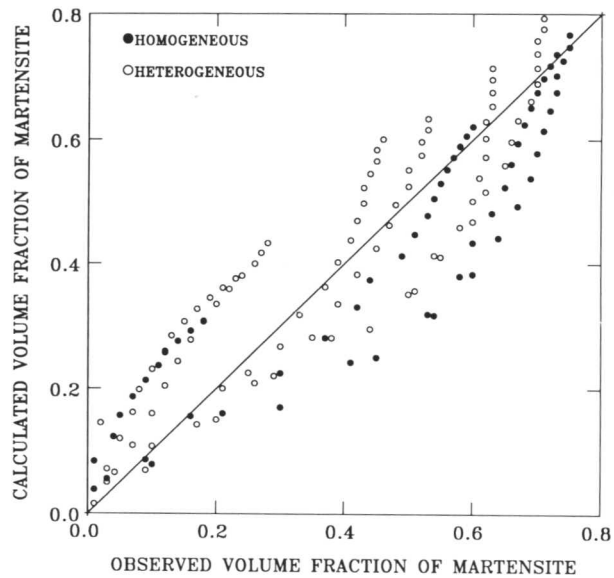


**Fig. 8.24:** *Comparison of experimental results with those calculated by the new model based on equation 8.9.*
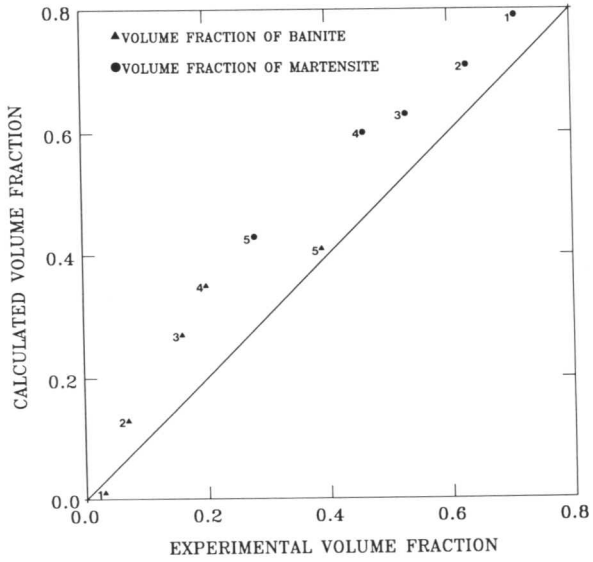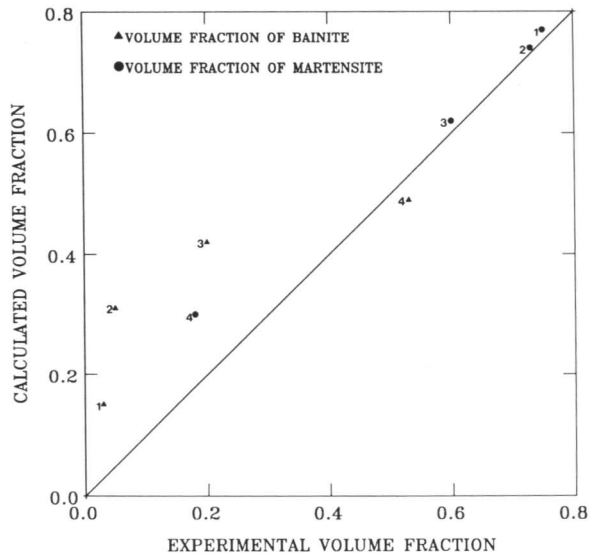
**Fig. 8.25:** *Comparison of the calculated and experimental maximum volume fractions of bainite and martensite in the "US83" steel. Data points marked with the same number are from the same heat treatment.*

*(a) Heterogeneous alloy.*

*(b) Homogeneous alloy.*

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# Chapter 9

# SUMMARY AND FURTHER WORK

## 9.1 Summary

Phase transformations in different heterogeneous steels have been investigated using thermodynamic analysis and phase transformation theory, backed by experimental confirmation. It is found that the maximum volume fraction of bainite formed at any temperature (except above the $B_s$ of homogeneous alloy) is lower in samples containing chemical segregation when compared with corresponding homogeneous alloy. A model has been developed which explains the results quantitatively, as long as the carbon distribution in the austenite does not homogenise during the course of bainite transformation. That it does not do so has been confirmed, since the $M_s$ temperatures of partially bainitic specimen have been found to be much higher than expected. It has also been shown that if an opportunity is provided for carbon to distribute evenly throughout the residual austenite during the development of the bainitic microstructure, then the extent of transformation is always larger for the heterogeneous samples when compared with the homogenised samples. The later case was found to be more applicable in the formation of allotriomorphic ferrite in a heterogeneous alloy, where due to higher transformation temperatures involved carbon can distribute evenly throughout the residual austenite to facilitate still more transformation.

The major effect of chemical segregation on martensite transformation, in the steel studied, is to extend the range over which the reaction occurs relative to homogenised samples. It was also found that the presence of bainitic ferrite does not significantly alter the way in which the subsequent transformation to martensite occurs. All the data from homogeneous and heterogeneous samples have been rationalised using a new model of athermal martensite kinetics, which includes an effect of autocatalytic nucleation

Reaustenitisation from a mixture of bainite and austenite, in homogeneous and heterogeneous samples has also been studied under isothermal conditions and in circumstances where the nucleation of austenite is not necessary. Dilatometric results can

be explained well by a published theory for reaustenitisation. As initially higher volume fractions of bainite were obtained in the homogeneous alloy its reaustenitisation start temperature will be lower than the heterogeneous alloy. The temperature at which the completion of reaustenitisation occurs, being dependent on average carbon content of the alloy should be the same for homogeneous and heterogeneous alloys.

## 9.2 Further Work

The present work has been on relatively higher Si content alloys, it will be interesting to study the effect of heterogeneities on the bainite reaction in alloys where carbide precipitation also accompanies ferrite formation. It will be worth checking for any correlation between banding and austenite grain structure. The existing model could be extended to investigate the phase transformations in heterogeneous austempered ductile cast irons which are becoming commercially important in automobile industry. Although this work is a part of a project into prediction of complete microstructure of steel weld deposits, all the experiments were done on wrought alloys. Some weld deposits should be tried and tested for this purpose. A study into a heterogeneous steel with an artificially modulated composition profile can help refine this model.

The model presented for the kinetics of martensitic transformation assumes that all the plates of martensite have identical volume. Moreover, it considers that all nucleation sites have the same activation energy. These approximations require much further research and characterisation.

This work needs to be related quantitatively to the influence of segregation on mechanical properties particularly as some qualitative and quantitative relationships can be found in the literature for homogeneous alloys.

More generally, it would be fascinating to investigate all the problems of heterogeneity using artificially modulated steels, in which not only the modulation wavelength but also its morphology can be controlled. The kinetics need to be developed further to treat the complete evolution of microstructure as a function of time, rather than just the maximum degrees of reaction obtained during isothermal reaction. In this respect, the experimental data accumulated here could be of considerable value in testing any overall transformation kinetics models for heterogeneous steels.

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C
C Program for the analysis of bainitic transformation in heterogeneous, Si
C containing steels. The steel is divided into slices of different compositions,
C the maximum volume fraction of bainite, for a given transformation temperature
C is then computed for each slice; taking care of nucleation (Bs temperature)
C & growth (T0 limit). Slices transform independent of each other and the
C carbon is not allowed to homogenise among the slices. The results averaged
C and compared with a steel of the corresponding average composition.
C This program calculates volume fraction of martensite also, Ms temperature is
C calculated from the carbon content of residual austenite left after the
C isothermally formed bainite at any specific temperature in every slice
C individually!!!
C Typical data set follows:
C 673 (temperature in Kelvin)
C 0.43 0.50 0.60 0.70 0.80 0.90 1.00 (Composition of slice 1 in wt.%)
C 0.43 0.60 0.60 0.70 0.80 0.90 1.90 (Composition of slice 2 in wt.%)
C C  Si  Mn  Ni  Mo  Cr  V
C

      IMPLICIT REAL*8(A-H,K-Z), INTEGER(I,J)
      DOUBLE PRECISION C(8),D(8),XTO(150),XTO400(150)
     &,E(8),F(8),MS(150),BS(150),IA(150),XGAMMA(150),VOLF(150)
     &,CN(150),SI(150),MN(150),NI(150),MO(150),V(150),FE(150)
     &,CR(150),WD(8),VG(150),CD(8),XG(150),VMF(150)
      VINCR=0.00005D+00
      ISTOP=0
      AVEVOL=0.0
      XGMS=0.00
      C1=0.0
      C2=0.0
      C3=0.0
      C4=0.0
      C5=0.0
      C6=0.0
      C7=0.0
      READ(5,*)KELVIN
      TISO=KELVIN-273.0
      XALPHA=XALPH(KELVIN)
      WRITE(6,9)KELVIN,XALPHA,VINCR
      DO 1 I=1,200
      READ(5,*,END=2)NIL,C(1),C(2),C(3),C(4),C(5),C(6),C(7)
      CN(I)=C(1)
      SI(I)=C(2)
      MN(I)=C(3)
      NI(I)=C(4)
      MO(I)=C(5)
      CR(I)=C(6)
      V(I)=C(7)
      FE(I)=100.0D+0-(C(1)+C(2)+C(3)+C(4)+C(5)+C(6)+C(7))
      C1=C1+C(1)
      C2=C2+C(2)
      C3=C3+C(3)
      C4=C4+C(4)
      C5=C5+C(5)
      C6=C6+C(6)
      C7=C7+C(7)
      DO 43 IJI=1,7
      E(IJI)=C(IJI)
43    CONTINUE
      CALL TZERO(C,KELVIN,XTO(I),XTO400(I))
      CALL MUC(E,MS,BS(I))
      XBAR=C(1)
      WRITE(6,10)I,XTO(I),BS(I)
1     CONTINUE
```

```
  2   ISLICE=I-1
      D(1)=C1/ISLICE
      D(2)=C2/ISLICE
      D(3)=C3/ISLICE
      D(4)=C4/ISLICE
      D(5)=C5/ISLICE
      D(6)=C6/ISLICE
      D(7)=C7/ISLICE
      DO 70 JII=1,7
      WD(JII)=D(JII)
 70   CONTINUE
      DO 56 JIJ=1,7
      F(JIJ)=D(JIJ)
 56   CONTINUE
      CALL TZERO(D,KELVIN,XTOH,XTO4H)
      CALL MUC(F,MS,BSH)
      WRITE(6,75)BSH,XTOH
 75   FORMAT( ' BSH= ',D10.4,' XTOH= ',D10.4)
      IF (BSH .LT. TISO) GOTO 789
      GOTO 85
 85   IF (XTOH .LE. D(1)) GOTO 789
      GOTO 79
 79   IF (XTOH .GT. XALPHA) GOTO 987
      GOTO 789
789   VOLH=0.00
      GOTO 678
987   VOLH=(XTOH-D(1))/(XTOH-XALPHA)
678   VGH=1.0D+0-VOLH
      XGM=WD(1)+((VOLH*WD(1))/(1.0D+00-VOLH))
C Getting new composition (wt%) of residual austenite for Ms calculation
      RTH=(100.0D+00-XGM)/(100.0D+00-WD(1))
      WD(1)=XGM
      DO 242 IIN=2,8
      WD(IIN)=WD(IIN)*RTH
242   CONTINUE
      CALL MUC(WD,MSH,BS)
      IF (MSH .GE. 20.0) GOTO 564
      GOTO 465
465   VMH=0.00
      GOTO 45
564   VMH=(1.0D+00-DEXP(-0.0054D+00*(MSH-20.0D+00)))*VGH
 45   WRITE(6,151)VMH
      WRITE(6,252)MSH
252   FORMAT( ' MSH= ', D10.4)
      WRITE(6,15)VOLH
      DO 6 I=1,100000
      IF(ISTOP .EQ. ISLICE) GOTO 14
      DO 4 J=1,ISLICE
      IF(IA(J) .EQ. 1) GOTO 4
      IF (BS(J) .LT. TISO) GOTO 5329
      GOTO 9352
5329  VOLF(J)=0.00
      GOTO 5
9352  VOLF(J)=VOLF(J) + VINCR
      XGAMMA(J)=XBAR + ((VOLF(J)*(XBAR-XALPHA))/
     &(1.0D+00-VOLF(J)))
      IF(XGAMMA(J) .GE. XTO(J)) GOTO 5
      GOTO 4
 5    IA(J)=1
      ISTOP=ISTOP+IA(J)
      VOLF(J)=VOLF(J)-VINCR
      IF (VOLF(J) .LE. 0.00) GOTO 115
      GOTO 4
115   VOLF(J)=0.00
      XGAMMA(J)=XBAR
 4    CONTINUE
 6    CONTINUE
 14   DO 12 J=1,ISLICE
      VG(J)=1.0D+00-VOLF(J)
```

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```
C Recalling the original composition(wt%) for each slice.....
      CD(1)=CN(J)
      CD(2)=SI(J)
      CD(3)=MN(J)
      CD(4)=NI(J)
      CD(5)=MO(J)
      CD(6)=CR(J)
      CD(7)=V(J)
      XG(J)=CD(1)+((VOLF(J)*CD(1))/(1.0D+00-VOLF(J)))
C Getting new composition (wt%) of residual austenite in each slice
C for Ms calculation...
      RT=(100.0D+00-XG(J))/(100.0D+00-CD(1))
      CD(1)=XG(J)
      DO 262 NIN=2,7
      CD(NIN)=CD(NIN)*RT
262   CONTINUE
      CALL MUC(CD,MS(J),BS)
      IF (MS(J) .GE. 20.0) GOTO 468
      GOTO 864
864   VMF(J)=0.00
      GOTO 464
468   VMF(J)=(1.0D+00-DEXP(-0.0054D+00*(MS(J)-20.0D+00)))*VG(J)
464   WRITE(6,909)J,MS(J),VMF(J),VOLF(J),XGAMMA(J)
909   FORMAT(' J= ',I3,' MS= ',D10.4,' VMF= ',D12.4,' VOLF= ',D12.4
     &,' XGM= ',D12.4)
      XGMS=XGMS+XGAMMA(J)
      AVEVOL=AVEVOL+VOLF(J)
      VMT=VMT+VMF(J)
      AVMS=AVMS+MS(J)
12    CONTINUE
      XGMS=XGMS/ISLICE
      AVEVOL=AVEVOL/ISLICE
      VMT=VMT/ISLICE
      AVMS=AVMS/ISLICE
      WRITE(6,166)XGMS
166   FORMAT(' Average carbon in residual austenite= ',F8.3)
      WRITE(6,13)AVEVOL
      WRITE(6,2539)AVMS
      WRITE(6,131)VMT
2539  FORMAT(' Average MS temperature= ',F8.3)
131   FORMAT(' Average volume fraction of MARTENSITE',
     &' in heterogeneous alloy =',F8.3)
151   FORMAT(' Maximum volume fraction of MARTENSITE in ',
     &' an alloy of average composition = ',F8.3)
13    FORMAT(' Average volume fraction of transformation',
     &' in heterogeneous alloy =',F8.3)
9     FORMAT(' KELVIN = ',F7.0,' XALPHA, mol. fraction =',D12.4
     &,' VOL INCREMENT=',D12.4)
10    FORMAT(' Slice Number ',I3,' XTO ',D12.4,
     &' BS ',D12.4/)
15    FORMAT(' Maximum volume fraction of bainitic ferrite in ',
     &' an alloy of average composition = ',F8.3)
      STOP
      END
C     Subroutine********MUC***************
      SUBROUTINE MUC(C,MS,BS)
      DOUBLE PRECISION X,X1,T,R,A,A1,AFE,A1FE,DA1,DA2,DA1FE,H,H1,S,S1
      INTEGER T1,I,NO,C100,U,B4,B5,J99,C99,C98,C97
      DOUBLE PRECISION D11,FTO,FTO400,XTO400,G9400,SHEART,DIFFT,
     1D44,A44,AFE44,DA44,DAFE44,DD44,F44,X44,DF441,DT4(40),DDFTO(40),
     1V13,V14,G9,V10,V11,V12,XTO,DFTO,INCEPT,SLOPE,CORR,
     1DEQ,ETEQ,T10,T20,XA,AFEQ,AEQ,ETEQ2,TEQ,
     1J,J1,D,D1,W,W1,F,TEST,GMAX,ERROR,T4,XEQ,FSON,FPRO
     1,C(8),B1,B2,P(7),Y(7),B3,BS,WS,WS1,MS
      C100=1
      DO 24 I=1,C100,1
      B5=111
      B3=0
      C(8)=(100.0-C(1)-C(2)-C(3)-C(4)-C(5)-C(6)-(C7))/55.84
```

```
        C(1)=C(1)/12.0115
        C(2)=C(2)/28.09
        C(3)=C(3)/54.94
        C(4)=C(4)/58.71
        C(5)=C(5)/95.94
        C(6)=C(6)/52.0
        C(7)=C(7)/50.94
        B1=C(1)+C(2)+C(3)+C(4)+C(5)+C(6)+C(7)+C(8)
        DO 107 U=2,7
        Y(U)=C(U)/C(8)
107   CONTINUE
        DO 106 U=1,7
        C(U)=C(U)/B1
106   CONTINUE
        B2=0.0
        T10=Y(2)*(-3)+Y(3)*2+Y(4)*12+Y(5)*(-9)+Y(6)*(-1)+Y(7)*(-12)
        T20=-3*Y(2)-37.5*Y(3)-6*Y(4)-26*Y(5)-19*Y(6)-44*Y(7)
        P(2)=2013.0341+763.8167*C(2)+45802.87*C(2)**2-280061.63*C(2)**3
      1+3.864D+06*C(2)**4-2.4233D+07*C(2)**5+6.9547D+07*C(2)**6
        P(3)=2012.067-1764.095*C(3)+6287.52*C(3)**2-21647.96*C(3)**3-
      12.0119D+06*C(3)**4+3.1716D+07*C(3)**5-1.3885D+08*C(3)**6
        P(4)=2006.8017+2330.2424*C(4)-54915.32*C(4)**2+1.6216D+06*C(4)**3
      1-2.4968D+07*C(4)**4+1.8838D+08*C(4)**5-5.5531D+08*C(4)**6
        P(5)=2006.834-2997.314*C(5)-37906.61*C(5)**2+1.0328D+06*C(5)**3
      1-1.3306D+07*C(5)**4+8.411D+07*C(5)**5-2.0826D+08*C(5)**6
        P(6)=2012.367-9224.2655*C(6)+33657.8*C(6)**2-566827.83*C(6)**3
      1+8.5676D+06*C(6)**4-6.7482D+07*C(6)**5 +2.0837D+08*C(6)**6
        P(7)=2011.9996-6247.9118*C(7)+5411.7566*C(7)**2
      1+250118.1085*C(7)**3-4.1676D+06*C(7)**4
        DO 108 U=2,7
        B3=B3+P(U)*Y(U)
        B2=B2+Y(U)
108   CONTINUE
        IF(B2 .EQ. 0.0) GOTO 455
        W=(B3/B2)*4.187
        GOTO 456
455   W=8054.0
456   FTO=1.0
        X1=C(1)
        XA=0.001
        R=8.31432
        W1=48570.0
        H=38575.0
        S=13.48
        XEQ=0.2
        XTO=0.07
        XTO400=0.06
        X44=0.1
        INCEPT=1.0D+00
        CORR=1.0D+00
        SLOPE=1.0D+00
        C98=0
        C97=0
        WS=0.0
        DO 9 T1=473,1173,20
        C98=C98+1
        J98=0
        J99=0
        XTO=XTO+0.0001
        XTO400=XTO400+0.0001
        X44=0.3*XEQ
        T=T1
        IF (T .LE. 1000) GOTO 20
        H1=105525
        S1=45.34521
        GOTO 19
20    H1=111918
        S1=51.44
19    F=ENERGY(T,T10,T20)
```

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```
        J=1-DEXP(-W/(R*T))
 51     DEQ=DSQRT(1-2*(1+2*J)*XEQ+(1+8*J)*XEQ*XEQ)
        TEQ=5*DLOG((1-XEQ)/(1-2*XEQ))
        TEQ=TEQ+DLOG(((1-2*J+(4*J-1)*XEQ-DEQ)/(2*J*(2*XEQ-1)))**6)
        TEQ=TEQ*R*T-F
        IF (DABS(TEQ) .LT. 1.0) GOTO 50
        ETEQ=5*((1/(XEQ-1))+2/(1-2*XEQ))
        ETEQ2=6*((4*J-1-(0.5/DEQ)*(-2-4*J+2*XEQ+16*XEQ*J))/(1-2*J+(4*J
        1-1)*XEQ-DEQ))+6*(4*J/(2*J*(2*XEQ-1)))
        ETEQ=(ETEQ+ETEQ2)*R*T
        XEQ=XEQ-TEQ/ETEQ
        GOTO 51
 50     AEQ=5*DLOG((1-2*XEQ)/XEQ)+6*W/(R*T)+((H)-(
        1S)*T)/(R*T)
        AEQ=AEQ+DLOG(((DEQ-1+3*XEQ)/(DEQ+1-3*XEQ))**6)
        AFEQ=5*DLOG((1-XEQ)/(1-2*XEQ))+DLOG(((1-2*J+(4*J-1)*XEQ-DEQ)/(2*J
        1*(2*XEQ-1)))**6)
        IF (XEQ .LT. X1) GOTO 2443
        GOTO 2442
 2443   IF(WS .EQ. 0.0) GOTO 2441
        GOTO 2444
 2441   WS=T4
        GOTO 2444
 2442   D=DSQRT(1-2*(1+2*J)*X1+(1+8*J)*X1*X1)
        A=6*W/(R*T)+DLOG(((D-1+3*X1)/(D+1-3*X1))**6)

        A=A+5*DLOG((1-2*X1)/X1)
        A=A+(H-S*T)/(R*T)
        AFE=5*DLOG((1-X1)/(1-2*X1))
        AFE=AFE+DLOG(((1-2*J+(4*J-1)*X1-D)/(2*J*(2*X1-1)))**6)
        FSON=R*T*(XA*(AEQ-A)+(1-XA)*(AFEQ-AFE))
        FPRO=R*T*(X1*(AEQ-A)+(1-X1)*(AFEQ-AFE))
        V14=3.251745029*(T-273)-2183.014
        IF (V14 .GE. 0.0) GOTO 452
        IF (FPRO .GE. V14) GOTO 105
 103    D44=DSQRT(1-2*(1+2*J)*X44+(1+8*J)*X44*X44)
        DD44=(0.5/D44)*(-2-4*J+2*X44+16*J*X44)
        A44=5*DLOG((1-2*X44)/X44)+6*W/(R*T)+((H)-(
        1S)*T)/(R*T)
        A44=A44+DLOG(((D44-1+3*X44)/(D44+1-3*X44))**6)
        AFE44=5*DLOG((1-X44)/(1-2*X44))+DLOG(((1-2*J+(4*J-1)*X44-D44

        1)/(2*J*(2*X44-1)))**6)
        F44=R*T*(X44*(AEQ-A44)+(1-X44)*(AFEQ-AFE44))
        F44=F44-V14
        IF (DABS(F44) .GE. 10.0) GOTO 101
        GOTO 102
 101    DA44=-((10/(1-2*X44))+(5/X44))+6*((DD44+3)/(D44-1+3*X44
        1)-(DD44-3)/(D44+1-3*X44))
        DAFE44=10/(1-2*X44)-5/(1-X44)+6*((4*J-1-DD44)/(1-2*J+(4*
        1J-1)*X44-D44)-2/(2*J*(2*X44-1)))
        DF441=R*T*(AEQ-X44*DA44-AFEQ+X44*DAFE44-DAFE44-A44+AFE44)
        X44=X44-F44/DF441
        GOTO 103
 105    X44=0.0
        IF (C97 .GT. 0) GOTO 102
        C97=1
        WS=T4
        GOTO 102
 452    X44=99999999999.99999
        IF(C97 .GT. 2) GOTO 9990
        C97=3
        WS1=T4
 9990   WS=T4
 102    FPROA=FPRO*((XEQ-XA)/(XEQ-X1))
        X=0.000001
        J1=1-DEXP(-W1/(R*T))
 7      D1=DSQRT(9-6*X*(2*J1+3)+(9+16*J1)*X*X)
        A1=3*DLOG((3-4*X)/X)+(4*W1/(R*T)
```

```
      A1=A1+DLOG(((D1-3+5*X)/(D1+3-5*X))**4)+(H1-S1*T)/(R*T)
      A1FE=DLOG(1-X)
      TEST=F+R*T*(A1FE-AFE) -R*T*(A1-A)
      IF (DABS(TEST) .GT. 10.0) GOTO 5
      GOTO 6
    5 DA1=(3*X/(3-4*X))*((4*X-3)/(X**2)-4/X)
      DA2=(0.5/D1)*(-12*J1-18+18*X+32*J1*X)
      DA2=4*(((DA2+5)/(D1-3+5*X))-((DA2-5)/(D1+3-5*X)))
      DA1=DA1+DA2
      DA1FE=1/(X-1)
      ERROR=TEST/(R*T*(DA1FE-DA1))
      IF (ERROR .GT. X) GOTO 30
      GOTO 29
   30 ERROR =0.3*X
   29 X=X-ERROR
      GOTO 7
    6 GMAX=R*T*(A1-A)
      D11=DSQRT(9-6*X1*(2*J1+3)+(9+16*J1)*X1*X1)
      T4=T-273
      IF (FTO .GE. 0.0) GOTO 22
      FTO=FTO1(H,S,X1,T,W,W1,H1,S1,F,J,J1)
      GOTO 21
   22 FTO =0.0
   21 DFTO=FTO1(H,S,XTO,T,W,W1,H1,S1,F,J,J1)
      J98=J98+1
      IF (DABS(DFTO) .LE. 10.0) GOTO 450
      G9=G91(XTO,T,W,W1,H1,S1,F,J,J1)
      IF (J98 .GE.9) GOTO 450
      XTO=XTO-DFTO/G9
      IF (XTO .LE. 0.0001) GOTO 94
      GOTO 21
   94 XTO=0.0000
  450 FTO400=FTO1(H,S,XTO400,T,W,W1,H1,S1,F,J,J1)+400.0
      J99=J99+1
      IF(J99 .GE. 9) GOTO 92
      IF (DABS(FTO400) .LE. 10.0) GOTO 92
      G9400=G91(XTO400,T,W,W1,H1,S1,F,J,J1)
      XTO400=XTO400-FTO400/G9400
      IF (XTO400 .LE. 0.0001) GOTO 451
      GOTO 450
  451 XTO400=0.0000
   92 V11=(XTO-X1)/(XTO-0.0013)
      V12=(XEQ-X1)/(XEQ-0.0013)
      V13=(X44-X1)/(X44-0.0013)
      V11=FFF(V11)
      V12=FFF(V12)
      V13=FFF(V13)
      SHEART=DEXP((0.2432D+06/(8.31432*T))-0.135D+03+20.0*DLOG(T)
     1-5*DLOG(DABS(GMAX)))
      DIFFT=DEXP((0.6031D+06/(8.31432*T))-0.1905D+03+20.0*DLOG(T)
     1-4*DLOG(DABS(GMAX)))
      IF (X44 .EQ. 0.0) GOTO 453
      GOTO 454
  453 SHEART=1D+20
  454 DDFTO(C98)=FTO
      DT4(C98)=T4
    9 CONTINUE
 2444 C98=C98-1
      CALL ANAL(C98,INCEPT,SLOPE,CORR,DT4,DDFTO)
      BS=(-400.0-INCEPT)/SLOPE
      MS=(-1120.0D+00-10568.0D+00*X1+94.1D+00-INCEPT)/SLOPE
      IF (WS .LT. BS) GOTO 9996
      GOTO 24
 9996 BS=WS
   24 CONTINUE
      RETURN
      END
C     Subroutine********TZERO*******************************************
      SUBROUTINE TZERO(C,T,XTO,XTO400)
```

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```
      DOUBLE PRECISION X,X1,T,R,H,H1,S,S1
      INTEGER I,U,B4,J99,C98,C97,B5
      DOUBLE PRECISION D11,FTO,FTO400,XTO400,G9400,G9,XTO,DFTO,T10,T20,
     1J,J1,D,W,W1,F,T4,C(8),B1,B2,P(7),Y(7),B3,WS
      B3=0
      C(8)=(100.0-C(1)-C(2)-C(3)-C(4)-C(5)-C(6)-(C(7))/55.84
C     DIVIDING BY ATOMIC WEIGHT........................................
      C(1)=C(1)/12.0115
      C(2)=C(2)/28.09
      C(3)=C(3)/54.94
      C(4)=C(4)/58.71
      C(5)=C(5)/95.94
      C(6)=C(6)/52.0
      C(7)=C(7)/50.94
      B1=C(1)+C(2)+C(3)+C(4)+C(5)+C(6)+C(7)+C(8)
      DO 107 U=2,7
      Y(U)=C(U)/C(8)
107   CONTINUE
C     CALCULATING MOLE FRACTIONS...........................................
      DO 106 U=1,7
      C(U)=C(U)/B1
106   CONTINUE
      B2=0.0
      T10=Y(2)*(-3)+Y(3)*2+Y(4)*12+Y(5)*(-9)+Y(6)*(-1)+Y(7)*(-12)
      T20=-3*Y(2)-37.5*Y(3)-6*Y(4)-26*Y(5)-19*Y(6)-44*Y(7)
      P(2)=2013.0341+763.8167*C(2)+45802.87*C(2)**2-280061.63*C(2)**3
     1+3.864D+06*C(2)**4-2.4233D+07*C(2)**5+6.9547D+07*C(2)**6
      P(3)=2012.067-1764.095*C(3)+6287.52*C(3)**2-21647.96*C(3)**3-
     12.0119D+06*C(3)**4+3.1716D+07*C(3)**5-1.3885D+08*C(3)**6
      P(4)=2006.8017+2330.2424*C(4)-54915.32*C(4)**2+1.6216D+06*C(4)**3
     1-2.4968D+07*C(4)**4+1.8838D+08*C(4)**5-5.5531D+08*C(4)**6
      P(5)=2006.834-2997.314*C(5)-37906.61*C(5)**2+1.0328D+06*C(5)**3
     1-1.3306D+07*C(5)**4+8.411D+07*C(5)**5-2.0826D+08*C(5)**6
      P(6)=2012.367-9224.2655*C(6)+33657.8*C(6)**2-566827.83*C(6)**3
     1+8.5676D+06*C(6)**4-6.7482D+07*C(6)**5 +2.0837D+08*C(6)**6
      P(7)=2011.9996-6247.9118*C(7)+5411.7566*C(7)**2
     1+250118.1085*C(7)**3-4.1676D+06*C(7)**4
      DO 108 U=2,7
      B3=B3+P(U)*Y(U)
      B2=B2+Y(U)
108   CONTINUE
      IF(B2 .EQ. 0.0) GOTO 455
      W=(B3/B2)*4.187
455   W=8054.0
      FTO=-1.0
      X1=C(1)
      R=8.31432
      W1=48570.0
C     ENTHALPY OF CARBON IN AUSTENITE....................................
      H=38575.0
C     ENTROPY OF CARBON IN AUSTENITE....................................
      S=13.48
      XTO=0.04
      XTO400=0.03
      C98=0
      C97=0
      WS=0.0
      J98=0
      J99=0
      IF (T .LE. 1000) GOTO 20
      H1=105525
      S1=45.34521
      GOTO 19
20    H1=111918
      S1=51.44
C     Calling subroutine ENERGY--------------------
C     DG FOR ALPHA---->GAMMA FOR PURE IRON............................
C     T10 & T20 ARE THE MAGNETIC & MAGN. EFFECTS OF ALLOY ADDITIONS ON
C     DG FOR ALPHA---->GAMMA FOR PURE IRON  (ZENER)
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19    F=ENERGY(T,T10,T20)
C     SITE EXCLUSION PARAMETER.............................................
      J=1-DEXP(-W/(R*T))
      J1=1.0-DEXP(-W1/(R*T))
      T4=T-273
C     Calling subroutine FTO1————————
      FTO=FTO1(H,S,X1,T,W,W1,H1,S1,F,J,J1)
C     Calling subroutine FTO1————————
21    DFTO=FTO1(H,S,XTO,T,W,W1,H1,S1,F,J,J1)
      J98=J98+1
      IF (DABS(DFTO) .LE. 10.0) GOTO 450
C     Calling subroutine G91————————
      G9=G91(XTO,T,W,W1,H1,S1,F,J,J1)
      IF (J98 .GE.9) GOTO 450
      XTO=XTO-DFTO/G9
      IF (XTO .LE. 0.0001) GOTO 94
      GOTO 21
94    XTO=0.0000
C     Calling subroutine FTO1————————
450   FTO400=FTO1(H,S,XTO400,T,W,W1,H1,S1,F,J,J1)+400.0
      J99=J99+1
      IF(J99 .GE. 10) GOTO 92
      IF (DABS(FTO400) .LE. 10.0) GOTO 92
C     Calling subroutine G91————————
      G9400=G91(XTO400,T,W,W1,H1,S1,F,J,J1)
      XTO400=XTO400-FTO400/G9400
      IF (XTO400 .LE. 0.0001) GOTO 451
      GOTO 450
451   XTO400=0.0000
92    CONTINUE
      RETURN
      END
C     Subroutine********FTO1****************************************
      DOUBLE PRECISION FUNCTION FTO1(H,S,X,T,W,W1,H1,S1,F,J,J1)
      DOUBLE PRECISION R,X,T,T60,ZEN1,ZEN2,ZENER,W,W1,H1,S1,F,
     1J,J1,D,D11,H,S
      D=DSQRT(1-2*(1+2*J)*X+(1+8*J)*X*X)
      D11=DSQRT(9-6*X*(2*J1+3)+(9+16*J1)*X*X)
      T60=T*(1-X)/(28080*X)
      IF (T60 .GT. 1.0) GOTO 18
      IF (T60 .GT. 0.25) GOTO 17
C     ZENER ORDERING.....................................
      ZEN1=0.2307+42.7974*T60-233.8631*T60*T60+645.4485*T60*T60*T60
     1-954.3995*(T60**4)+711.8095*(T60**5)-211.5136*(T60**6)
      ZEN2=-2.6702+45.6337*T60-225.3965*T60*T60+567.7112*(T60**3)
     1-771.6466*(T60**4)+538.1778*(T60**5)-151.3818*(T60**6)
      GOTO 16
17    ZEN2=1
      ZEN1=3.295
16    ZENER=(((ZEN2*X)**2)*(-50898.56)/(1-X))+ZEN1*T*X*0.6623741
      ZENER=ZENER*4.187
      GOTO 15
18    ZENER=0.0
15    R=8.31432
      FTO1=X*R*T*DLOG(X*X)+X*(H1-(H)-(S1-(S)
     1)*T+4*W1-6*W)-R*T*(1-X)*DLOG((1-X)**4)+5*R*T*(1-2*X)*DLOG(1-2*X)
     1-R*T*X*DLOG(((D-1+3*X)/(D+1-3*X))**6)-R*T*(1-X)*DLOG(((1-2*J+(4
     1*J-1)*X-D)/(2*J*(2*X-1)))**6)+3*R*T*X*DLOG(3-4*X)+R*T*
     1X*DLOG(((D11-3+5*X)/(D11+3-5*X))**4)+(1-X)*F+ZENER
      RETURN
      END
C     Subroutine********G91****************************************
      DOUBLE PRECISION FUNCTION G91(XTO,T,W,W1,H1,S1,F,J,J1)
      DOUBLE PRECISION R,XTO,T,W,W1,H1,S1,F,J,J1,FD,FD1,DT5,
     1DT6,DZEN1,DZEN2,DZEN3,V1,V2,V3,V4,V5,V6,V7,V8,V9,G1,
     1DZEN6,DZEN7,DZEN8
      R=8.31432
      FD=DSQRT(1-2*(1+2*J)*XTO+(1+8*J)*XTO*XTO)
      FD1=DSQRT(9-6*XTO*(2*J1+3)+(9+16*J1)*XTO*XTO)
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       DT5=28080*XTO/(1-XTO)
       DT6=T/DT5
       IF (DT6 .GT. 1.0) GOTO 48
       IF (DT6 .LT. 0.25) GOTO 47
       DZEN1=0.2307+42.7974*DT6-233.8631*(DT6**2)+645.4485*(DT6**3)
      1-954.3995*(DT6**4)+711.8095*(DT6**5)-211.5136*(DT6**6)
       DZEN2=-2.6702+45.6337*DT6-225.3965*(DT6**2)+567.7112*(DT6**3)
      1-771.6466*(DT6**4)+538.1778*(DT6**5)-151.3818*(DT6**6)
       GOTO 46
47     DZEN2=1
       DZEN1=3.295
46     DZEN3=(((DZEN2*XTO)**2)*(-50898.56)/(1-XTO))+DZEN1*T*XTO*
      1(0.6623741)
       DZEN3=DZEN3*4.187
       GOTO 45
48     DZEN3=0.0
45     V1=FD-1+3*XTO
       V2=FD+1-3*XTO
       V3=1-2*J+(4*J-1)*XTO-FD
       V4=2*J*(2*XTO-1)
       V5=FD1-3+5*XTO
       V6=FD1+3-5*XTO
       V7=(XTO-1-2*J+8*XTO*J)/FD
       V8=(9*XTO-9-6*J1+16*J1*XTO)/FD1
       V9=H1-(H)-(S1-(S))*T-6*W+4*W1
       G1=2+DLOG(XTO**2)+4+DLOG((1-XTO)**4)-10-DLOG((1-2*XTO)**10)
      1-DLOG((V1/V2)**6)-6*((XTO/V1)*(V7+3+V1*(3-V7)/V2))
      1+DLOG((V3/V4)**6)-6*((1-XTO)/V3)*(4*J*(1-(V3/V4))-V7)
      1+3*(DLOG(3-4*XTO)-4*XTO/(3-4*XTO))+DLOG((V5/V6)**4)+4*(XTO
      1/V5)*(V8+5+(V5/V6)*(5-V8))
       IF (DT6 .GT. 1.0) GOTO 90
       DZEN6=(-3.3948+13.6112*DT6-13.4376*(DT6**2))*T/(28080*
      1((1-XTO)**2))
       DZEN7=(-3.3118+15.7462*DT6-23.2449*(DT6**2))*T/(28080*
      1((1-XTO)**2))
       DZEN8=50898*((DZEN2*XTO)**2)/((1-XTO)**2)+(-50898*(2*
      1DZEN2*DZEN6*(XTO**2)+2*XTO*(DZEN2**2))/(1-XTO))+DZEN1
      1*T*0.6623741+DZEN7*T*XTO*0.6623741
       GOTO 91
90     DZEN8=0.0
91     G91=V9+R*T*G1+DZEN8-F
       RETURN
       END
C      Subroutine*******FFF*******************************************
       DOUBLE PRECISION FUNCTION FFF(V)
       DOUBLE PRECISION V
       IF (V .LE. 0.0) GOTO 1
       IF (V .GT. 1.0) GOTO 1
2      GOTO 3
1      FFF=0.0
       GOTO 4
3      FFF=V
4      RETURN
       END
C      Subroutine*******ENERGY***************************************
       DOUBLE PRECISION FUNCTION ENERGY(T,T10,T20)
       DOUBLE PRECISION T,T10,T20,F,T7
       T7=T-100*T20
       IF (T7 .LT. 300) GOTO 1
       IF (T7 .LT. 700) GOTO 2
       IF (T7 .LT. 940) GOTO 3
       F=-8.88909+0.26557*(T7-1140)-1.04923D-3*((T7-1140)**2)
       F=F+2.70013D-6*((T7-1140)**3)-3.58434D-9*((T7-1140)**4)
       GOTO 4
1      F=1.38*T7-1499
       GOTO 4
2      F=1.65786*T7-1581
       GOTO 4
3      F=1.30089*T7-1331
```

```
4      ENERGY=(141*T10 + F)*4.187
       RETURN
       END
       DOUBLE PRECISION FUNCTION XALPH(T)
       DOUBLE PRECISION T,CTEMP
       CTEMP=(T-273.0D+00)/900.0D+00
       XALPH=0.1528D-02-0.8816D-02*CTEMP+0.2450D-01*CTEMP*CTEMP
     &-0.2417D-01*CTEMP*CTEMP*CTEMP+
     &0.6966D-02*CTEMP*CTEMP*CTEMP*CTEMP
       RETURN
       END
       SUBROUTINE ANAL(C98,INCEPT,SLOPE,CORR,X,Y)
       DOUBLE PRECISION AX,AX2,AY,AY2,AXY,INCEPT,CORR,SLOPE,
     &X(40),Y(40)
       INTEGER I,C98,I1
       I1=C98
       C98=C98-10
       AX=0.0D+00
       AY=0.0D+00
       AX2=0.0D+00
       AY2=0.0D+00
       AXY=0.0D+00
       DO 1 I=1,C98
       AX=AX+X(I)
       AY=AY+Y(I)
       AXY=AXY+X(I)*Y(I)
       AX2=AX2+X(I)*X(I)
       AY2=AY2+Y(I)*Y(I)
1      CONTINUE
       INCEPT=(AY*AX2-AX*AXY)/(C98*AX2-AX*AX)
       SLOPE=((C98*AXY-AX*AY)/(C98*AX2-AX*AX))
       CORR=(C98*AXY-AX*AY)/(DSQRT((C98*AX2-AX*AX)*
     &(C98*AY2-AY*AY)))
       C98=I1
       RETURN
       END
```

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C Copyright S. A. Khan and H. K. D. H. Bhadeshia
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C
C Program for the analysis of bainitic transformation in heterogeneous, Si
C containing steels. The steel is divided into slices of different compositions,
C the maximum volume fraction of bainite, for a given transformation temperature
C is then computed for each slice; taking care of nucleation (Bs temperature)
C & growth (T0 limit). The carbon is allowed to redistribute among the slices
C after each increment of transformation.
C The results averaged and compared with a steel of the corresponding average
C composition.
C
C Typical data set follows:
C 673 (temperature in Kelvin)
C 0.43 0.50 0.60 0.70 0.80 0.90 1.00 (Composition of slice 1 in wt.%)
C 0.43 0.60 0.60 0.70 0.80 0.90 1.90 (Composition of slice 2 in wt.%)
C C   Si  Mn  Ni  Mo  Cr  V
C
      IMPLICIT REAL*8(A-H,K-Z), INTEGER(I,J)
      DOUBLE PRECISION C(8),D(8),XTO(100),XTO400(100)
     &,E(8),F(8),MS(100),BS(100),IA(100),XGAMMA(100),VOLF(100)
     &,CN(100),SI(100),MN(100),NI(100),MO(100),V(100),FE(100)
     &,CR(100),WD(8),VG(100),CD(8),XG(100),VMF(100)
      VINCR=0.00005D+00
      ISTOP=0
      AVEVOL=0.0
      C1=0.0
      C2=0.0
      C3=0.0
      C4=0.0
      C5=0.0
      C6=0.0
      C7=0.0
      READ(5,*)KELVIN
      TISO=KELVIN-273.0
      XALPHA=XALPH(KELVIN)
      WRITE(6,4444)
4444  FORMAT( ' YOU ARE ALLOWING CARBON TO HOMOGENIZE!!! ' )
      WRITE(6,9)KELVIN,XALPHA,VINCR
      DO 1 I=1,100
      READ(5,*,END=2)C(1),C(2),C(3),C(4),C(5),C(6),C(7)
      CN(I)=C(1)
      SI(I)=C(2)
      MN(I)=C(3)
      NI(I)=C(4)
      MO(I)=C(5)
      CR(I)=C(6)
      V(I)=C(7)
      FE(I)=100.0D+0-(C(1)+C(2)+C(3)+C(4)+C(5)+C(6)+C(7))
      C1=C1+C(1)
      C2=C2+C(2)
      C3=C3+C(3)
      C4=C4+C(4)
      C5=C5+C(5)
      C6=C6+C(6)
      C7=C7+C(7)
      DO 43 IJI=1,7
      E(IJI)=C(IJI)
43    CONTINUE
      CALL TZERO(C,KELVIN,XTO(I),XTO400(I))
      CALL MUC(E,MS,BS(I))
      XBAR=C(1)
      WRITE(6,10)I,XTO(I),BS(I)
1     CONTINUE
2     ISLICE=I-1
      D(1)=C1/ISLICE
```

```fortran
      D(2)=C2/ISLICE
      D(3)=C3/ISLICE
      D(4)=C4/ISLICE
      D(5)=C5/ISLICE
      D(6)=C6/ISLICE
      D(7)=C7/ISLICE
      DO 70 JII=1,7
      WD(JII)=D(JII)
70    CONTINUE
      DO 56 JIJ=1,7
      F(JIJ)=D(JIJ)
56    CONTINUE
      CALL TZERO(D,KELVIN,XTOH,XTO4H)
      CALL MUC(F,MS,BSH)
      WRITE(6,75)BSH,XTOH
75    FORMAT( ' BSH= ',D10.4,' XTOH= ',D10.4)
      IF (BSH .LT. TISO) GOTO 789
      GOTO 85
85    IF (XTOH .LE. D(1)) GOTO 789
      GOTO 79
79    IF (XTOH .GT. XALPHA) GOTO 987
      GOTO 789
789   VOLH=0.00
      GOTO 678
987   VOLH=(XTOH-D(1))/(XTOH-XALPHA)
678   VGH=1.0D+0-VOLH
      DO 101 III=1,ISLICE
      XGAMMA(III)=D(1)
      VOLF(III)=0.0
      IA(III)=0
101   CONTINUE
      AVEX=D(1)
      WRITE(6,15)VOLH
      DO 6 I=1,100000
      IF(ISTOP .EQ. ISLICE) GOTO 14
      DO 4 J=1,ISLICE
      IF(IA(J) .EQ. 1) GOTO 4
      IF (BS(J) .LT. TISO) GOTO 5329
      GOTO 9352
5329  VOLF(J)=0.00
      GOTO 5
9352  VOLF(J)=VOLF(J) + VINCR
      XGAMMA(J)=AVEX
      IF(XGAMMA(J) .GE. XTO(J)) GOTO 5
      GOTO 4
5     IA(J)=1
      ISTOP=ISTOP+IA(J)
      VOLF(J)=VOLF(J)-VINCR
      IF (VOLF(J) .LE. 0.00) GOTO 115
      GOTO 4
115   VOLF(J)=0.00
      XGAMMA(J)=AVEX
4     CONTINUE
      AVEVOL=0.0D+00
      DO 90 J33=1,ISLICE
      AVEVOL=AVEVOL+VOLF(J33)
90    CONTINUE
      AVEVOL=AVEVOL/ISLICE
      AVEX=D(1)+(AVEVOL*(D(1)-XALPHA))/(1.0D+00-AVEVOL)
6     CONTINUE
14    AVEVOL=0.0
      DO 12 J=1,ISLICE
      AVEVOL=AVEVOL+VOLF(J)
12    CONTINUE
      XGMS=XGMS/ISLICE
      AVEVOL=AVEVOL/ISLICE
      WRITE(6,166)XGMS
166   FORMAT(' Average carbon in residual austenite= ',F8.3)
      WRITE(6,13)AVEVOL
```

```fortran
13    FORMAT(' Average volume fraction of transformation',
     &' in heterogeneous alloy =',F8.3)
9     FORMAT(' KELVIN = ',F7.0,' XALPHA, mol. fraction =',D12.4
     &,' VOL INCREMENT=',D12.4)
10    FORMAT(' Slice Number ',I3,' XTO ',D12.4,
     &' BS  ',D12.4/)
15    FORMAT(' Maximum volume fraction of bainitic ferrite in ',
     &' an alloy of average composition = ',F8.3)
      STOP
      END
C     Subroutine********MUC***************
      SUBROUTINE MUC(C,MS,BS)
      DOUBLE PRECISION X,X1,T,R,A,A1,AFE,A1FE,DA1,DA2,DA1FE,H,H1,S,S1
      INTEGER T1,I,NO,C100,U,B4,B5,J99,C99,C98,C97
      DOUBLE PRECISION D11,FTO,FTO400,XTO400,G9400,SHEART,DIFFT,
     1D44,A44,AFE44,DA44,DAFE44,DD44,F44,X44,DF441,DT4(40),DDFTO(40),
     1V13,V14,G9,V10,V11,V12,XTO,DFTO,INCEPT,SLOPE,CORR,
     1DEQ,ETEQ,T10,T20,XA,AFEQ,AEQ,ETEQ2,TEQ,
     1J,J1,D,D1,W,W1,F,TEST,GMAX,ERROR,T4,XEQ,FSON,FPRO
     1,C(8),B1,B2,P(7),Y(7),B3,BS,WS,WS1,MS
      C100=1
      DO 24 I=1,C100,1
      B5=111
      B3=0
      C(8)=(100.0-C(1)-C(2)-C(3)-C(4)-C(5)-C(6)-(C7))/55.84
      C(1)=C(1)/12.0115
      C(2)=C(2)/28.09
      C(3)=C(3)/54.94
      C(4)=C(4)/58.71
      C(5)=C(5)/95.94
      C(6)=C(6)/52.0
      C(7)=C(7)/50.94
      B1=C(1)+C(2)+C(3)+C(4)+C(5)+C(6)+C(7)+C(8)
      DO 107 U=2,7
      Y(U)=C(U)/C(8)
107   CONTINUE
      DO 106 U=1,7
      C(U)=C(U)/B1
106   CONTINUE
      B2=0.0
      T10=Y(2)*(-3)+Y(3)*2+Y(4)*12+Y(5)*(-9)+Y(6)*(-1)+Y(7)*(-12)
      T20=-3*Y(2)-37.5*Y(3)-6*Y(4)-26*Y(5)-19*Y(6)-44*Y(7)
      P(2)=2013.0341+763.8167*C(2)+45802.87*C(2)**2-280061.63*C(2)**3
     1+3.864D+06*C(2)**4-2.4233D+07*C(2)**5+6.9547D+07*C(2)**6
      P(3)=2012.067-1764.095*C(3)+6287.52*C(3)**2-21647.96*C(3)**3-
     12.0119D+06*C(3)**4+3.1716D+07*C(3)**5-1.3885D+08*C(3)**6
      P(4)=2006.8017+2330.2424*C(4)-54915.32*C(4)**2+1.6216D+06*C(4)**3
     1-2.4968D+07*C(4)**4+1.8838D+08*C(4)**5-5.5531D+08*C(4)**6
      P(5)=2006.834-2997.314*C(5)-37906.61*C(5)**2+1.0328D+06*C(5)**3
     1-1.3306D+07*C(5)**4+8.411D+07*C(5)**5-2.0826D+08*C(5)**6
      P(6)=2012.367-9224.2655*C(6)+33657.8*C(6)**2-566827.83*C(6)**3
     1+8.5676D+06*C(6)**4-6.7482D+07*C(6)**5 +2.0837D+08*C(6)**6
      P(7)=2011.9996-6247.9118*C(7)+5411.7566*C(7)**2
     1+250118.1085*C(7)**3-4.1676D+06*C(7)**4
      DO 108 U=2,7
      B3=B3+P(U)*Y(U)
      B2=B2+Y(U)
108   CONTINUE
      IF(B2 .EQ. 0.0) GOTO 455
      W=(B3/B2)*4.187
      GOTO 456
455   W=8054.0
456   FTO=-1.0
      X1=C(1)
      XA=0.001
      R=8.31432
      W1=48570.0
      H=38575.0
      S=13.48
```

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```
      XEQ=0.2
      XTO=0.07
      XTO400=0.06
      X44=0.1
      INCEPT=1.0D+00
      CORR=1.0D+00
      SLOPE=1.0D+00
      C98=0
      C97=0
      WS=0.0
      DO 9 T1=473,1173,20
      C98=C98+1
      J98=0
      J99=0
      XTO=XTO+0.0001
      XTO400=XTO400+0.0001
      X44=0.3*XEQ
      T=T1
      IF (T .LE. 1000) GOTO 20
      H1=105525
      S1=45.34521
      GOTO 19
20    H1=111918
      S1=51.44
19    F=ENERGY(T,T10,T20)
      J=1-DEXP(-W/(R*T))
51    DEQ=DSQRT(1-2*(1+2*J)*XEQ+(1+8*J)*XEQ*XEQ)
      TEQ=5*DLOG((1-XEQ)/(1-2*XEQ))
      TEQ=TEQ+DLOG(((1-2*J+(4*J-1)*XEQ-DEQ)/(2*J*(2*XEQ-1)))**6)
      TEQ=TEQ*R*T-F
      IF (DABS(TEQ) .LT. 1.0) GOTO 50
      ETEQ=5*((1/(XEQ-1))+2/(1-2*XEQ))
      ETEQ2=6*((4*J-1-(0.5/DEQ)*(-2-4*J+2*XEQ+16*XEQ*J))/(1-2*J+(4*J
     1-1)*XEQ-DEQ))+6*(4*J/(2*J*(2*XEQ-1)))
      ETEQ=(ETEQ+ETEQ2)*R*T
      XEQ=XEQ-TEQ/ETEQ
      GOTO 51
50    AEQ=5*DLOG((1-2*XEQ)/XEQ)+6*W/(R*T)+((H)-(
     1S)*T)/(R*T)
      AEQ=AEQ+DLOG(((DEQ-1+3*XEQ)/(DEQ+1-3*XEQ))**6)
      AFEQ=5*DLOG((1-XEQ)/(1-2*XEQ))+DLOG(((1-2*J+(4*J-1)*XEQ-DEQ)/(2*J
     1*(2*XEQ-1)))**6)
      IF (XEQ .LT. X1) GOTO 2443
      GOTO 2442
2443  IF(WS .EQ. 0.0) GOTO 2441
      GOTO 2444
2441  WS=T4
      GOTO 2444
2442  D=DSQRT(1-2*(1+2*J)*X1+(1+8*J)*X1*X1)
      A=6*W/(R*T)+DLOG(((D-1+3*X1)/(D+1-3*X1))**6)

      A=A+5*DLOG((1-2*X1)/X1)
      A=A+(H-S*T)/(R*T)
      AFE=5*DLOG((1-X1)/(1-2*X1))
      AFE=AFE+DLOG(((1-2*J+(4*J-1)*X1-D)/(2*J*(2*X1-1)))**6)
      FSON=R*T*(XA*(AEQ-A)+(1-XA)*(AFEQ-AFE))
      FPRO=R*T*(X1*(AEQ-A)+(1-X1)*(AFEQ-AFE))
      V14=3.251745029*(T-273)-2183.014
      IF (V14 .GE. 0.0) GOTO 452
      IF (FPRO .GE. V14) GOTO 105
103   D44=DSQRT(1-2*(1+2*J)*X44+(1+8*J)*X44*X44)
      DD44=(0.5/D44)*(-2-4*J+2*X44+16*J*X44)
      A44=5*DLOG((1-2*X44)/X44)+6*W/(R*T)+((H)-(
     1S)*T)/(R*T)
      A44=A44+DLOG(((D44-1+3*X44)/(D44+1-3*X44))**6)
      AFE44=5*DLOG((1-X44)/(1-2*X44))+DLOG(((1-2*J+(4*J-1)*X44-D44

     1)/(2*J*(2*X44-1)))**6)
      F44=R*T*(X44*(AEQ-A44)+(1-X44)*(AFEQ-AFE44))
```

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```
        F44=F44-V14
        IF (DABS(F44) .GE. 10.0) GOTO 101
        GOTO 102
101   DA44=-((10/(1-2*X44))+(5/X44))+6*((DD44+3)/(D44-1+3*X44
      1)-(DD44-3)/(D44+1-3*X44))
        DAFE44=10/(1-2*X44)-5/(1-X44)+6*((4*J-1-DD44)/(1-2*J+(4*
      1J-1)*X44-D44)-2/(2*J*(2*X44-1)))
        DF441=R*T*(AEQ-X44*DA44-AFEQ+X44*DAFE44-DAFE44-A44+AFE44)
        X44=X44-F44/DF441
        GOTO 103
105   X44=0.0
        IF (C97 .GT. 0) GOTO 102
        C97=1
        WS=T4
        GOTO 102
452   X44=99999999999.99999
        IF(C97 .GT. 2) GOTO 9990
        C97=3
        WS1=T4
9990  WS=T4
102   FPROA=FPRO*((XEQ-XA)/(XEQ-X1))
        X=0.000001
        J1=1-DEXP(-W1/(R*T))
7       D1=DSQRT(9-6*X*(2*J1+3)+(9+16*J1)*X*X)
        A1=3*DLOG((3-4*X)/X)+(4*W1)/(R*T)
        A1=A1+DLOG(((D1-3+5*X)/(D1+3-5*X))**4)+(H1-S1*T)/(R*T)
        A1FE=DLOG(1-X)
        TEST=F+R*T*(A1FE-AFE) -R*T*(A1-A)
        IF (DABS(TEST) .GT. 10.0) GOTO 5
        GOTO 6
5       DA1=(3*X/(3-4*X))*((4*X-3)/(X**2)-4/X)
        DA2=(0.5/D1)*(-12*J1-18+18*X+32*J1*X)
        DA2=4*(((DA2+5)/(D1-3+5*X))-((DA2-5)/(D1+3-5*X)))
        DA1=DA1+DA2
        DA1FE=1/(X-1)
        ERROR=TEST/(R*T*(DA1FE-DA1))
        IF (ERROR .GT. X) GOTO 30
        GOTO 29
30    ERROR =0.3*X
29    X=X-ERROR
        GOTO 7
6       GMAX=R*T*(A1-A)
        D11=DSQRT(9-6*X1*(2*J1+3)+(9+16*J1)*X1*X1)
        T4=T-273
        IF (FTO .GE. 0.0) GOTO 22
        FTO=FTO1(H,S,X1,T,W,W1,H1,S1,F,J,J1)
        GOTO 21
22    FTO =0.0
21    DFTO=FTO1(H,S,XTO,T,W,W1,H1,S1,F,J,J1)
        J98=J98+1
        IF (DABS(DFTO) .LE. 10.0) GOTO 450
        G9=G91(XTO,T,W,W1,H1,S1,F,J,J1)
        IF (J98 .GE.9) GOTO 450
        XTO=XTO-DFTO/G9
        IF (XTO .LE. 0.0001) GOTO 94
        GOTO 21
94    XTO=0.0000
450   FTO400=FTO1(H,S,XTO400,T,W,W1,H1,S1,F,J,J1)+400.0
        J99=J99+1
        IF(J99 .GE. 9) GOTO 92
        IF (DABS(FTO400) .LE. 10.0) GOTO 92
        G9400=G91(XTO400,T,W,W1,H1,S1,F,J,J1)
        XTO400=XTO400-FTO400/G9400
        IF (XTO400 .LE. 0.0001) GOTO 451
        GOTO 450
451   XTO400=0.0000
92    V11=(XTO-X1)/(XTO-0.0013)
        V12=(XEQ-X1)/(XEQ-0.0013)
        V13=(X44-X1)/(X44-0.0013)
```

```
      V11=FFF(V11)
      V12=FFF(V12)
      V13=FFF(V13)
      SHEART=DEXP((0.2432D+06/(8.31432*T))-0.135D+03+20.0*DLOG(T)
     1-5*DLOG(DABS(GMAX)))
      DIFFT=DEXP((0.6031D+06/(8.31432*T))-0.1905D+03+20.0*DLOG(T)
     1-4*DLOG(DABS(GMAX)))
      IF (X44 .EQ. 0.0) GOTO 453
      GOTO 454
453   SHEART=1D+20
454   DDFTO(C98)=FTO
      DT4(C98)=T4
9     CONTINUE
2444  C98=C98-1
      CALL ANAL(C98,INCEPT,SLOPE,CORR,DT4,DDFTO)
      BS=(-400.0-INCEPT)/SLOPE
      MS=(-1120.0D+00-10568.0D+00*X1+94.1D+00-INCEPT)/SLOPE
      IF (WS .LT. BS) GOTO 9996
      GOTO 24
9996  BS=WS
24    CONTINUE
      RETURN
      END
C     Subroutine*******TZERO****************************************
      SUBROUTINE TZERO(C,T,XTO,XTO400)
      DOUBLE PRECISION X,X1,T,R,H,H1,S,S1
      INTEGER I,U,B4,J99,C98,C97,B5
      DOUBLE PRECISION D11,FTO,FTO400,XTO400,G9400,G9,XTO,DFTO,T10,T20,
     1J,J1,D,W,W1,F,T4,C(8),B1,B2,P(7),Y(7),B3,WS
      B3=0
      C(8)=(100.0-C(1)-C(2)-C(3)-C(4)-C(5)-C(6)-(C7))/55.84
C     DIVIDING BY ATOMIC WEIGHT..........................................
      C(1)=C(1)/12.0115
      C(2)=C(2)/28.09
      C(3)=C(3)/54.94
      C(4)=C(4)/58.71
      C(5)=C(5)/95.94
      C(6)=C(6)/52.0
      C(7)=C(7)/50.94
      B1=C(1)+C(2)+C(3)+C(4)+C(5)+C(6)+C(7)+C(8)
      DO 107 U=2,7
      Y(U)=C(U)/C(8)
107   CONTINUE
C     CALCULATING MOLE FRACTIONS.........................................
      DO 106 U=1,7
      C(U)=C(U)/B1
106   CONTINUE
      B2=0.0
      T10=Y(2)*(-3)+Y(3)*2+Y(4)*12+Y(5)*(-9)+Y(6)*(-1)+Y(7)*(-12)
      T20=-3*Y(2)-37.5*Y(3)-6*Y(4)-26*Y(5)-19*Y(6)-44*Y(7)
      P(2)=2013.0341+763.8167*C(2)+45802.87*C(2)**2-280061.63*C(2)**3
     1+3.864D+06*C(2)**4-2.4233D+07*C(2)**5+6.9547D+07*C(2)**6
      P(3)=2012.067-1764.095*C(3)+6287.52*C(3)**2-21647.96*C(3)**3-
     12.0119D+06*C(3)**4+3.1716D+07*C(3)**5-1.3885D+08*C(3)**6
      P(4)=2006.8017+2330.2424*C(4)-54915.32*C(4)**2+1.6216D+06*C(4)**3
     1-2.4968D+07*C(4)**4+1.8838D+08*C(4)**5-5.5531D+08*C(4)**6
      P(5)=2006.834-2997.314*C(5)-37906.61*C(5)**2+1.0328D+06*C(5)**3
     1-1.3306D+07*C(5)**4+8.411D+07*C(5)**5-2.0826D+08*C(5)**6
      P(6)=2012.367-9224.2655*C(6)+33657.8*C(6)**2-566827.83*C(6)**3
     1+8.5676D+06*C(6)**4-6.7482D+07*C(6)**5 +2.0837D+08*C(6)**6
      P(7)=2011.9996-6247.9118*C(7)+5411.7566*C(7)**2
     1+250118.1085*C(7)**3-4.1676D+06*C(7)**4
      DO 108 U=2,7
      B3=B3+P(U)*Y(U)
      B2=B2+Y(U)
108   CONTINUE
      IF(B2 .EQ. 0.0) GOTO 455
      W=(B3/B2)*4.187
455   W=8054.0
```

```
        FTO=-1.0
        X1=C(1)
        R=8.31432
        W1=48570.0
C    ENTHALPY OF CARBON IN AUSTENITE.................................
        H=38575.0
C    ENTROPY OF CARBON IN AUSTENITE...........................
        S=13.48
        XTO=0.04
        XTO400=0.03
        C98=0
        C97=0
        WS=0.0
        J98=0
        J99=0
        IF (T .LE. 1000) GOTO 20
        H1=105525
        S1=45.34521
        GOTO 19
20      H1=111918
        S1=51.44
C    Calling subroutine ENERGY————————————
C    DG FOR ALPHA—→GAMMA FOR PURE IRON............................
C    T10 & T20 ARE THE MAGNETIC & MAGN. EFFECTS OF ALLOY ADDITIONS ON
C    DG FOR ALPHA—→GAMMA FOR PURE IRON  (ZENER)
19      F=ENERGY(T,T10,T20)
C    SITE EXCLUSION PARAMETER...........................................
        J=1-DEXP(-W/(R*T))
        J1=1.0-DEXP(-W1/(R*T))
        T4=T-273
C    Calling subroutine FTO1————————————
        FTO=FTO1(H,S,X1,T,W,W1,H1,S1,F,J,J1)
C    Calling subroutine FTO1————————————
21      DFTO=FTO1(H,S,XTO,T,W,W1,H1,S1,F,J,J1)
        J98=J98+1
        IF (DABS(DFTO) .LE. 10.0) GOTO 450
C    Calling subroutine G91————————————
        G9=G91(XTO,T,W,W1,H1,S1,F,J,J1)
        IF (J98 .GE.9) GOTO 450
        XTO=XTO-DFTO/G9
        IF (XTO .LE. 0.0001) GOTO 94
        GOTO 21
94      XTO=0.0000
C    Calling subroutine FTO1————————————
450     FTO400=FTO1(H,S,XTO400,T,W,W1,H1,S1,F,J,J1)+400.0
        J99=J99+1
        IF(J99 .GE. 10) GOTO 92
        IF (DABS(FTO400) .LE. 10.0) GOTO 92
C    Calling subroutine G91————————————
        G9400=G91(XTO400,T,W,W1,H1,S1,F,J,J1)
        XTO400=XTO400-FTO400/G9400
        IF (XTO400 .LE. 0.0001) GOTO 451
        GOTO 450
451     XTO400=0.0000
92      CONTINUE
        RETURN
        END
C    Subroutine********FTO1****************************************
        DOUBLE PRECISION FUNCTION FTO1(H,S,X,T,W,W1,H1,S1,F,J,J1)
        DOUBLE PRECISION R,X,T,T60,ZEN1,ZEN2,ZENER,W,W1,H1,S1,F,
        1J,J1,D,D11,H,S
        D=DSQRT(1-2*(1+2*J)*X+(1+8*J)*X*X)
        D11=DSQRT(9-6*X*(2*J1+3)+(9+16*J1)*X*X)
        T60=T*(1-X)/(28080*X)
        IF (T60 .GT. 1.0) GOTO 18
        IF (T60 .GT. 0.25) GOTO 17
C    ZENER ORDERING.......................................................
        ZEN1=0.2307+42.7974*T60-233.8631*T60*T60+645.4485*T60*T60*T60
        1-954.3995*(T60**4)+711.8095*(T60**5)-211.5136*(T60**6)
```

```fortran
      ZEN2=-2.6702+45.6337*T60-225.3965*T60*T60+567.7112*(T60**3)
     1-771.6466*(T60**4)+538.1778*(T60**5)-151.3818*(T60**6)
      GOTO 16
17    ZEN2=1
      ZEN1=3.295
16    ZENER=(((ZEN2*X)**2)*(-50898.56)/(1-X))+ZEN1*T*X*0.6623741
      ZENER=ZENER*4.187
      GOTO 15
18    ZENER=0.0
15    R=8.31432
      FTO1=X*R*T*DLOG(X*X)+X*(H1-(H)-(S1-(S)
     1)*T+4*W1-6*W)-R*T*(1-X)*DLOG((1-X)**4)+5*R*T*(1-2*X)*DLOG(1-2*X)
     1-R*T*X*DLOG(((D-1+3*X)/(D+1-3*X))**6)-R*T*(1-X)*DLOG(((1-2*J+(4
     1*J-1)*X-D)/(2*J*(2*X-1)))**6)+3*R*T*X*DLOG(3-4*X)+R*T*
     1X*DLOG(((D11-3+5*X)/(D11+3-5*X))**4)+(1-X)*F+ZENER
      RETURN
      END
C     Subroutine********G91****************************************
      DOUBLE PRECISION FUNCTION G91(XTO,T,W,W1,H1,S1,F,J,J1)
      DOUBLE PRECISION R,XTO,T,W,W1,H1,S1,F,J,J1,FD,FD1,DT5,
     1DT6,DZEN1,DZEN2,DZEN3,V1,V2,V3,V4,V5,V6,V7,V8,V9,G1,
     1DZEN6,DZEN7,DZEN8
      R=8.31432
      FD=DSQRT(1-2*(1+2*J)*XTO+(1+8*J)*XTO*XTO)
      FD1=DSQRT(9-6*XTO*(2*J1+3)+(9+16*J1)*XTO*XTO)
      DT5=28080*XTO/(1-XTO)
      DT6=T/DT5
      IF (DT6 .GT. 1.0) GOTO 48
      IF (DT6 .LT. 0.25) GOTO 47
      DZEN1=0.2307+42.7974*DT6-233.8631*(DT6**2)+645.4485*(DT6**3)
     1-954.3995*(DT6**4)+711.8095*(DT6**5)-211.5136*(DT6**6)
      DZEN2=-2.6702+45.6337*DT6-225.3965*(DT6**2)+567.7112*(DT6**3)
     1-771.6466*(DT6**4)+538.1778*(DT6**5)-151.3818*(DT6**6)
      GOTO 46
47    DZEN2=1
      DZEN1=3.295
46    DZEN3=(((DZEN2*XTO)**2)*(-50898.56)/(1-XTO))+DZEN1*T*XTO*
     1(0.6623741)
      DZEN3=DZEN3*4.187
      GOTO 45
48    DZEN3=0.0
45    V1=FD-1+3*XTO
      V2=FD+1-3*XTO
      V3=1-2*J+(4*J-1)*XTO-FD
      V4=2*J*(2*XTO-1)
      V5=FD1-3+5*XTO
      V6=FD1+3-5*XTO
      V7=(XTO-1-2*J+8*XTO*J)/FD
      V8=(9*XTO-9-6*J1+16*J1*XTO)/FD1
      V9=H1-(H)-(S1-(S))*T-6*W+4*W1
      G1=2+DLOG(XTO**2)+4+DLOG((1-XTO)**4)-10-DLOG((1-2*XTO)**10)
     1-DLOG((V1/V2)**6)-6*((XTO/V1)*(V7+3+V1*(3-V7)/V2))
     1+DLOG((V3/V4)**6)-6*((1-XTO)/V3)*(4*J*(1-(V3/V4))-V7)
     1+3*(DLOG(3-4*XTO)-4*XTO/(3-4*XTO))+DLOG((V5/V6)**4)+4*(XTO
     1/V5)*(V8+5+(V5/V6)*(5-V8))
       IF (DT6 .GT. 1.0) GOTO 90
      DZEN6=(-3.3948+13.6112*DT6-13.4376*(DT6**2))*T/(28080*
     1((1-XTO)**2))
      DZEN7=(-3.3118+15.7462*DT6-23.2449*(DT6**2))*T/(28080*
     1((1-XTO)**2))
      DZEN8=50898*((DZEN2*XTO)**2)/((1-XTO)**2)+(-50898*(2*
     1DZEN2*DZEN6*(XTO**2)+2*XTO*(DZEN2**2))/(1-XTO))+DZEN1
     1*T*0.6623741+DZEN7*T*XTO*0.6623741
      GOTO 91
90    DZEN8=0.0
91    G91=V9+R*T*G1+DZEN8-F
      RETURN
      END
C     Subroutine********FFF****************************************
```

```
       DOUBLE PRECISION FUNCTION FFF(V)
       DOUBLE PRECISION V
       IF (V .LE. 0.0) GOTO 1
       IF (V .GT. 1.0) GOTO 1
2      GOTO 3
1      FFF=0.0
       GOTO 4
3      FFF=V
4      RETURN
       END
C    Subroutine********ENERGY*********************************************
       DOUBLE PRECISION FUNCTION ENERGY(T,T10,T20)
       DOUBLE PRECISION T,T10,T20,F,T7
       T7=T-100*T20
       IF (T7 .LT. 300) GOTO 1
       IF (T7 .LT. 700) GOTO 2
       IF (T7 .LT. 940) GOTO 3
       F=-8.88909+0.26557*(T7-1140)-1.04923D-3*((T7-1140)**2)
       F=F+2.70013D-6*((T7-1140)**3)-3.58434D-9*((T7-1140)**4)
       GOTO 4
1      F=1.38*T7-1499
       GOTO 4
2      F=1.65786*T7-1581
       GOTO 4
3      F=1.30089*T7-1331
4      ENERGY=(141*T10 + F)*4.187
       RETURN
       END
       DOUBLE PRECISION FUNCTION XALPH(T)
       DOUBLE PRECISION T,CTEMP
       CTEMP=(T-273.0D+00)/900.0D+00
       XALPH=0.1528D-02-0.8816D-02*CTEMP+0.2450D-01*CTEMP*CTEMP
      &-0.2417D-01*CTEMP*CTEMP*CTEMP+
      &0.6966D-02*CTEMP*CTEMP*CTEMP*CTEMP
       RETURN
       END
       SUBROUTINE ANAL(C98,INCEPT,SLOPE,CORR,X,Y)
       DOUBLE PRECISION AX,AX2,AY,AY2,AXY,INCEPT,CORR,SLOPE,
      &X(40),Y(40)
       INTEGER I,C98,I1
       I1=C98
       C98=C98-10
       AX=0.0D+00
       AY=0.0D+00
       AX2=0.0D+00
       AY2=0.0D+00
       AXY=0.0D+00
       DO 1 I=1,C98
       AX=AX+X(I)
       AY=AY+Y(I)
       AXY=AXY+X(I)*Y(I)
       AX2=AX2+X(I)*X(I)
       AY2=AY2+Y(I)*Y(I)
1      CONTINUE
       INCEPT=(AY*AX2-AX*AXY)/(C98*AX2-AX*AX)
       SLOPE=((C98*AXY-AX*AY)/(C98*AX2-AX*AX))
       CORR=(C98*AXY-AX*AY)/(DSQRT((C98*AX2-AX*AX)*
      &(C98*AY2-AY*AY)))
       C98=I1
       RETURN
       END
```

```
C Copyright S. A. Khan and H. K. D. H. Bhadeshia
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C
C PROG. FOR THE ANALYSIS OF ALLOTRIOMORPHIC FERRITE TRANSFORMATION IN
C HETEROGENEOUS STEELS.
C
C The motion of austenite/ferrite interface is considered to be parallel to the
C isoconcentration planes.
C
C The steel is divided into slices of different compositions, Ae3 temperature
C of each slice is calculated and transformation is allowed only in slices
C whose Ae3 temperature is higher than the concerned transformation
C temeprature. The exetent of transformation is limited by paraequilibrium
C mechanism. The carbon is permitted to redistribute among the slices after
C each increment of transformation. The results averaged and compared with a
C steel of the corresponding average composition.
C Typical data set follows:
C 673 (temperature in Kelvin)
C 0.43 0.50 0.60 0.70 0.80 0.90 1.00 (Composition of slice 1 in wt.%)
C 0.43 0.60 0.60 0.70 0.80 0.90 1.90 (Composition of slice 2 in wt.%)
C C   Si  Mn  Ni  Mo  Cr  V
C
      IMPLICIT REAL*8(A-H,K-Z), INTEGER(I,J)
      DOUBLE PRECISION C(8),D(8),XEQ(200)
     &,E(8),F(8),MS(100),IA(100),XGAMMA(200),VOLF(200)
     &,CN(200),SI(200),MN(200),NI(200),MO(200),V(200),FE(200)
     &,CR(200),WD(8),VG(200),CD(8),XG(200),TAE3(200)
     &,TAE3H,XEQH,TVOLF,AVEVOL,MOMENT,TISO
      VINCR=0.00005D+00
      ISTOP=0
      AVEVOL=0.0D+0
      TVOLF=0.0D+0
      C1=0.0
      C2=0.0
      C3=0.0
      C4=0.0
      C5=0.0
      C6=0.0
      C7=0.0
      READ(5,*)KELVIN
      TISO=KELVIN-273.0D+0
      XALPHA=XALPH(KELVIN)
      WRITE(6,4444)
4444  FORMAT( ' ****CARBON  IS ALLOWED TO DIFFUSE!!!!**********')
      WRITE(6,9)KELVIN,XALPHA,VINCR
      WRITE(6,9090)
9090  FORMAT('————————————————————————————————————
     &——————————')
      DO 1 I=1,101
      READ(5,*,END=2)C(1),C(2),C(3),C(4),C(5),C(6),C(7)
      CN(I)=C(1)
      SI(I)=C(2)
      MN(I)=C(3)
      NI(I)=C(4)
      MO(I)=C(5)
      CR(I)=C(6)
      V(I)=C(7)
      FE(I)=100.0D+0-(C(1)+C(2)+C(3)+C(4)+C(5)+C(6)+C(7))
      C1=C1+C(1)
      C2=C2+C(2)
      C3=C3+C(3)
      C4=C4+C(4)
      C5=C5+C(5)
      C6=C6+C(6)
      C7=C7+C(7)
      DO 43 IJI=1,7
```

```
          E(IJI)=C(IJI)
43    CONTINUE
      CALL XEQ3(KELVIN,C,XEQ(I))
      CALL TEMP3(E,TAE3(I))
      XBAR=C(1)
      WRITE(6,10)I,XEQ(I),TAE3(I)
      WRITE(6,6161)
6161  FORMAT('********************************************************
     &*********************')
1     CONTINUE
2     ISLICE=I-1
      WRITE(*,*) ISLICE
      D(1)=C1/ISLICE
      D(2)=C2/ISLICE
      D(3)=C3/ISLICE
      D(4)=C4/ISLICE
      D(5)=C5/ISLICE
      D(6)=C6/ISLICE
      D(7)=C7/ISLICE
      DO 70 JII=1,7
      WD(JII)=D(JII)
70    CONTINUE
      DO 56 JIJ=1,7
      F(JIJ)=D(JIJ)
56    CONTINUE
      CALL XEQ3(KELVIN,D,XEQH)
      CALL TEMP3(F,TAE3H)
      WRITE(6,75)TAE3H
75    FORMAT(' Ae3H= ',D10.4)
      WRITE(*,*)D(1)
      IF (TAE3H .LT. TISO) GOTO 789
      GOTO 85
85    IF (XEQH .LE. D(1)) GOTO 789
      GOTO 79
79    IF (XEQH .GT. XALPHA) GOTO 987
      GOTO 789
789   VOLH=0.00
      GOTO 678
987   VOLH=(XEQH-D(1))/(XEQH-XALPHA)
678   VGH=1.0D+0-VOLH
      WRITE(6,15)VOLH
      DO 1020 III=1,ISLICE
      XGAMMA(III)=D(1)
      VOLF(III)=0.0D+0
1020  CONTINUE
      AVEX=D(1)
      DO 6 I=1,100000
      IF (ISTOP .EQ. ISLICE) GO TO 14
      DO 4 J=1,ISLICE
      IF (IA(J) .EQ. 1) GOTO 4
      IF (TAE3(J) .LT. TISO) GOTO 5329
      GOTO 9352
5329  VOLF(J)=0.00
      GOTO 5
9352  VOLF(J)=VOLF(J)+VINCR
      XGAMMA(J)=AVEX
      IF (XGAMMA(J) .GT. XEQ(J)) GOTO 5
      GOTO 4
5     IA(J)=1
      ISTOP=ISTOP+IA(J)
      VOLF(J)=VOLF(J)-VINCR
      IF (VOLF(J) .LE. 0.0D+0) GOTO 115
      GOTO 4
115   VOLF(J)=0.0D+0
      XGAMMA(J)=AVEX
4     CONTINUE
      AVEVOL=0.0D+0
      DO 90 J33=1,ISLICE
      AVEVOL=AVEVOL+VOLF(J33)
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90    CONTINUE
      AVEVOL=AVEVOL/ISLICE
      AVEX=D(1)+(AVEVOL*(D(1)-XALPHA))/(1.0D+0-AVEVOL)
6     CONTINUE
14    AVEVOL=0.0D+0
      DO 12 J=1,ISLICE
      AVEVOL=AVEVOL+VOLF(J)
      WRITE(6,786)J,VOLF(J),XGAMMA(J),XEQ(J),TAE3(J),D(1),AVEVOL
786   FORMAT(' SLICE=',I3,' VOLF=',D10.3,' XGAMMA=',D10.3,' XEQ=',
     &D10.3,' TAE3=',D10.3,' D(1)=',D10.3,' AVEVOL=',D10.3)
12    CONTINUE
      AVEVOL=AVEVOL/ISLICE
      WRITE(6,13)AVEVOL
13    FORMAT(' Average volume fraction of transformation',
     &' in heterogeneous alloy =',D8.3)
9     FORMAT(' KELVIN = ',F7.0,' XALPHA, mol. fraction =',D12.4
     &,' VOL INCREMENT=',D12.4)
10    FORMAT(' Slice Number= ',I3,'      XEQ = ',D10.4,
     &'        AE3-T= ',D10.4/)
15    FORMAT(' Maximum volume fraction of bainitic ferrite in ',
     &' an alloy of average composition = ',D8.3)
      STOP
      END


C********************************************************
      SUBROUTINE TEMP3(C,AE3T)
      DOUBLE PRECISION X,X1,R,A,A1,AFE,A1FE,DA1,DA2,DA1FE,H,H1,S,S1
      INTEGER T1,I,NO,U,B4,J99,C99,C98,C97
      DOUBLE PRECISION D11,DTQ(40),DXEQ(40),
     1INCEPT,SLOPE,CORR,
     1DEQ,ETEQ,T10,T20,XA,AFEQ,AEQ,ETEQ2,TEQ,
     1J,J1,D,D1,W,W1,F,TEST,ERROR,T4,XEQ,FPRO
     1,C(8),B1,B2,P(7),Y(7),B3,AE3T,EE(8)
      WRITE(6,1100)C(1),C(2),C(3),C(4),C(5),C(6),C(7)
1100  FORMAT(7D11.3)
      B3=0
      C(8)=(100.0-C(1)-C(2)-C(3)-C(4)-C(5)-C(6)-(C(7))/55.84
      C(1)=C(1)/12.0115
      C(2)=C(2)/28.09
      C(3)=C(3)/54.94
      C(4)=C(4)/58.71
      C(5)=C(5)/95.94
      C(6)=C(6)/52.0
      C(7)=C(7)/50.94
      B1=C(1)+C(2)+C(3)+C(4)+C(5)+C(6)+C(7)+C(8)
      DO 107 U=2,7
      Y(U)=C(U)/C(8)
107   CONTINUE
      DO 106 U=1,7
      C(U)=C(U)/B1
106   CONTINUE
      B2=0.0
      T10=Y(2)*(-3)+Y(3)*2+Y(4)*12+Y(5)*(-9)+Y(6)*(-1)+Y(7)*(-12)
      T20=-3*Y(2)-37.5*Y(3)-6*Y(4)-26*Y(5)-19*Y(6)-44*Y(7)
      P(2)=2013.0341+763.8167*C(2)+45802.87*C(2)**2-280061.63*C(2)**3
     1+3.864D+06*C(2)**4-2.4233D+07*C(2)**5+6.9547D+07*C(2)**6
      P(3)=2012.067-1764.095*C(3)+6287.52*C(3)**2-21647.96*C(3)**3-
     12.0119D+06*C(3)**4+3.1716D+07*C(3)**5-1.3885D+08*C(3)**6
      P(4)=2006.8017+2330.2424*C(4)-54915.32*C(4)**2+1.6216D+06*C(4)**3
     1-2.4968D+07*C(4)**4+1.8838D+08*C(4)**5-5.5531D+08*C(4)**6
      P(5)=2006.834-2997.314*C(5)-37906.61*C(5)**2+1.0328D+06*C(5)**3
     1-1.3306D+07*C(5)**4+8.411D+07*C(5)**5-2.0826D+08*C(5)**6
      P(6)=2012.367-9224.2655*C(6)+33657.8*C(6)**2-566827.83*C(6)**3
     1+8.5676D+06*C(6)**4-6.7482D+07*C(6)**5 +2.0837D+08*C(6)**6
      P(7)=2011.9996-6247.9118*C(7)+5411.7566*C(7)**2
     1+250118.1085*C(7)**3-4.1676D+06*C(7)**4
      DO 108 U=2,7
      B3=B3+P(U)*Y(U)
      B2=B2+Y(U)
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108    CONTINUE
       IF(B2 .EQ. 0.0) GOTO 455
       W=(B3/B2)*4.187
       GOTO 456
455    W=8054.0
456    CONTINUE
       X1=C(1)
       R=8.31432
       W1=48570.0
       H=38575.0
       S=13.48
       II1=873
       II2=1173
       II3=15
       II=0
201    XEQ=0.1
       INCEPT=1.0D+00
       CORR=1.0D+00
       SLOPE=1.0D+00
       C98=0
       C97=0
       DO 9 T1=II1,II2,II3
       C98=C98+1
       T=T1
       IF (T .LE. 1000) GOTO 20
       H1=105525
       S1=45.34521
       GOTO 19
20     H1=111918
       S1=51.44
19     F=ENERGY(T,T10,T20)
       J=1-DEXP(-W/(R*T))
51     DEQ=DSQRT(1-2*(1+2*J)*XEQ+(1+8*J)*XEQ*XEQ)
       TEQ=5*DLOG((1-XEQ)/(1-2*XEQ))
       TEQ=TEQ+DLOG(((1-2*J+(4*J-1)*XEQ-DEQ)/(2*J*(2*XEQ-1)))**6)
       TEQ=TEQ*R*T-F
       IF (DABS(TEQ) .LT. 1.0) GOTO 50
       ETEQ=5*((1/(XEQ-1))+2/(1-2*XEQ))
       ETEQ2=6*((4*J-1-(0.5/DEQ)*(-2-4*J+2*XEQ+16*XEQ*J))/(1-2*J+(4*J
       1-1)*XEQ-DEQ))+6*(4*J/(2*J*(2*XEQ-1)))
       ETEQ=(ETEQ+ETEQ2)*R*T
       XEQ=XEQ-TEQ/ETEQ
       GOTO 51
50     IF (XEQ .LT. 0.001) GOTO 2444
       T4=T1-273.0
       DTQ(C98)=T4
       DXEQ(C98)=XEQ
9      CONTINUE
2444   C98=C98-1
       CALL ANAL(C98,INCEPT,SLOPE,CORR,DTQ,DXEQ)
       AE3T=(X1-INCEPT)/SLOPE
       IF(II .GT. 0) GOTO 802
       II=AE3T
       II1=II-9+273
       II2=II+9+273
       II3=1
       GOTO 201
802    RETURN
       END
       SUBROUTINE ANAL(C98,INCEPT,SLOPE,CORR,X,Y)
       DOUBLE PRECISION AX,AX2,AY,AY2,AXY,INCEPT,CORR,SLOPE,
       &X(40),Y(40)
       INTEGER I,C98,I1
       I1=C98
       C98=C98-10
       AX=0.0D+00
       AY=0.0D+00
       AX2=0.0D+00
       AY2=0.0D+00
```

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      AXY=0.0D+00
      DO 1 I=1,C98
      AX=AX+X(I)
      AY=AY+Y(I)
      AXY=AXY+X(I)*Y(I)
      AX2=AX2+X(I)*X(I)
      AY2=AY2+Y(I)*Y(I)
1     CONTINUE
      INCEPT=(AY*AX2-AX*AXY)/(C98*AX2-AX*AX)
      SLOPE=((C98*AXY-AX*AY)/(C98*AX2-AX*AX))
      CORR=(C98*AXY-AX*AY)/(DSQRT((C98*AX2-AX*AX)*
     &(C98*AY2-AY*AY)))
      C98=I1
      RETURN
      END
      DOUBLE PRECISION FUNCTION ENERGY(T,T10,T20)
      DOUBLE PRECISION T,T10,T20,F,T7
      T7=T-100*T20
      IF (T7 .LT. 300) GOTO 1
      IF (T7 .LT. 700) GOTO 2
      IF (T7 .LT. 940) GOTO 3
      F=-8.88909+0.26557*(T7-1140)-1.04923D-3*((T7-1140)**2)
      F=F+2.70013D-6*((T7-1140)**3)-3.58434D-9*((T7-1140)**4)
      GOTO 4
1     F=1.38*T7-1499
      GOTO 4
2     F=1.65786*T7-1581
      GOTO 4
3     F=1.30089*T7-1331
4     ENERGY=(141*T10 + F)*4.187
      RETURN
      END


C***************************************************************
      SUBROUTINE XEQ3(TT,C,XEQ)
      DOUBLE PRECISION X,X1,T,R,A,A1,AFE,A1FE,DA1,DA2,DA1FE,H,H1,S,S1
     &,TT
      INTEGER I,NO,U,B4,J99,C99,C98,C97
      DOUBLE PRECISION D11,
     1DEQ,ETEQ,T10,T20,XA,AFEQ,AEQ,ETEQ2,TEQ,
     1J,J1,D,D1,W,W1,F,TEST,ERROR,T4,XEQ,FPRO
     1,C(8),B1,B2,P(7),Y(7),B3,AE3T,CC(8)

      B3=0
      C(8)=(100.0-C(1)-C(2)-C(3)-C(4)-C(5)-C(6)-(C7))/55.84
      C(1)=C(1)/12.0115
      C(2)=C(2)/28.09
      C(3)=C(3)/54.94
      C(4)=C(4)/58.71
      C(5)=C(5)/95.94
      C(6)=C(6)/52.0
      C(7)=C(7)/50.94
      B1=C(1)+C(2)+C(3)+C(4)+C(5)+C(6)+C(7)+C(8)
      DO 107 U=2,7
      Y(U)=C(U)/C(8)
107   CONTINUE
      DO 106 U=1,7
      C(U)=C(U)/B1
106   CONTINUE
      B2=0.0
      T10=Y(2)*(-3)+Y(3)*2+Y(4)*12+Y(5)*(-9)+Y(6)*(-1)+Y(7)*(-12)
      T20=-3*Y(2)-37.5*Y(3)-6*Y(4)-26*Y(5)-19*Y(6)-44*Y(7)
      P(2)=2013.0341+763.8167*C(2)+45802.87*C(2)**2-280061.63*C(2)**3
     1+3.864D+06*C(2)**4-2.4233D+07*C(2)**5+6.9547D+07*C(2)**6
      P(3)=2012.067-1764.095*C(3)+6287.52*C(3)**2-21647.96*C(3)**3-
     12.0119D+06*C(3)**4+3.1716D+07*C(3)**5-1.3885D+08*C(3)**6
      P(4)=2006.8017+2330.2424*C(4)-54915.32*C(4)**2+1.6216D+06*C(4)**3
     1-2.4968D+07*C(4)**4+1.8838D+08*C(4)**5-5.5531D+08*C(4)**6
      P(5)=2006.834-2997.314*C(5)-37906.61*C(5)**2+1.0328D+06*C(5)**3
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     1-1.3306D+07*C(5)**4+8.411D+07*C(5)**5-2.0826D+08*C(5)**6
     P(6)=2012.367-9224.2655*C(6)+33657.8*C(6)**2-566827.83*C(6)**3
     1+8.5676D+06*C(6)**4-6.7482D+07*C(6)**5 +2.0837D+08*C(6)**6
     P(7)=2011.9996-6247.9118*C(7)+5411.7566*C(7)**2
     1+250118.1085*C(7)**3-4.1676D+06*C(7)**4
     DO 108 U=2,7
     B3=B3+P(U)*Y(U)
     B2=B2+Y(U)
108  CONTINUE
     IF(B2 .EQ. 0.0) GOTO 455
     W=(B3/B2)*4.187
     GOTO 456
455  W=8054.0
456  CONTINUE
     X1=C(1)
     R=8.31432
     W1=48570.0
     H=38575.0
     S=13.48
201  XEQ=0.1
     T=TT
     IF (T .LE. 1000) GOTO 20
     H1=105525
     S1=45.34521
     GOTO 19
20   H1=111918
     S1=51.44
19   F=ENERGY(T,T10,T20)
     J=1-DEXP(-W/(R*T))
51   DEQ=DSQRT(1-2*(1+2*J)*XEQ+(1+8*J)*XEQ*XEQ)
     TEQ=5*DLOG((1-XEQ)/(1-2*XEQ))
     TEQ=TEQ+DLOG(((1-2*J+(4*J-1)*XEQ-DEQ)/(2*J*(2*XEQ-1)))**6)
     TEQ=TEQ*R*T-F
     IF (DABS(TEQ) .LT. 1.0) GOTO 50
     ETEQ=5*((1/(XEQ-1))+2/(1-2*XEQ))
     ETEQ2=6*((4*J-1-(0.5/DEQ)*(-2-4*J+2*XEQ+16*XEQ*J))/(1-2*J+(4*J
     1-1)*XEQ-DEQ))+6*(4*J/(2*J*(2*XEQ-1)))
     ETEQ=(ETEQ+ETEQ2)*R*T
     XEQ=XEQ-TEQ/ETEQ
     GOTO 51
50   RETURN
     END
     DOUBLE PRECISION FUNCTION ENERGY(T,T10,T20)
     DOUBLE PRECISION T,T10,T20,F,T7
     T7=T-100*T20
     IF (T7 .LT. 300) GOTO 1
     IF (T7 .LT. 700) GOTO 2
     IF (T7 .LT. 940) GOTO 3
     F=-8.88909+0.26557*(T7-1140)-1.04923D-3*((T7-1140)**2)
     F=F+2.70013D-6*((T7-1140)**3)-3.58434D-9*((T7-1140)**4)
     GOTO 4
1    F=1.38*T7-1499
     GOTO 4
2    F=1.65786*T7-1581
     GOTO 4
3    F=1.30089*T7-1331
4    ENERGY=(141*T10 + F)*4.187
     RETURN
     END

     DOUBLE PRECISION FUNCTION XALPH(T)
     DOUBLE PRECISION T,CTEMP
     CTEMP=(T-273.0D+00)/900.0D+00
     XALPH=0.1528D-02-0.8816D-02*CTEMP+0.2450D-01*CTEMP*CTEMP
    &-0.2417D-01*CTEMP*CTEMP*CTEMP+
    &0.6966D-02*CTEMP*CTEMP*CTEMP*CTEMP
     RETURN
     END
```

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C
C PROG. FOR THE ANALYSIS OF ALLOTRIOMORPHIC FERRITE TRANSFORMATION IN
C HETEROGENEOUS STEELS.
C
C The motion of austenite/ferrite interface is considered to be parallel to the
C isoconcentration planes.
C
C The steel is divided into slices of different compositions, Ae3 temperature
C of each slice is calculated and transformation is allowed only in slices
C whose Ae3 temperature is higher than the concerned transformation
C temeprature. The exetent of transformation is limited by paraequilibrium
C mechanism.
C
C The carbon is not allowed to redistribute among the slices after each
C increment of transformation. The results averaged and compared with a steel
C of the corresponding average composition.
C Typical data set follows:
C 673 (temperature in Kelvin)
C 0.43 0.50 0.60 0.70 0.80 0.90 1.00 (Composition of slice 1 in wt.%)
C 0.43 0.60 0.60 0.70 0.80 0.90 1.90 (Composition of slice 2 in wt.%)
C C   Si  Mn  Ni  Mo  Cr  V
C
      IMPLICIT REAL*8(A-H,K-Z), INTEGER(I,J)
      DOUBLE PRECISION C(8),D(8),XEQ(300)
     &,E(8),F(8),MS(300),IA(300),XGAMMA(300),VOLF(300)
     &,CN(300),SI(300),MN(300),NI(300),MO(300),V(300),FE(300)
     &,CR(300),WD(8),VG(300),CD(8),XG(300),TAE3(300)
     &,TAE3H,XEQH,TVOLF,AVEVOL,MOMENT,TISO
      VINCR=0.00005D+00
      ISTOP=0
      AVEVOL=0.0D+0
      TVOLF=0.0D+0
      C1=0.0
      C2=0.0
      C3=0.0
      C4=0.0
      C5=0.0
      C6=0.0
      C7=0.0
      READ(5,*)KELVIN
      TISO=KELVIN-273.0D+0
      XALPHA=XALPH(KELVIN)
      WRITE(6,9)KELVIN,XALPHA,VINCR
      WRITE(6,9090)
9090  FORMAT('——————————————————————————————
     &——————————')
      DO 1 I=1,300
      READ(5,*,END=2)C(1),C(2),C(3),C(4),C(5),C(6),C(7)
      CN(I)=C(1)
      SI(I)=C(2)
      MN(I)=C(3)
      NI(I)=C(4)
      MO(I)=C(5)
      CR(I)=C(6)
      V(I)=C(7)
      FE(I)=100.0D+0-(C(1)+C(2)+C(3)+C(4)+C(5)+C(6)+C(7))
      C1=C1+C(1)
      C2=C2+C(2)
      C3=C3+C(3)
      C4=C4+C(4)
      C5=C5+C(5)
      C6=C6+C(6)
      C7=C7+C(7)
      DO 43 IJI=1,7
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      E(IJI)=C(IJI)
43    CONTINUE
      CALL XEQ3(KELVIN,C,XEQ(I))
      CALL TEMP3(E,TAE3(I))
      XBAR=C(1)
      WRITE(6,10)I,XEQ(I),TAE3(I)
      WRITE(6,6161)
6161  FORMAT('***************************************************************
     &************************')
1     CONTINUE
2     ISLICE=I-1
      WRITE(*,*) ISLICE
      D(1)=C1/ISLICE
      D(2)=C2/ISLICE
      D(3)=C3/ISLICE
      D(4)=C4/ISLICE
      D(5)=C5/ISLICE
      D(6)=C6/ISLICE
      D(7)=C7/ISLICE
      DO 70 JII=1,7
      WD(JII)=D(JII)
70    CONTINUE
      DO 56 JIJ=1,7
      F(JIJ)=D(JIJ)
56    CONTINUE
      CALL XEQ3(KELVIN,D,XEQH)
      CALL TEMP3(F,TAE3H)
      WRITE(6,75)TAE3H
75    FORMAT( ' Ae3H= ',D10.4)
      WRITE(*,*)D(1)
      IF (TAE3H .LT. TISO) GOTO 789
      GOTO 85
85    IF (XEQH .LE. D(1)) GOTO 789
      GOTO 79
79    IF (XEQH .GT. XALPHA) GOTO 987
      GOTO 789
789   VOLH=0.00
      GOTO 678
987   VOLH=(XEQH-D(1))/(XEQH-XALPHA)
678   VGH=1.0D+0-VOLH
      WRITE(6,15)VOLH
      DO 6 I=1,100000
      IF (ISTOP .EQ. ISLICE) GOTO 14
      DO 4 J=1,ISLICE
      IF (IA(J) .EQ. 1) GOTO 4
      IF (TAE3(J) .LT. TISO) GOTO 5329
      GOTO 9352
5329  VOLF(J)=0.00
      GOTO 5
9352  VOLF(J)=VOLF(J)+VINCR
      XGAMMA(J)=XBAR+((VOLF(J)*(XBAR-XALPHA))/
     &(1.0D+0-VOLF(J)))
      IF (XGAMMA(J) .GE. XEQ(J)) GOTO 5
      GOTO 4
5     IA(J)=1
      ISTOP =ISTOP+IA(J)
      VOLF(J)=VOLF(J)-VINCR
      IF (VOLF(J) .LE. 0.0D+0) GOTO 115
      GOTO 4
115   VOLF(J)=0.0D+0
      XGAMMA(J)=XBAR
4     CONTINUE
6     CONTINUE
14    DO 12 JJ=1,ISLICE
      AVEVOL=AVEVOL+VOLF(JJ)
      WRITE(6,786)JJ,VOLF(JJ),XGAMMA(JJ),XEQ(JJ),TAE3(JJ),XBAR,AVEVOL
786   FORMAT(' SLICE=',I3,' VOLF=',D10.3,' XGAMMA=',D10.3,' XEQ=',
     &D10.3,' TAE3=',D10.3,' XBAR=',D10.3,' AVEVOL(RUNNING SUM)=',D10.3)
12    CONTINUE
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      WRITE(6,13)AVEVOL
13    FORMAT(' Average volume fraction of transformation',
     &' in heterogeneous alloy =',D8.3)
9     FORMAT(' KELVIN = ',F7.0,' XALPHA, mol. fraction =',D12.4
     &,' VOL INCREMENT=',D12.4)
10    FORMAT(' Slice Number= ',I3,'       XEQ = ',D10.4,
     &'       AE3-T= ',D10.4/)
15    FORMAT(' Maximum volume fraction of bainitic ferrite in ',
     &' an alloy of average composition = ',D8.3)
      STOP
      END

C***********************************************************
      SUBROUTINE TEMP3(C,AE3T)
      DOUBLE PRECISION X,X1,R,A,A1,AFE,A1FE,DA1,DA2,DA1FE,H,H1,S,S1
      INTEGER T1,I,NO,U,B4,J99,C99,C98,C97
      DOUBLE PRECISION D11,DTQ(40),DXEQ(40),
     1INCEPT,SLOPE,CORR,
     1DEQ,ETEQ,T10,T20,XA,AFEQ,AEQ,ETEQ2,TEQ,
     1J,J1,D,D1,W,W1,F,TEST,ERROR,T4,XEQ,FPRO
     1,C(8),B1,B2,P(7),Y(7),B3,AE3T,EE(8)
      WRITE(6,1100)C(1),C(2),C(3),C(4),C(5),C(6),C(7)
1100  FORMAT(7D11.3)
      B3=0
      C(8)=(100.0-C(1)-C(2)-C(3)-C(4)-C(5)-C(6)-(C(7))/55.84
      C(1)=C(1)/12.0115
      C(2)=C(2)/28.09
      C(3)=C(3)/54.94
      C(4)=C(4)/58.71
      C(5)=C(5)/95.94
      C(6)=C(6)/52.0
      C(7)=C(7)/50.94
      B1=C(1)+C(2)+C(3)+C(4)+C(5)+C(6)+C(7)+C(8)
      DO 107 U=2,7
      Y(U)=C(U)/C(8)
107   CONTINUE
      DO 106 U=1,7
      C(U)=C(U)/B1
106   CONTINUE
      B2=0.0
      T10=Y(2)*(-3)+Y(3)*2+Y(4)*12+Y(5)*(-9)+Y(6)*(-1)+Y(7)*(-12)
      T20=-3*Y(2)-37.5*Y(3)-6*Y(4)-26*Y(5)-19*Y(6)-44*Y(7)
      P(2)=2013.0341+763.8167*C(2)+45802.87*C(2)**2-280061.63*C(2)**3
     1+3.864D+06*C(2)**4-2.4233D+07*C(2)**5+6.9547D+07*C(2)**6
      P(3)=2012.067-1764.095*C(3)+6287.52*C(3)**2-21647.96*C(3)**3-
     12.0119D+06*C(3)**4+3.1716D+07*C(3)**5-1.3885D+08*C(3)**6
      P(4)=2006.8017+2330.2424*C(4)-54915.32*C(4)**2+1.6216D+06*C(4)**3
     1-2.4968D+07*C(4)**4+1.8838D+08*C(4)**5-5.5531D+08*C(4)**6
      P(5)=2006.834-2997.314*C(5)-37906.61*C(5)**2+1.0328D+06*C(5)**3
     1-1.3306D+07*C(5)**4+8.411D+07*C(5)**5-2.0826D+08*C(5)**6
      P(6)=2012.367-9224.2655*C(6)+33657.8*C(6)**2-566827.83*C(6)**3
     1+8.5676D+06*C(6)**4-6.7482D+07*C(6)**5 +2.0837D+08*C(6)**6
      P(7)=2011.9996-6247.9118*C(7)+5411.7566*C(7)**2
     1+250118.1085*C(7)**3-4.1676D+06*C(7)**4
      DO 108 U=2,7
      B3=B3+P(U)*Y(U)
      B2=B2+Y(U)
108   CONTINUE
      IF(B2 .EQ. 0.0) GOTO 455
      W=(B3/B2)*4.187
      GOTO 456
455   W=8054.0
456   CONTINUE
      X1=C(1)
      R=8.31432
      W1=48570.0
      H=38575.0
      S=13.48
      II1=873
```

```
        II2=1173
        II3=15
        II=0
201   XEQ=0.1
        INCEPT=1.0D+00
        CORR=1.0D+00
        SLOPE=1.0D+00
        C98=0
        C97=0
        DO 9 T1=II1,II2,II3
        C98=C98+1
        T=T1
        IF (T .LE. 1000) GOTO 20
        H1=105525
        S1=45.34521
        GOTO 19
20      H1=111918
        S1=51.44
19    F=ENERGY(T,T10,T20)
        J=1-DEXP(-W/(R*T))
51    DEQ=DSQRT(1-2*(1+2*J)*XEQ+(1+8*J)*XEQ*XEQ)
        TEQ=5*DLOG((1-XEQ)/(1-2*XEQ))
        TEQ=TEQ+DLOG(((1-2*J+(4*J-1)*XEQ-DEQ)/(2*J*(2*XEQ-1)))**6)
        TEQ=TEQ*R*T-F
        IF (DABS(TEQ) .LT. 1.0) GOTO 50
        ETEQ=5*((1/(XEQ-1))+2/(1-2*XEQ))
        ETEQ2=6*((4*J-1-(0.5/DEQ)*(-2-4*J+2*XEQ+16*XEQ*J))/(1-2*J+(4*J
        1-1)*XEQ-DEQ))+6*(4*J/(2*J*(2*XEQ-1)))
        ETEQ=(ETEQ+ETEQ2)*R*T
        XEQ=XEQ-TEQ/ETEQ
        GOTO 51
50    IF (XEQ .LT. 0.001) GOTO 2444
        T4=T1-273.0
        DTQ(C98)=T4
        DXEQ(C98)=XEQ
9       CONTINUE
2444  C98=C98-1
        CALL ANAL(C98,INCEPT,SLOPE,CORR,DTQ,DXEQ)
        AE3T=(X1-INCEPT)/SLOPE
        IF(II .GT. 0) GOTO 802
        II=AE3T
        II1=II-9+273
        II2=II+9+273
        II3=1
        GOTO 201
802   RETURN
        END
        SUBROUTINE ANAL(C98,INCEPT,SLOPE,CORR,X,Y)
        DOUBLE PRECISION AX,AX2,AY,AY2,AXY,INCEPT,CORR,SLOPE,
        &X(40),Y(40)
        INTEGER I,C98,I1
        I1=C98
        C98=C98-10
        AX=0.0D+00
        AY=0.0D+00
        AX2=0.0D+00
        AY2=0.0D+00
        AXY=0.0D+00
        DO 1 I=1,C98
        AX=AX+X(I)
        AY=AY+Y(I)
        AXY=AXY+X(I)*Y(I)
        AX2=AX2+X(I)*X(I)
        AY2=AY2+Y(I)*Y(I)
1       CONTINUE
        INCEPT=(AY*AX2-AX*AXY)/(C98*AX2-AX*AX)
        SLOPE=((C98*AXY-AX*AY)/(C98*AX2-AX*AX))
        CORR=(C98*AXY-AX*AY)/(DSQRT((C98*AX2-AX*AX)*
        &(C98*AY2-AY*AY)))
```

```
        C98=I1
        RETURN
        END
        DOUBLE PRECISION FUNCTION ENERGY(T,T10,T20)
        DOUBLE PRECISION T,T10,T20,F,T7
        T7=T-100*T20
        IF (T7 .LT. 300) GOTO 1
        IF (T7 .LT. 700) GOTO 2
        IF (T7 .LT. 940) GOTO 3
        F=-8.88909+0.26557*(T7-1140)-1.04923D-3*((T7-1140)**2)
        F=F+2.70013D-6*((T7-1140)**3)-3.58434D-9*((T7-1140)**4)
        GOTO 4
1       F=1.38*T7-1499
        GOTO 4
2       F=1.65786*T7-1581
        GOTO 4
3       F=1.30089*T7-1331
4       ENERGY=(141*T10 + F)*4.187
        RETURN
        END


C*************************************************************
        SUBROUTINE XEQ3(TT,C,XEQ)
        DOUBLE PRECISION X,X1,T,R,A,A1,AFE,A1FE,DA1,DA2,DA1FE,H,H1,S,S1
       &,TT
        INTEGER I,NO,U,B4,J99,C99,C98,C97
        DOUBLE PRECISION D11,
       1DEQ,ETEQ,T10,T20,XA,AFEQ,AEQ,ETEQ2,TEQ,
       1J,J1,D,D1,W,W1,F,TEST,ERROR,T4,XEQ,FPRO
       1,C(8),B1,B2,P(7),Y(7),B3,AE3T,CC(8)

        B3=0
        C(8)=(100.0-C(1)-C(2)-C(3)-C(4)-C(5)-C(6)-(C7))/55.84
        C(1)=C(1)/12.0115
        C(2)=C(2)/28.09
        C(3)=C(3)/54.94
        C(4)=C(4)/58.71
        C(5)=C(5)/95.94
        C(6)=C(6)/52.0
        C(7)=C(7)/50.94
        B1=C(1)+C(2)+C(3)+C(4)+C(5)+C(6)+C(7)+C(8)
        DO 107 U=2,7
        Y(U)=C(U)/C(8)
107     CONTINUE
        DO 106 U=1,7
        C(U)=C(U)/B1
106     CONTINUE
        B2=0.0
        T10=Y(2)*(-3)+Y(3)*2+Y(4)*12+Y(5)*(-9)+Y(6)*(-1)+Y(7)*(-12)
        T20=-3*Y(2)-37.5*Y(3)-6*Y(4)-26*Y(5)-19*Y(6)-44*Y(7)
        P(2)=2013.0341+763.8167*C(2)+45802.87*C(2)**2-280061.63*C(2)**3
       1+3.864D+06*C(2)**4-2.4233D+07*C(2)**5+6.9547D+07*C(2)**6
        P(3)=2012.067-1764.095*C(3)+6287.52*C(3)**2-21647.96*C(3)**3-
       12.0119D+06*C(3)**4+3.1716D+07*C(3)**5-1.3885D+08*C(3)**6
        P(4)=2006.8017+2330.2424*C(4)-54915.32*C(4)**2+1.6216D+06*C(4)**3
       1-2.4968D+07*C(4)**4+1.8838D+08*C(4)**5-5.5531D+08*C(4)**6
        P(5)=2006.834-2997.314*C(5)-37906.61*C(5)**2+1.0328D+06*C(5)**3
       1-1.3306D+07*C(5)**4+8.411D+07*C(5)**5-2.08826D+08*C(5)**6
        P(6)=2012.367-9224.2655*C(6)+33657.8*C(6)**2-566827.83*C(6)**3
       1+8.5676D+06*C(6)**4-6.7482D+07*C(6)**5 +2.0837D+08*C(6)**6
        P(7)=2011.9996-6247.9118*C(7)+5411.7566*C(7)**2
       1+250118.1085*C(7)**3-4.1676D+06*C(7)**4
        DO 108 U=2,7
        B3=B3+P(U)*Y(U)
        B2=B2+Y(U)
108     CONTINUE
        IF(B2 .EQ. 0.0) GOTO 455
        W=(B3/B2)*4.187
        GOTO 456
```

```
455   W=8054.0
456   CONTINUE
      X1=C(1)
      R=8.31432
      W1=48570.0
      H=38575.0
      S=13.48
201   XEQ=0.1
      T=TT
      IF (T .LE. 1000) GOTO 20
      H1=105525
      S1=45.34521
      GOTO 19
20    H1=111918
      S1=51.44
19    F=ENERGY(T,T10,T20)
      J=1-DEXP(-W/(R*T))
51    DEQ=DSQRT(1-2*(1+2*J)*XEQ+(1+8*J)*XEQ*XEQ)
      TEQ=5*DLOG((1-XEQ)/(1-2*XEQ))
      TEQ=TEQ+DLOG(((1-2*J+(4*J-1)*XEQ-DEQ)/(2*J*(2*XEQ-1)))**6)
      TEQ=TEQ*R*T-F
      IF (DABS(TEQ) .LT. 1.0) GOTO 50
      ETEQ=5*((1/(XEQ-1))+2/(1-2*XEQ))
      ETEQ2=6*((4*J-1-(0.5/DEQ)*(-2-4*J+2*XEQ+16*XEQ*J))/(1-2*J+(4*J
      1-1)*XEQ-DEQ))+6*(4*J/(2*J*(2*XEQ-1)))
      ETEQ=(ETEQ+ETEQ2)*R*T
      XEQ=XEQ-TEQ/ETEQ
      GOTO 51
50    RETURN
      END
      DOUBLE PRECISION FUNCTION ENERGY(T,T10,T20)
      DOUBLE PRECISION T,T10,T20,F,T7
      T7=T-100*T20
      IF (T7 .LT. 300) GOTO 1
      IF (T7 .LT. 700) GOTO 2
      IF (T7 .LT. 940) GOTO 3
      F=-8.88909+0.26557*(T7-1140)-1.04923D-3*((T7-1140)**2)
      F=F+2.70013D-6*((T7-1140)**3)-3.58434D-9*((T7-1140)**4)
      GOTO 4
1     F=1.38*T7-1499
      GOTO 4
2     F=1.65786*T7-1581
      GOTO 4
3     F=1.30089*T7-1331
4     ENERGY=(141*T10 + F)*4.187
      RETURN
      END

      DOUBLE PRECISION FUNCTION XALPH(T)
      DOUBLE PRECISION T,CTEMP
      CTEMP=(T-273.0D+00)/900.0D+00
      XALPH=0.1528D-02-0.8816D-02*CTEMP+0.2450D-01*CTEMP*CTEMP
     &-0.2417D-01*CTEMP*CTEMP*CTEMP+
     &0.6966D-02*CTEMP*CTEMP*CTEMP*CTEMP
      RETURN
      END
```

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```
C Copyright S. A. Khan, H. K. D. H. Bhadeshia.
C
C Program calculates volume fraction of martensite from dilatometric data.
C Typical dataset follows
C VBAIN-wt% C in residual aust.-Ms
C 0.142 0.508 262.0
C relative length change-respective temp
C 0.0057 100.00
C 0.0053 120.00
C VBAIN calculated from dilatometery using prog .length
C wt% C in residual aust.from dilatometery using prog .length
C Ms from cooling curve from dilatometery
C Relative length change-&-respective temp obtained  from cooling curve
C A1, C1, G1 are the martensite a, martensite c and austenite lattice parameters
C See Andrews and Speich for details of parameters as a function of alloy
C For lattice parameter equations, substitutional alloy content in atomic %
C   but carbon in wt.%
C VBAIN = bainite volume fraction
C MS = martensite start temperature   XWT = carbon content of residual austenite
C T = Centigrade (all temps in these units) L = relative length change
      IMPLICIT REAL*8 (A-H,L-Z), INTEGER (I-K)
      DOUBLE PRECISION X(500),Y(500),RESULT(200)
      READ(5,*) VBAIN,XWT,MS
      VG=1.0D+00-VBAIN
      WRITE(6,9)VG
9     FORMAT( 'VOLUME FRACTION OF AUSTENITE=',F8.4)
      EXA=1.1103E-05
      EXY=1.7951E-05
      WRITE(6,4)VBAIN,XWT,MS
      WRITE(6,6)EXA,EXY
      MN=0.66
      SI=3.35
      VAN=0.1
      CR=0.86
      NI=1.70
      MO=0.22
      WRITE (6,7) XWT,SI,MN,NI,MO,CR,VAN
      ALLOY1=0.0010*MN-0.0002*NI+0.0006*CR+0.0053*MO+0.0017*VAN
      ALLOY2=0.0006*MN+0.0007*NI+0.0005*CR-0.0003*SI
      G1=3.573+ALLOY1+0.033*XWT
      A1=2.8661+ALLOY2- 0.013*XWT
      C1=2.8661+ALLOY2+0.116*XWT
      WRITE(6,5)
      DO 1 K=1,500
      READ(5,*,END=2)L,T
C Calculation of lattice parameters at temprature T
      G2=G1*(1.0D+00+(T-20)*EXY)
      A2=A1*(1.0D+00+(T-20)*EXA)
      C2=C1*(1.0D+00+(T-20)*EXA)
C Calculation of the volume fraction of martensite
      V2=(3*L*G2**3)/(VG*(2*A2*A2*C2-G2**3))
C V2 is the fraction of residual austenite that transforms into martensite
C V2 = f = VM/Vg
C Calculation of ln(1-f)
      IF (V2 .GT. 1) GOTO 22
      GOTO 23
22    V2=0.999
23    Y(K)=DLOG(1.0D+00-(V2))
      X(K)=MS-T
      VGR=VG-(V2*VG)
C TO read every 3rd data from the computed (dilatometric) length change data.
      NO=NO+1
      IF (NO .EQ. 3) GOTO 67
      GOTO 68
C Not to consider data below 15.0 degree centigrade.
67    IF (T .LT. 15.0) GOTO 68
      GOTO 71
```

```
71      WRITE (6,3) L,T,V2,G2,A2,C2,X(K),Y(K),VGR
C Calculation of the absolute volume fraction
        IF (T .LE. 20.0) GOTO 123
        GOTO 321
123     VAB=V2*VG
        WRITE(6,66)T,VAB
66      FORMAT( ' ABSOLUTE VALUE OF MARTENSITE AT',F4.0,' IS= ',F8.3)
321     NO=0
68      III=III+1
3       FORMAT (F8.5,F5.0,F7.3,F10.5,F10.5,F10.5,F7.0,F10.3,F10.4)
1       CONTINUE
2       III=K-1
        STOP
4       FORMAT(' Volume Fraction of Bainite = ', F8.4/
        &' C in residual austenite, at ',
        &' termination of bainite reaction, wt.%, =', F8.3/
        &' Martensite start temperature, centigrade, = ',F8.2)
7       FORMAT(' C, wt.% =',F8.3,2X, 'Si, At.% =',
        &F8.2,2X,'Mn, At.% =',F8.2,
        &2X,'Ni, At.% =',F10.4/' Mo, At.% =',F10.4,2X,
        &' Cr, At.% =',F8.2,2X,'V, At.% =',F10.4//)
6       FORMAT(' Linear Expansivity, alpha = ',D12.4/
        &' Linear Expansivity, gamma = ',D12.4)
5       FORMAT(' Length Ctemp Vmart    G2      A2      C2 ',
        &'    Ms-Tq    LN(1-F)   VGR')
        END
```

```
C Copyright S. A. Khan and H. K. D. H. Bhadeshia
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C Pembroke Street, Cambridge CB2 3QZ, U. K.
C
C PROG. FOR THE ANALYSIS OF ALLOTRIOMORPHIC FERRITE TRANSFORMATION IN
C HETEROGENEOUS ALLOY, AS INTERFACE MOTION IS NORMAL TO THE ISOCONCENTRATION
C PLANES.
C
C The steel is divided into slices of different compositions,
C Ae3 temperature and XEQ of the first slice (solute depleted) is calculated.
C Transformation is allowed to go to 100% in slice J=1 if its Ae3 temperature
C is higher than the isothermal temperature, the carbon thus
C rejected is allowed to homogenise in the residual austenite.
C Transformation now shifts to slice J=2 if its Ae3 temperature, calculated
C from the its new composition (i.e., due to increase in carbon content), is
C higher than the concerned transformation temeprature. The exetent of
C transformation is limited by paraequilibrium mechanism.
C The results averaged and compared with a steel of the corresponding average
C composition.
C Typical data set follows:
C 673 (temperature in Kelvin)
C 0.43 0.50 0.60 0.70 0.80 0.90 1.00 (Composition of slice 1 in wt.%)
C 0.43 0.60 0.60 0.70 0.80 0.90 1.90 (Composition of slice 2 in wt.%)
C C  Si  Mn  Ni  Mo  Cr  V
C
      IMPLICIT REAL*8(A-H,K-Z), INTEGER(I,J)
      DOUBLE PRECISION C(8),D(8),XEQ(200)
     &,E(8),F(8),MS(100),IA(100),XGAMMA(200),VOLF(200)
     &,CN(200),SI(200),MN(200),NI(200),MO(200),V(200),FE(200)
     &,CR(200),WD(8),VG(200),CD(8),XG(200),TAE3(200)
     &,TAE3H,XEQH,TVOLF,AVEVOL,MOMENT,TISO,CE(8),SLICEN,TSLICE
      DIMENSION VOLFD(200)
      VINCR=0.00005D+00
      ISTOP=0
      AVEVOL=0.0D+0
      TVOLF=0.0D+0
      C1=0.0
      C2=0.0
      C3=0.0
      C4=0.0
      C5=0.0
      C6=0.0
      C7=0.0
      READ(5,*)KELVIN
      TISO=KELVIN-273.0D+0
      XALPHA=XALPH(KELVIN)
      WRITE(6,4444)
4444  FORMAT( ' ****CARBON  IS ALLOWED TO DIFFUSE!!!!**********')
      WRITE(6,9)KELVIN,XALPHA,VINCR
      WRITE(6,9090)
9090  FORMAT('————————————————————————————
     &————————')
      DO 1 I=1,200
      READ(5,*,END=2)C(1),C(2),C(3),C(4),C(5),C(6),C(7)
      CN(I)=C(1)
      SI(I)=C(2)
      MN(I)=C(3)
      NI(I)=C(4)
      MO(I)=C(5)
      CR(I)=C(6)
      V(I)=C(7)
      FE(I)=100.0D+0-(C(1)+C(2)+C(3)+C(4)+C(5)+C(6)+C(7))
      C1=C1+C(1)
      C2=C2+C(2)
      C3=C3+C(3)
      C4=C4+C(4)
      C5=C5+C(5)
```

```fortran
      C6=C6+C(6)
      C7=C7+C(7)
      DO 43 IJI=1,7
      E(IJI)=C(IJI)
43    CONTINUE
      CALL XEQ3(KELVIN,C,XEQ(I))
      CALL TEMP3(E,TAE3(I))
      XBAR=C(1)
      WRITE(6,10)I,XEQ(I),TAE3(I)
      WRITE(6,6161)
6161  FORMAT('***************************************************************
     &***********************')
1     CONTINUE
2     ISLICE=I-1
      WRITE(*,*) ISLICE
      D(1)=C1/ISLICE
      D(2)=C2/ISLICE
      D(3)=C3/ISLICE
      D(4)=C4/ISLICE
      D(5)=C5/ISLICE
      D(6)=C6/ISLICE
      D(7)=C7/ISLICE
      DO 70 JII=1,7
      WD(JII)=D(JII)
70    CONTINUE
      DO 56 JIJ=1,7
      F(JIJ)=D(JIJ)
56    CONTINUE
      CALL XEQ3(KELVIN,D,XEQH)
      CALL TEMP3(F,TAE3H)
      WRITE(6,75)TAE3H
75    FORMAT(' Ae3H= ',D10.4)
C     IF (TAE3H .LT. TISO) GOTO 789
C     GOTO 85
      IF (XEQH .LE. D(1)) GOTO 789
      GOTO 79
79    IF (XEQH .GT. XALPHA) GOTO 987
      GOTO 789
789   VOLH=0.00
      GOTO 678
987   VOLH=(XEQH-D(1))/(XEQH-XALPHA)
678   VGH=1.0D+0-VOLH
      WRITE(6,15)VOLH
      AVEX=D(1)
      DO 4 J=1,ISLICE
      SLICEN=J
      TSLICE=ISLICE
      IF (XEQ(J) .LE. AVEX) GOTO 5
      GOTO 7007
7007  IF (TAE3(J) .LT. TISO) GOTO 5
      GOTO 9352
9352  AVEVOL=SLICEN/TSLICE
      VOLF(J)=AVEVOL
      AVEX=D(1)+(AVEVOL*(D(1)-XALPHA))/(1.0D+0-AVEVOL)
      WRITE(6,886)J,XEQ(J),TAE3(J),D(1),AVEVOL,AVEX,VOLF(J)
886   FORMAT(' SLICE=',I3,' XEQ=',
     &D10.3,' TAE3=',D10.3,' D(1)=',D10.3,' AVEVOL=',D10.3,' AVEX=',
     &D10.3,' VOLF(J)=', D10.3)
C Recalling the original composition(wt%) for each slice.....
      CD(1)=CN(J+1)
      CD(2)=SI(J+1)
      CD(3)=MN(J+1)
      CD(4)=NI(J+1)
      CD(5)=MO(J+1)
      CD(6)=CR(J+1)
      CD(7)=V(J+1)
      XG(J+1)=CD(1)+((VOLF(J)*CD(1))/(1.0D+00-VOLF(J)))
C Getting new composition (wt%) of residual austenite in each slice
      RT=(100.0D+00-XG(J+1))/(100.0D+00-CD(1))
```

```
      CD(1)=XG(J+1)
      DO 262 NIN=2,7
      CD(NIN)=CD(NIN)*RT
262   CONTINUE
      DO 161 NO=1,7
      CE(NO)=CD(NO)
161   CONTINUE
      CALL XEQ3(KELVIN,CD,XEQ(J+1))
      CALL TEMP3(CE,TAE3(J+1))
      GOTO 4
5     GOTO 786
4     CONTINUE
786       WRITE(6,13)AVEVOL
13    FORMAT(' Average volume fraction of transformation',
     &' in heterogeneous alloy =',D8.3)
9     FORMAT(' KELVIN = ',F7.0,' XALPHA, mol. fraction =',D12.4
     &,' VOL INCREMENT=',D12.4)
10    FORMAT(' Slice Number= ',I3,'       XEQ = ',D10.4,
     &'        AE3-T= ',D10.4/)
15    FORMAT(' Maximum volume fraction of bainitic ferrite in ',
     &' an alloy of average composition = ',D8.3)
      STOP
      END


C***********************************************************
      SUBROUTINE TEMP3(C,AE3T)
      DOUBLE PRECISION X,X1,R,A,A1,AFE,A1FE,DA1,DA2,DA1FE,H,H1,S,S1
      INTEGER T1,I,NO,U,B4,J99,C99,C98,C97
      DOUBLE PRECISION D11,DTQ(40),DXEQ(40),
     1INCEPT,SLOPE,CORR,
     1DEQ,ETEQ,T10,T20,XA,AFEQ,AEQ,ETEQ2,TEQ,
     1J,J1,D,D1,W,W1,F,TEST,ERROR,T4,XEQ,FPRO
     1,C(8),B1,B2,P(7),Y(7),B3,AE3T,EE(8)
      WRITE(6,1100)C(1),C(2),C(3),C(4),C(5),C(6),C(7)
1100  FORMAT(7D11.3)
      B3=0
      C(8)=(100.0-C(1)-C(2)-C(3)-C(4)-C(5)-C(6)-(C7))/55.84
      C(1)=C(1)/12.0115
      C(2)=C(2)/28.09
      C(3)=C(3)/54.94
      C(4)=C(4)/58.71
      C(5)=C(5)/95.94
      C(6)=C(6)/52.0
      C(7)=C(7)/50.94
      B1=C(1)+C(2)+C(3)+C(4)+C(5)+C(6)+C(7)+C(8)
      DO 107 U=2,7
      Y(U)=C(U)/C(8)
107   CONTINUE
      DO 106 U=1,7
      C(U)=C(U)/B1
106   CONTINUE
      B2=0.0
      T10=Y(2)*(-3)+Y(3)*2+Y(4)*12+Y(5)*(-9)+Y(6)*(-1)+Y(7)*(-12)
      T20=-3*Y(2)-37.5*Y(3)-6*Y(4)-26*Y(5)-19*Y(6)-44*Y(7)
      P(2)=2013.0341+763.8167*C(2)+45802.87*C(2)**2-280061.63*C(2)**3
     1+3.864D+06*C(2)**4-2.4233D+07*C(2)**5+6.9547D+07*C(2)**6
      P(3)=2012.067-1764.095*C(3)+6287.52*C(3)**2-21647.96*C(3)**3-
     12.0119D+06*C(3)**4+3.1716D+07*C(3)**5-1.3885D+08*C(3)**6
      P(4)=2006.8017+2330.2424*C(4)-54915.32*C(4)**2+1.6216D+06*C(4)**3
     1-2.4968D+07*C(4)**4+1.8838D+08*C(4)**5-5.5531D+08*C(4)**6
      P(5)=2006.834-2997.314*C(5)-37906.61*C(5)**2+1.0328D+06*C(5)**3
     1-1.3306D+07*C(5)**4+8.411D+07*C(5)**5-2.0826D+08*C(5)**6
      P(6)=2012.367-9224.2655*C(6)+33657.8*C(6)**2-566827.83*C(6)**3
     1+8.5676D+06*C(6)**4-6.7482D+07*C(6)**5 +2.0837D+08*C(6)**6
      P(7)=2011.9996-6247.9118*C(7)+5411.7566*C(7)**2
     1+250118.1085*C(7)**3-4.1676D+06*C(7)**4
      DO 108 U=2,7
      B3=B3+P(U)*Y(U)
      B2=B2+Y(U)
```

```fortran
108   CONTINUE
      IF(B2 .EQ. 0.0) GOTO 455
      W=(B3/B2)*4.187
      GOTO 456
455   W=8054.0
456   CONTINUE
      X1=C(1)
      R=8.31432
      W1=48570.0
      H=38575.0
      S=13.48
      II1=873
      II2=1173
      II3=15
      II=0
201   XEQ=0.1
      INCEPT=1.0D+00
      CORR=1.0D+00
      SLOPE=1.0D+00
      C98=0
      C97=0
      DO 9 T1=II1,II2,II3
      C98=C98+1
      T=T1
      IF (T .LE. 1000) GOTO 20
      H1=105525
      S1=45.34521
      GOTO 19
20    H1=111918
      S1=51.44
19    F=ENERGY(T,T10,T20)
      J=1-DEXP(-W/(R*T))
51    DEQ=DSQRT(1-2*(1+2*J)*XEQ+(1+8*J)*XEQ*XEQ)
      TEQ=5*DLOG((1-XEQ)/(1-2*XEQ))
      TEQ=TEQ+DLOG(((1-2*J+(4*J-1)*XEQ-DEQ)/(2*J*(2*XEQ-1)))**6)
      TEQ=TEQ*R*T-F
      IF (DABS(TEQ) .LT. 1.0) GOTO 50
      ETEQ=5*((1/(XEQ-1))+2/(1-2*XEQ))
      ETEQ2=6*((4*J-1-(0.5/DEQ)*(-2-4*J+2*XEQ+16*XEQ*J))/(1-2*J+(4*J
     1-1)*XEQ-DEQ))+6*(4*J/(2*J*(2*XEQ-1)))
      ETEQ=(ETEQ+ETEQ2)*R*T
      XEQ=XEQ-TEQ/ETEQ
      GOTO 51
50    IF (XEQ .LT. 0.001) GOTO 2444
      T4=T1-273.0
      DTQ(C98)=T4
      DXEQ(C98)=XEQ
9     CONTINUE
2444  C98=C98-1
      CALL ANAL(C98,INCEPT,SLOPE,CORR,DTQ,DXEQ)
      AE3T=(X1-INCEPT)/SLOPE
      IF(II .GT. 0) GOTO 802
      II=AE3T
      II1=II-9+273
      II2=II+9+273
      II3=1
      GOTO 201
802   RETURN
      END
      SUBROUTINE ANAL(C98,INCEPT,SLOPE,CORR,X,Y)
      DOUBLE PRECISION AX,AX2,AY,AY2,AXY,INCEPT,CORR,SLOPE,
     &X(40),Y(40)
      INTEGER I,C98,I1
      I1=C98
      C98=C98-10
      AX=0.0D+00
      AY=0.0D+00
      AX2=0.0D+00
      AY2=0.0D+00
```

```fortran
      AXY=0.0D+00
      DO 1 I=1,C98
      AX=AX+X(I)
      AY=AY+Y(I)
      AXY=AXY+X(I)*Y(I)
      AX2=AX2+X(I)*X(I)
      AY2=AY2+Y(I)*Y(I)
1     CONTINUE
      INCEPT=(AY*AX2-AX*AXY)/(C98*AX2-AX*AX)
      SLOPE=((C98*AXY-AX*AY)/(C98*AX2-AX*AX))
      CORR=(C98*AXY-AX*AY)/(DSQRT((C98*AX2-AX*AX)*
     &(C98*AY2-AY*AY)))
      C98=I1
      RETURN
      END
      DOUBLE PRECISION FUNCTION ENERGY(T,T10,T20)
      DOUBLE PRECISION T,T10,T20,F,T7
      T7=T-100*T20
      IF (T7 .LT. 300) GOTO 1
      IF (T7 .LT. 700) GOTO 2
      IF (T7 .LT. 940) GOTO 3
      F=-8.88909+0.26557*(T7-1140)-1.04923D-3*((T7-1140)**2)
      F=F+2.70013D-6*((T7-1140)**3)-3.58434D-9*((T7-1140)**4)
      GOTO 4
1     F=1.38*T7-1499
      GOTO 4
2     F=1.65786*T7-1581
      GOTO 4
3     F=1.30089*T7-1331
4     ENERGY=(141*T10 + F)*4.187
      RETURN
      END


C***********************************************************
      SUBROUTINE XEQ3(TT,C,XEQ)
      DOUBLE PRECISION X,X1,T,R,A,A1,AFE,A1FE,DA1,DA2,DA1FE,H,H1,S,S1
     &,TT
      INTEGER I,NO,U,B4,J99,C99,C98,C97
      DOUBLE PRECISION D11,
     1DEQ,ETEQ,T10,T20,XA,AFEQ,AEQ,ETEQ2,TEQ,
     1J,J1,D,D1,W,W1,F,TEST,ERROR,T4,XEQ,FPRO
     1,C(8),B1,B2,P(7),Y(7),B3,AE3T,CC(8)

      B3=0
      C(8)=(100.0-C(1)-C(2)-C(3)-C(4)-C(5)-C(6)-(C7))/55.84
      C(1)=C(1)/12.0115
      C(2)=C(2)/28.09
      C(3)=C(3)/54.94
      C(4)=C(4)/58.71
      C(5)=C(5)/95.94
      C(6)=C(6)/52.0
      C(7)=C(7)/50.94
      B1=C(1)+C(2)+C(3)+C(4)+C(5)+C(6)+C(7)+C(8)
      DO 107 U=2,7
      Y(U)=C(U)/C(8)
107   CONTINUE
      DO 106 U=1,7
      C(U)=C(U)/B1
106   CONTINUE
      B2=0.0
      T10=Y(2)*(-3)+Y(3)*2+Y(4)*12+Y(5)*(-9)+Y(6)*(-1)+Y(7)*(-12)
      T20=-3*Y(2)-37.5*Y(3)-6*Y(4)-26*Y(5)-19*Y(6)-44*Y(7)
      P(2)=2013.0341+763.8167*C(2)+45802.87*C(2)**2-280061.63*C(2)**3
     1+3.864D+06*C(2)**4-2.4233D+07*C(2)**5+6.9547D+07*C(2)**6
      P(3)=2012.067-1764.095*C(3)+6287.52*C(3)**2-21647.96*C(3)**3-
     12.0119D+06*C(3)**4+3.1716D+07*C(3)**5-1.3885D+08*C(3)**6
      P(4)=2006.8017+2330.2424*C(4)-54915.32*C(4)**2+1.6216D+06*C(4)**3
     1-2.4968D+07*C(4)**4+1.8838D+08*C(4)**5-5.5531D+08*C(4)**6
      P(5)=2006.834-2997.314*C(5)-37906.61*C(5)**2+1.0328D+06*C(5)**3
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      1-1.3306D+07*C(5)**4+8.411D+07*C(5)**5-2.0826D+08*C(5)**6
      P(6)=2012.367-9224.2655*C(6)+33657.8*C(6)**2-566827.83*C(6)**3
      1+8.5676D+06*C(6)**4-6.7482D+07*C(6)**5 +2.0837D+08*C(6)**6
      P(7)=2011.9996-6247.9118*C(7)+5411.7566*C(7)**2
      1+250118.1085*C(7)**3-4.1676D+06*C(7)**4
      DO 108 U=2,7
      B3=B3+P(U)*Y(U)
      B2=B2+Y(U)
108   CONTINUE
      IF(B2 .EQ. 0.0) GOTO 455
      W=(B3/B2)*4.187
      GOTO 456
455   W=8054.0
456   CONTINUE
      X1=C(1)
      R=8.31432
      W1=48570.0
      H=38575.0
      S=13.48
201   XEQ=0.1
      T=TT
      IF (T .LE. 1000) GOTO 20
      H1=105525
      S1=45.34521
      GOTO 19
20    H1=111918
      S1=51.44
19    F=ENERGY(T,T10,T20)
      J=1-DEXP(-W/(R*T))
51    DEQ=DSQRT(1-2*(1+2*J)*XEQ+(1+8*J)*XEQ*XEQ)
      TEQ=5*DLOG((1-XEQ)/(1-2*XEQ))
      TEQ=TEQ+DLOG(((1-2*J+(4*J-1)*XEQ-DEQ)/(2*J*(2*XEQ-1)))**6)
      TEQ=TEQ*R*T-F
      IF (DABS(TEQ) .LT. 1.0) GOTO 50
      ETEQ=5*((1/(XEQ-1))+2/(1-2*XEQ))
      ETEQ2=6*((4*J-1-(0.5/DEQ)*(-2-4*J+2*XEQ+16*XEQ*J))/(1-2*J+(4*J
      1-1)*XEQ-DEQ))+6*(4*J/(2*J*(2*XEQ-1)))
      ETEQ=(ETEQ+ETEQ2)*R*T
      XEQ=XEQ-TEQ/ETEQ
      GOTO 51
50    RETURN
      END
      DOUBLE PRECISION FUNCTION ENERGY(T,T10,T20)
      DOUBLE PRECISION T,T10,T20,F,T7
      T7=T-100*T20
      IF (T7 .LT. 300) GOTO 1
      IF (T7 .LT. 700) GOTO 2
      IF (T7 .LT. 940) GOTO 3
      F=-8.88909+0.26557*(T7-1140)-1.04923D-3*((T7-1140)**2)
      F=F+2.70013D-6*((T7-1140)**3)-3.58434D-9*((T7-1140)**4)
      GOTO 4
1     F=1.38*T7-1499
      GOTO 4
2     F=1.65786*T7-1581
      GOTO 4
3     F=1.30089*T7-1331
4     ENERGY=(141*T10 + F)*4.187
      RETURN
      END

      DOUBLE PRECISION FUNCTION XALPH(T)
      DOUBLE PRECISION T,CTEMP
      CTEMP=(T-273.0D+00)/900.0D+00
      XALPH=0.1528D-02-0.8816D-02*CTEMP+0.2450D-01*CTEMP*CTEMP
     &-0.2417D-01*CTEMP*CTEMP*CTEMP+
     &0.6966D-02*CTEMP*CTEMP*CTEMP*CTEMP
      RETURN
      END
```