

PAPER 1. A DISLOCATION MODEL FOR THE PLASTIC DEFORMATION OF SINGLE-PHASE ALPHA-IRON

1. Introduction

The plastic forming of metals and alloys plays an important technical and economical role in modern society and it is therefore not surprising that the physical mechanisms behind the plastic deformation process have been the subject of extensive experimental and theoretical studies over the years.

The first great step towards an increased understanding of the plastic deformation of crystalline materials was taken in the early 1930's when the dislocation concept was introduced to explain the stress – strain behaviour of metals (1). It was then realised that the plastic deformation process was not homogeneous but localised around moving linear defects called dislocations. The dislocation concept was also capable of explaining the comparatively low shear stresses needed to activate the plastic deformation process and thereby ended a long dispute that had gone on to physically explain this fact.

In one of the first attempts to formulate a dislocation theory for the work hardening of metals it was assumed that the mean free path of the mobile dislocations was strain independent and that the dislocations were homogeneously distributed in the material (1). Proceeding from these assumptions and the stress fields around dislocations a parabolic strain – hardening law was derived.

A second important step was taken in the middle 1950's when transmission electron microscopy (TEM) was applied to study the dislocations and dislocation structures in deformed materials (2,3). These studies revealed that the assumptions made concerning the general behaviour of dislocations during straining had on a large scale been correct and it was demonstrated that the total dislocation density raises with increasing strain for example. However, the original assumption of a homogeneous distribution of dislocations proved to be wrong since the dislocations were observed to heap up in tangles and cells. To-day, with modern technologies to analyse strain distribution, it is obvious that the plastic deformation process in most cases is inhomogeneous. Typical examples illustrating this are well-developed dislocation cells with high dislocation densities in the cell walls and low densities in the interior of the cells, pronounced strain gradients inside the grains as well as between grains. Other typical inhomogeneous phenomena are the Lüders strain in steel and the serrations in the stress-strain curves during dynamic strain ageing. It is also reasonable to assume that the high strain hardening rates in dual phase steels are due to some type of inhomogeneous deformation behaviour originating from the hard second phase (4,5)

In order to mathematically describe the stress – strain behaviour of metals and alloys a number of empirical relationships have been proposed. The most well-known of these are the ones proposed by Ludwik (6)

$$\sigma = \sigma_{0L} + L \cdot \varepsilon^m \quad (1)$$

where σ is the true stress, ε the true strain and σ_{0L} , L and m are material constants and by Hollomon (7)

$$\sigma = K \cdot \varepsilon^n \quad (2)$$

where σ and ε are the true stress and strain respectively and K and n material constants.

The Hollomon equation is the most well-known of the two, mainly because it is frequently used to describe the stretch formability of sheets via the n – value which is assumed to be equal to the true strain to necking.

It should be underlined, however, that neither of these two equations are capable of giving a good description of the stress – strain behaviour of metals and alloys. It should also be pointed out that the material parameters involved are lacking a physical meaning. In most cases a “double- n ” or “triple- n ” behaviour is required to describe experimental data (8)

During the last 50 years numerous theoretical relationships have been proposed for the plastic deformation of metals and most of them are based on various types of assumptions regarding the creation, the immobilisation and the annihilation of dislocations (9), (10), (11), (12), (13), (14), (15). Quite often advanced mathematics is applied. However, so far, no generally accepted physically founded theory has been proposed not even for simple cases like uniaxial work hardening in pure single-phase metals.

The situation for the new advanced high strength steels like dual phase steels and martensitic steels is even more unclear.

It is the objective of this homepage to present the various steps taken to develop the Bergström dislocation theory (9) for the plastic behaviour of metals and alloys. The first version, dealing with single-phase bcc metals, was presented almost 40 years ago. The last version incorporating materials containing a soft matrix and a hard second phase, was presented recently. The first theories were based on the assumption that the deformation process was almost homogeneous. In the latest theories e.g. for dual phase steel, account is taken for the inhomogeneous behavior in this type of material.

2. Theoretical Background

It is well established, both experimentally and theoretically, that the true flow stress, $\sigma(\varepsilon)$, in crystalline materials and alloys is related to the total dislocation density $\rho(\varepsilon)$ as (1)

$$\sigma(\varepsilon) = \sigma_{i0} + \alpha Gb\sqrt{\rho(\varepsilon)} \quad (3)$$

where, σ_{i0} , is the friction stress, α , a dislocation strengthening constant, G the shear modulus, b the nominal value of the Burgers vector and, ε , the true strain. If the validity of equation (3) is accepted then the main problem in formulating a dislocation theory for the true stress-true strain behaviour of metals and alloys is to derive a relationship for $\rho(\varepsilon)$. This, however, is a complicated task due to the fact that the total dislocation density is very high already after small strains, of the order of 10^{13} - 10^{15} m^{-2} and consequently it is not possible to distinguish the individual behaviour of the dislocations. The way to proceed is thus to consider the average behaviour of a large number of dislocations. There are also other complicating factors that must be taken into account, i.e.:

- the dislocations are not homogeneously distributed in the material during deformation but form dislocation tangles and dislocation cells

- the virgin microstructure consisting of for instance precipitates, solute atoms, “grown-in” dislocations etc. affect dislocation motion and dislocation substructure formation
- the modus of deformation has an effect on several parameters controlling the plastic deformation process

Further, in order to formulate a theory for $\rho(\varepsilon)$ the following points must be considered:

- is it possible to distinguish between mobile and immobile dislocations and to estimate their densities?
- is the density of mobile dislocations strain independent?
- where and how are the mobile dislocations generated, how do they move and how far a distance do they move before they are immobilized?
- is it possible for immobilized dislocations to remobilize and if so what factors control the rate at which this occurs?
- at what rate do the dislocations annihilate and can this process be neglected at low and moderate temperatures?

The literature provides answers to some of these questions. Michalak (16), for instance, investigated α -iron and concluded that the density of mobile dislocations, L , is small and approximately strain independent. This has also been verified by Bergström and Hallén (17) by analysing strain-rate change data. In the low alloy steels investigated L was observed to be small – in the order of 10^8 m^{-2} – and approximately strain independent. In-situ studies of the plastic deformation process in HVEM have, further on, revealed that

- dislocation cells are rapidly formed during straining, especially in bcc-metals and in fcc-metals with high stacking fault energy
- mobile dislocations are predominantly generated at cell walls and move in one rapid step towards opposite cell walls where they are immobilized
- immobile dislocations are observed to remobilize

Although some of the observations are uncertain they indicate the existence of a mean free path, s , of mobile dislocations which in one way or another is related to the average dislocation cell diameter. They also indicate that dislocation remobilization may occur. It has also been concluded that the annihilation of dislocations may be ignored at least at low and moderate temperatures.

3. Theory

By introducing these concepts into a dislocation model for *single-phase* metals and alloys, Bergström (9) derived the following expression for the variation of the total dislocation density with strain

$$\frac{d\rho}{d\varepsilon} = \frac{m}{b \cdot s(\varepsilon)} - \Omega \cdot \rho \quad (4)$$

where ρ is the total dislocation density, $s(\varepsilon)$ is the mean free path of dislocation motion, b is the nominal value of Burger’s vector, Ω is a strain independent material constant representing the remobilization (dynamic recovery) of immobile dislocations and, at higher temperatures annihilation, m is the Taylor constant.

In the original Bergström theory it was assumed that the mean free path of dislocation motion was strain independent and equal to s_0 in iron and steel which implies that eqn(2) may be written

$$\frac{d\rho}{d\varepsilon} = \frac{\bar{m}}{b \cdot s_0} - \Omega \cdot \rho \quad (5)$$

By introducing

$$U_0 = \frac{m}{b \cdot s_0} \quad (6)$$

where U_0 is a strain independent dislocation creation rate-constant, eqn(3) may be re-written

$$\frac{d\rho}{d\varepsilon} = U_0 - \Omega \cdot \rho \quad (7)$$

The physical meaning of the components in this equation is roughly the following:

$\frac{d\rho}{d\varepsilon}$	the <u>net rate</u> of dislocation generation
U_0	the <u>rate</u> of dislocation creation
$\Omega \cdot \rho$	the <u>rate</u> of dislocation re-mobilisation and/or annihilation

Now, with a strain independent mean free path s_0 and thus U_0 , eqn(7) is easily integrated:

$$\rho(\varepsilon) = \frac{U_0}{\Omega} \cdot (1 - e^{-\Omega \cdot \varepsilon}) + \rho_0 \cdot e^{-\Omega \cdot \varepsilon} \quad (8)$$

where ρ_0 is the “grown-in” dislocation density, that is the total dislocation density present in the metal at the start of plastic deformation.

Combining eqn(8) with eqn(1) we obtain the following relationship for the true stress – strain behaviour of iron and steel

$$\sigma = \sigma_{i0} + \alpha \cdot G \cdot b \cdot \left(\frac{U_0}{\Omega} \cdot (1 - e^{-\Omega \cdot \varepsilon}) + \rho_0 \cdot e^{-\Omega \cdot \varepsilon} \right)^{\frac{1}{2}} \quad (9)$$

In well annealed materials the “grown-in” dislocation density, ρ_0 , is small and may as a first approximation be neglected and eqn(7) becomes

$$\sigma = \sigma_{i0} + H \cdot \left(\frac{1 - e^{-\Omega \cdot \varepsilon}}{\Omega} \right)^{\frac{1}{2}} \quad (10)$$

where $H = \alpha \cdot G \cdot b \cdot \sqrt{U_0}$ is a constant. This equation contains only three parameters and may in that respect be compared to the empirical Ludwik equation, see eqn(1). Now, at smaller strains and/or if the remobilisation constant Ω is small then the term $e^{-\Omega \cdot \varepsilon} \approx 1 - \Omega \cdot \varepsilon$ and eqn(10) may be written

$$\sigma = \sigma_{i0} + H \cdot \varepsilon^{\frac{1}{2}} \quad (11)$$

which is identical to the famous Taylor equation for work hardening.. However the best agreement with experimental data is obtained with eqn(9).

By combining eqn(9) and eqn(6) we obtain the following expression for the true stress-strain behaviour of bcc metals like ferritic steel.

$$\sigma = \sigma_{i0} + \alpha \cdot G \cdot b \cdot \left(\frac{m}{\Omega \cdot b \cdot s_{\alpha}} \cdot (1 - e^{-\Omega \cdot \varepsilon}) + \rho_0 \cdot e^{-\Omega \cdot \varepsilon} \right)^{\frac{1}{2}} \quad (12)$$

4.1 Experimental

In order to avoid the Lüders phenomenon and hence to maximise the homogeneous part of the true stress – strain curve a Ti-stabilised steel was investigated.

Tensile testing was carried out at 25C and a strain rate of 10^{-3} s^{-1} .

Transmission electron microscopy investigations of both unstrained and deformed specimens were performed. From these studies the “grown-in” dislocation density, ρ_0 , the strain dependence of the total dislocation density, ρ , and the dislocation strengthening parameter, α , were experimentally estimated.

4.2. Experimental results

In Fig 1 experimentally recorded dislocation densities for the investigated Ti – stabilised steel – red squares - are plotted versus prestrain. The bars represent the estimated errors. The grown-in dislocation density, ρ_0 , was estimated to be $2 \times 10^{12} \text{ m}^{-2}$. The black curve in Fig 1 is the corresponding theoretically calculated $\rho - \varepsilon$ curve, see below.

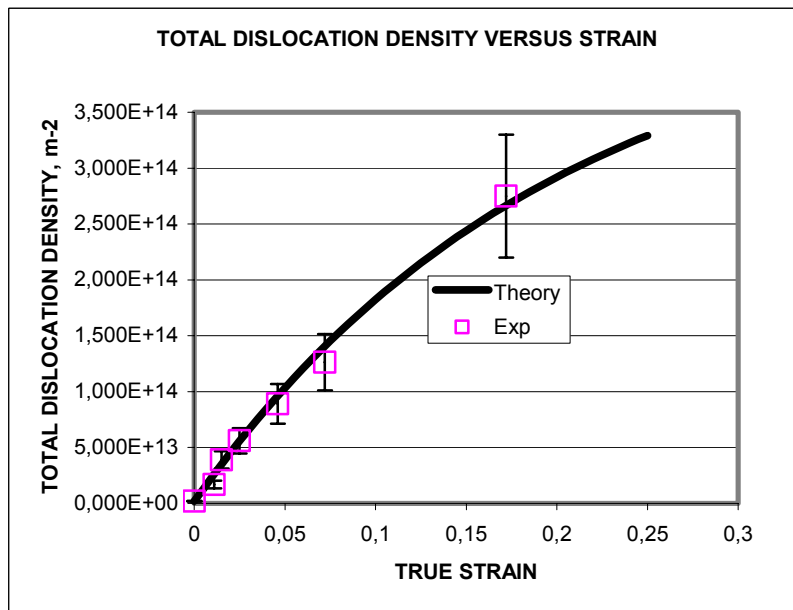


Fig. 1. Total dislocation density versus strain for a Ti-stabilised steel. The test was carried out at RT and at a strain rate of 10^{-3} s^{-1} .

In Fig 2 the flow stress is plotted versus the square root of the total dislocation density at various pre-strains.

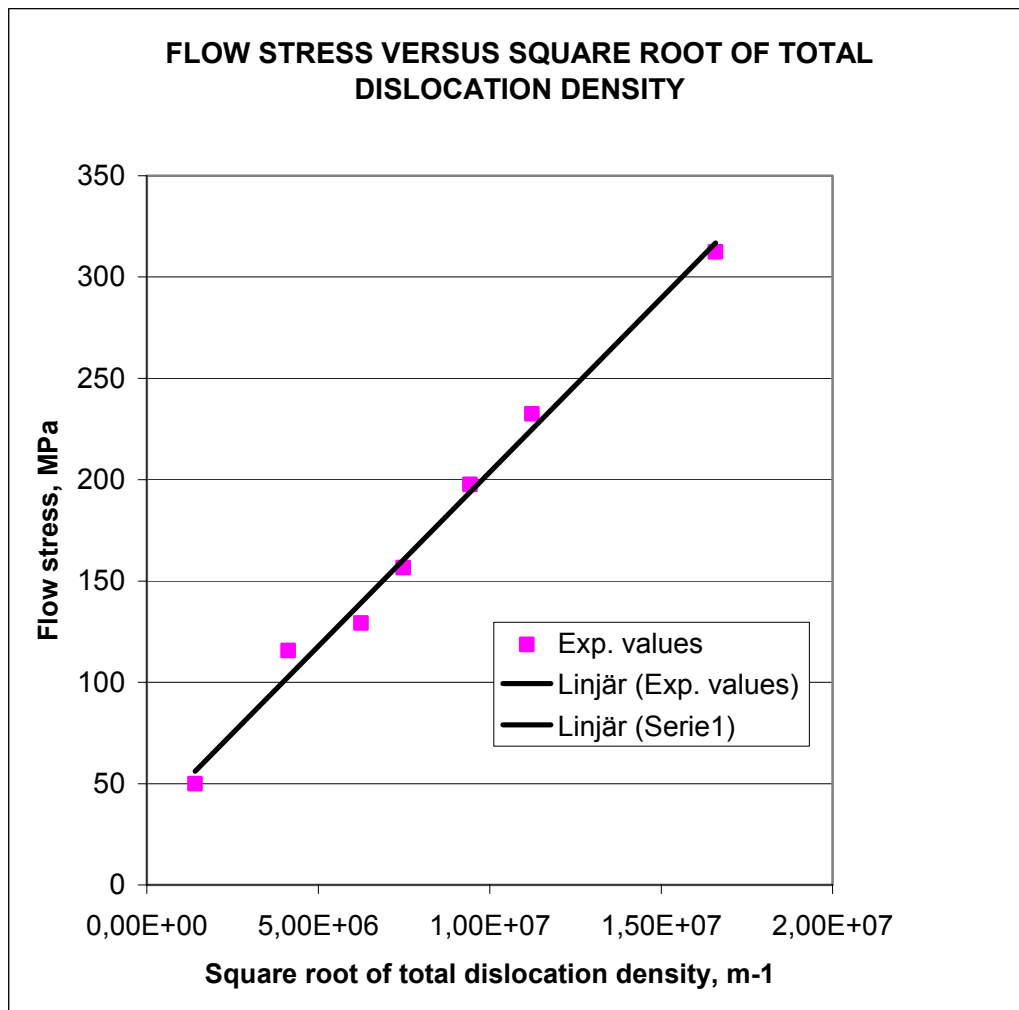


Fig 2. Flow stress versus square root of the total dislocation density in Ti-stabilised α -iron.

In analysing the experimental results the shear modulus G and the Burgers vector b are assigned the values of 80 000 MPa and $2.5 \cdot 10^{-10}$ m respectively. From the slope of the experimental $\sigma - \rho^{1/2}$ plot, see Fig 2, the parameter α is evaluated to be 0.88. From the same plot σ_{i0} is estimated to be approximately equal to 25 MPa.

From the dislocation density measurements the value of the “grown-in” dislocation density ρ_0 is calculated to be approximately equal to $2 \cdot 10^{12} \text{ m}^{-2}$.

From the slope of the experimental ρ - ϵ curve at smaller strains the parameter U_0 is estimated to be approximately $2.3 \cdot 10^{14} \text{ m}^{-2}$.

6. Theoretical analysis and results

A specially designed program based on the MATLAB Curve Fitting Toolbox has been used to fit eqn(12) to the experimental true stress – true strain data. In the fitting-procedure the following parameters were kept constant; $G = 80\,000$ MPa, $b = 2.5 \cdot 10^{-10}$ m, $m = 2$ and $\alpha =$

0.88, see above. The parameters σ_{i0} , Ω , s_0 and ρ_0 are allowed to vary freely, within physically reasonable limits, until the best fit is obtained. An example of the result obtained from the fitting procedure is presented in Fig 1.

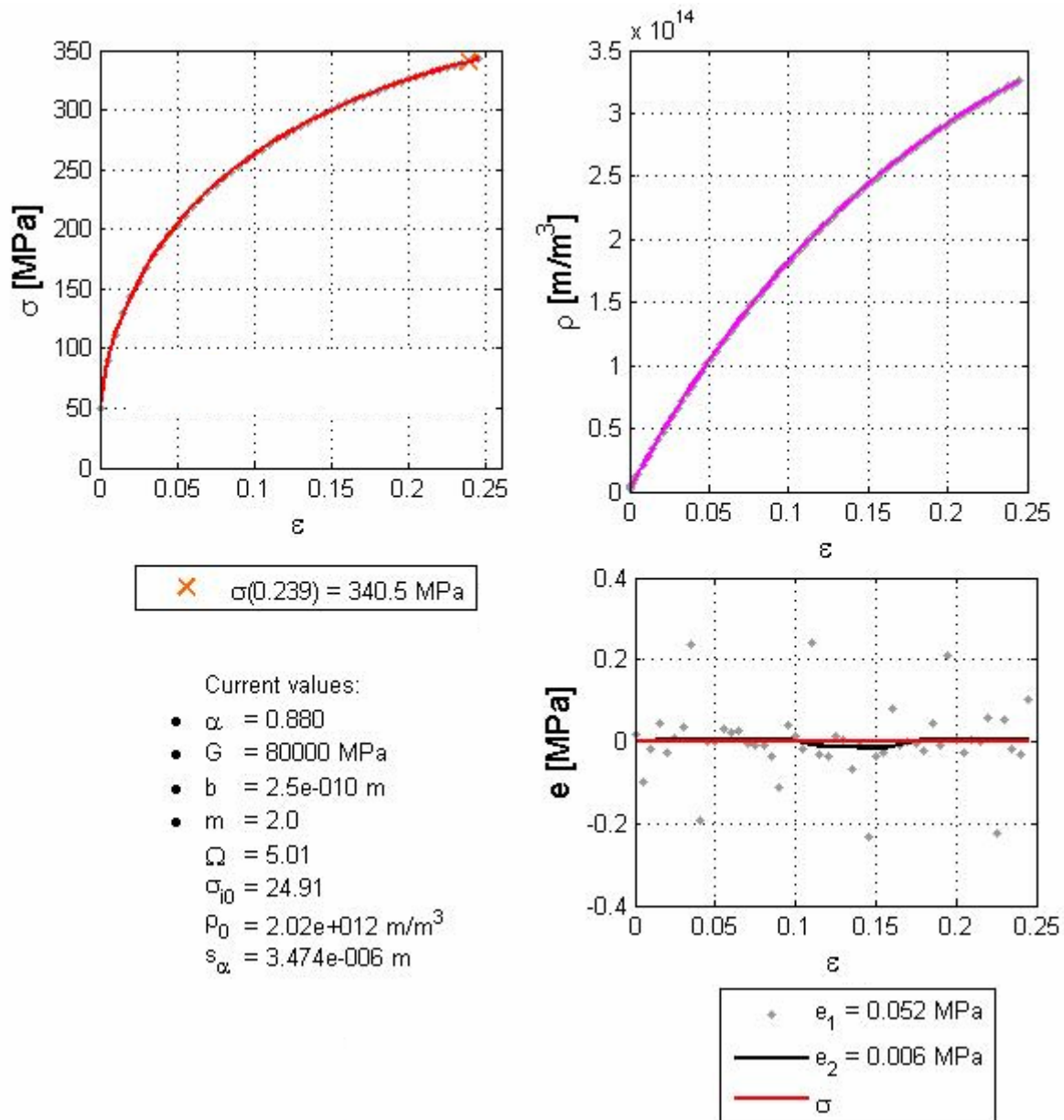


Fig. 3

The fitting of eqn(12) to experimental uniaxial true stress – strain data recorded from a Ti-stabilised ferritic steel (for details, see text).

In the figure – upper left - we can see that the fitted stress – strain curve (red) covers the experimental data. The red cross indicates the strain to necking and the corresponding flow stress. The obtained parameter values are depicted in the table below the stress – strain curve. The corresponding strain dependence of the total dislocation density is shown to the upper right.

To the lower right the scattering of the experimental data points – black dots - around the calculated stress strain – curve is seen. The maximum error of fit is less than 0.6 MPa while the running minimum error is approximated to be 0.006 MPa.

The mean free path, s , of mobile dislocations

It is reasonable to believe that the mean free path of mobile dislocations is intimately correlated to the mean diameter of the dislocation cells. This was observed in-situ in a 1 MV electron microscope and the results in Fig. 4 point in the same direction. In this case the Ti-stabilised steel has been tensile tested at various temperatures in the range R.T. to 600C and eqns.(3) and (12) were fitted to the corresponding stress – strain curves. The fixed parameter values of α , G , b , m were the same as in Fig 3 above with the exception that the temperature dependence of G was taken into account. This means that the parameters σ_{i0} , s , Ω and ρ_0 were allowed to vary freely until the best fit was obtained. As can be seen in Fig. 4 the experimentally measured cell diameters agree well with the calculated s_0 values based on the model.

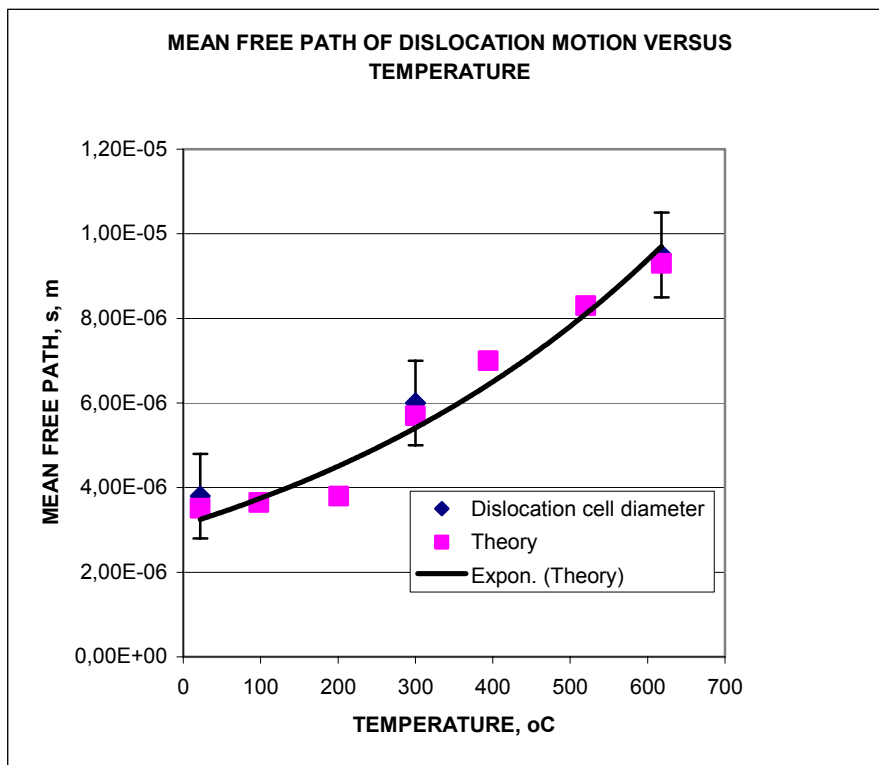


Fig 4. Mean free path of dislocation motion and dislocation cell diameter versus temperature in a Ti – stabilised steel

The temperature dependence of the remobilisation factor Ω for the presently investigated Ti – stabilised steel is presented in Fig. 6.

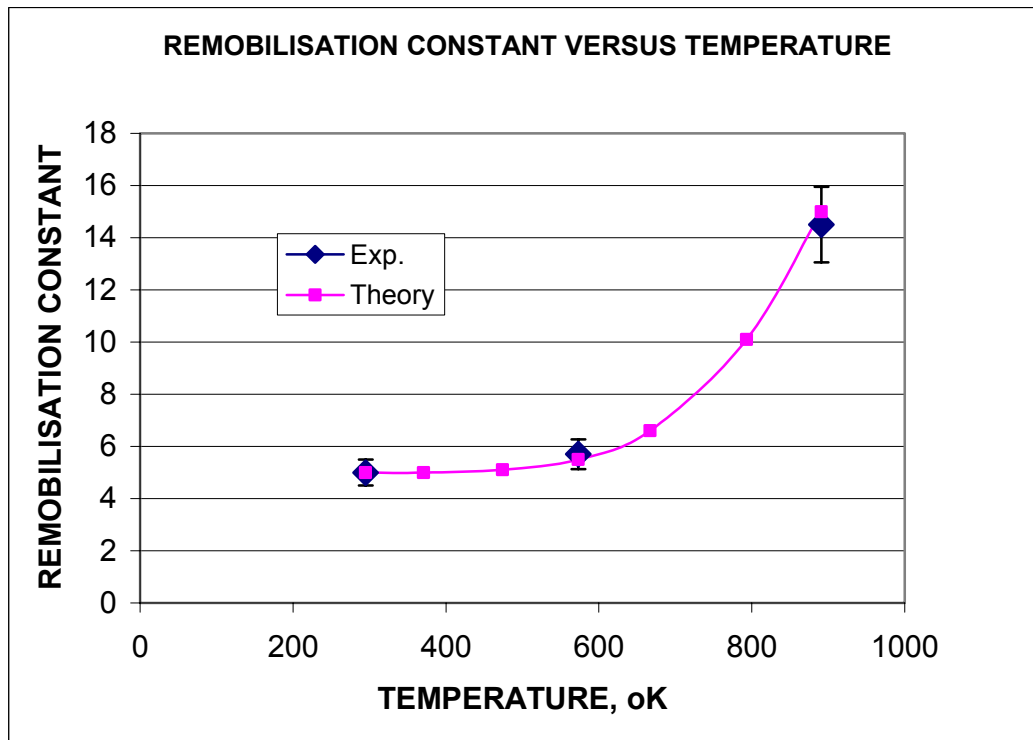


Fig. 6. The temperature dependence of Ω in the investigated Ti – stabilised steel. The theoretical points are calculated according to a theory presented in PAPER 3.

It is reasonable to assume, according to Fig. 6 that Ω consists of an athermal component, Ω_0 , and a thermal component $\Omega(\dot{\epsilon}, T)$, i.e.

$$\Omega = \Omega_0 + \Omega(\dot{\epsilon}, T) \quad (15)$$

In the present case it seems that Ω_0 is approximately equal to 5 and that Ω presumably increases with increasing temperature according to some type of thermally activated process. A similar behaviour can be noted for the temperature dependence of the mean free path s , see Fig. 4.

A simple theory for Ω and its temperature and strain rate dependences will be presented in PAPER 3.

SUMMARY (17)

A dislocation model for bcc iron, based on the following assumptions, is proposed:

- the mobile dislocation density is small and strain independent
- the increase in dislocation density with increasing strain is controlled by the creation, the immobilisation and the remobilisation of dislocations
- the mean free path of dislocation motion is strain independent
- the Taylor equation describes the relationship between flow stress and total dislocation density

The following expression for the stress – strain dependence of bcc iron is derived:

$$\sigma = \sigma_{i0} + \alpha \cdot G \cdot b \cdot \left(\frac{m}{\Omega \cdot b \cdot s_0} \cdot (1 - e^{-\Omega \cdot \varepsilon}) + \rho_0 \cdot e^{-\Omega \cdot \varepsilon} \right)^{\frac{1}{2}} \quad (16)$$

where:

σ = true stress

ε = true strain

σ_{i0} = friction stress

α = dislocation strengthening constant

G = shear modulus

b = value of the Burgers vector

m = Taylor constant (~ 2 for bcc materials)

Ω = dislocation remobilisation constant

S_0 = dislocation mean free path (strain independent)

ρ_0 = “grown-in” dislocation density

A specially designed program based on the MATLAB Curve Fitting Toolbox has been used to fit eqn(12) to the experimental true stress – true strain data. In the fitting-procedure the following parameters were kept constant; $G = 80\,000$ MPa, $b = 2.5 \cdot 10^{-10}$ m, $m = 2$ and $\alpha = 0.88$, see above.

The parameters σ_{i0} , Ω , s_a are allowed to vary freely, within physically reasonable limits, until the best fit is obtained. In Ti – stabilised iron or H_2 – treated iron where most of the carbon and nitrogen content has been eliminated from the matrix the following values are normally obtained:

$\sigma_{i0} = 10 - 40$ MPa (depending on grain size)

$\Omega = 4 - 6$

$S_0 = 3 - 5$ μm

REFERENCES

1. G.I. Taylor, Proc. Roy. Soc. A145, 362(1934)
2. W. Bollman, Phys. Rev. 103, 1588 (1956)
3. P.B. Hirsch, R.W. Harve, M.J. Whelan. Phil. Mag. 1, 677(1956)
4. D.A. Korzekwa, D.K. Matlock,, G. Krauss, Met. Trans. A 15A, 1221(1984)
5. U. Liedl, S. Traint, E.A. Werner, Comp.Mat.Sci. 25, 122(2002)
6. P. Ludwik, in: Elemente der Technologischen Mechanik, Julius Springer, Berlin, 32(1909)
7. J.H. Hollomon, Trans AIME, 162, 268(1945)
8. W.B. Morrison, Met. Trans. 2,331(1971)
9. Y. Bergström, Mater. Sci. Eng. 5(193)1969/70
10. M.F. Ashby, The deformation of plastically non-homogeneous alloys, Applied Science Publishers LTD, London, 1971
11. U.F. Kocks, J. Eng. Mater. Technolo., 98, (1976)72

12. W.D. Nix, J.C. Gibeling and K.P. Fuchs, in *Mechanical Testing for Deformation Model Development*, ASTM, STP 765, R.W. Rhode and J.C. Swearingen eds., ASTM 301(1982)
13. F.P. Prinz and A.S. Argon, *Acta Metall.*, 32(1984)1021
14. E. Nes, *Prog. Materials Sci.*, 41(1998)129
15. Y. Estrin, L.S. Toth, A. Molinari and Y. Brechet, *Acta mater.*, 46(1998)5509
16. J.T. Michalak, *Acta Met.*, 13(1965)213
17. Y. Bergström, *Reviews on powder metallurgy and physical ceramics*, vol 2. No. 2&3, 1983.