A DISLOCATION MODEL FOR THE PLASTIC DEFORMATION OF FCC METALS – AN ANALYSIS OF PURE COPPER AND AUSTENITIC STEEL

Background

In the bcc model for work hardening in single phase materials, see (6), it is assumed that the plastic deformation behaviour is controlled by three processes, namely the creation, the immobilisation and the remobilisation of dislocations. *It is also assumed, as a first approximation, that the mean free path, s, of dislocation motion is strain independent*. Based on these assumptions the following expression for the increase of the total dislocation density, ρ, with strain, ε, is derived(1):

$$\frac{d\rho}{d\varepsilon} = \frac{m}{b \cdot s_0} - \Omega \cdot \rho \qquad (1)$$

where m is the Taylor factor, b is the nominal value of the Burgers vector, s_0 is the strain independent mean free path of dislocation motion and Ω is the dislocation remobilisation constant.

The following equation, proposed by Taylor (2), is used to describe the strain dependence of the true stress, σ(ε)

$$\sigma(\varepsilon) = \sigma_{i0} + \alpha \cdot G \cdot b \cdot \sqrt{\rho(\varepsilon)} \qquad (2)$$

where σ_{i0} is the friction stress, α is a dislocation strengthening constant, G is the shear modulus and b is the nominal value of the Burgers vector.

Integration of eqn(1) yields

$$\rho(\varepsilon) = \frac{m}{b \cdot s_0}(1 - e^{-\Omega \cdot \varepsilon}) + \rho_0 \cdot e^{-\Omega \cdot \varepsilon} \qquad (3)$$

where ρ_0 is the "grown-in" dislocation density. By combining eqn(2) and (3) we obtain the following expression for the stress – strain behaviour of bcc metals like iron (1,3).

$$\sigma(\varepsilon) = \sigma_{i0} + \alpha \cdot G \cdot b \cdot \left[\frac{m}{b \cdot s_0}(1 - e^{-\Omega \cdot \varepsilon}) + \rho_0 \cdot e^{-\Omega \cdot \varepsilon} \right]^{1/2} \qquad (4)$$

For many fcc metals the stacking fault energy, γ, is low, at least in comparison with α-iron, and experiments have shown that $\gamma \approx 45$ erg/cm^2 for copper, ref, $\gamma \approx 20$ erg/cm^2 for austenitic stainless steel, ref, and $\gamma \approx 5$erg/cm^2 for certain copper-alloys, (3). This implies that the dislocations are strongly dissociated and since also the number of slip systems is less than in bcc crystals the probability of cross slip is comparatively small. Hence there are strong reasons to believe that dislocation pile-ups are easily formed and as a result of this the mean free path, s, is supposed to decrease with increasing strain – as the number of dislocations in the pile-up increases, the distance between the dislocation generator and the last dislocation in the pile-up decreases. Such a strain dependence of s implies that the bcc approach, see

above, cannot be used and that an expression for the strain dependence of s in fcc metals must be derived.

Theory for fcc single phase metals

Making the assumption that the mean free path s(ε) approaches on deformation, some equilibrium value, s_0 – defined by the final dislocation cell diameter for example – at a rate determined by the difference $(s - s_0)$, then (3)

$$\frac{ds}{d\varepsilon} = -k(s - s_0) \tag{5}$$

where k is a rate constant.

After integration of eqn(5) the following expression is obtained

$$s(\varepsilon) = s_0 + (s_1 - s_0) \cdot e^{-k \cdot \varepsilon} \tag{6}$$

where s_1 is the initial mean free path of dislocation motion.
(s_0 is presumably intimately related to the "grown-in" dislocation density ρ_0, see (6), PAPER 4).

Now, by combining eqn(1) and (6) the following expression for the strain dependence of ρ in single phase fcc metals is obtained (3)

$$\frac{d\rho}{d\varepsilon} = \frac{m}{b \cdot \left[s_0 + (s_1 - s_0) \cdot e^{-k \cdot \varepsilon} \right]} - \Omega \cdot \rho \tag{7}$$

For the special case Ω = 0, this equation can be integrated analytically to give the strain dependence of ρ (3)

$$\rho(\varepsilon) = \rho_0 + \frac{m}{b \cdot s_0} \cdot \varepsilon + \frac{m}{b \cdot s_0} \cdot \ln \left[\frac{s_0 + (s_1 - s_0) \cdot e^{-k \cdot \varepsilon}}{s_1} \right] \tag{8}$$

where ρ_0 is the "grown-in" dislocation density.

A combination of eqns(8) and (2) results in the following expression for the stress – strain dependence of single-phase fcc-metals in the case of zero remobilisation.

$$\sigma = \sigma_{i0} + \alpha \cdot G \cdot b \cdot \left[\rho_0 + \frac{m}{b \cdot s_0} \cdot \varepsilon + \frac{m}{b \cdot s_0} \cdot \frac{1}{k} \cdot \ln \frac{s_0 + (s_1 - s_0) \cdot e^{-k \cdot \varepsilon}}{s_1} \right]^{1/2} \tag{9}$$

It is reasonable to believe that eqn(9) holds for fcc materials with an extremely low stacking fault energy or at extremely low temperatures in which cases the probability of thermally activated dislocation remobilisation is presumably negligible. Austenitic steels deformed at room temperature or below is such an example. For high stacking fault energy fcc metals

tested at high temperatures the rate constant, k, is large and the bcc approach may therefore be used in such cases.

In all other cases, however, eqn(7) together with eqn(2) must be applied.

Since eqn(7) can not be solved analytically, numerical methods must be applied. The routines for fitting the fcc-theory to experimental data are explained in detail below.

Pure copper – an analysis

Experiments

The tensile tests were carried out on 99.99% polycrystalline copper (grain size 30 μm) at a strain rate of 7.4 x 10^{-4} s^{-1} and at various temperatures in the range 298K to 764 K. Experimentally recorded true stress-true strain curves at the different temperatures are presented in Fig. 1. It is obvious from this figure that an increase in testing temperature gives rise to a decrease in the rate of work hardening while the friction stress seems to be almost independent of temperature. It can also be seen that the strain to necking decreases with increasing temperature.

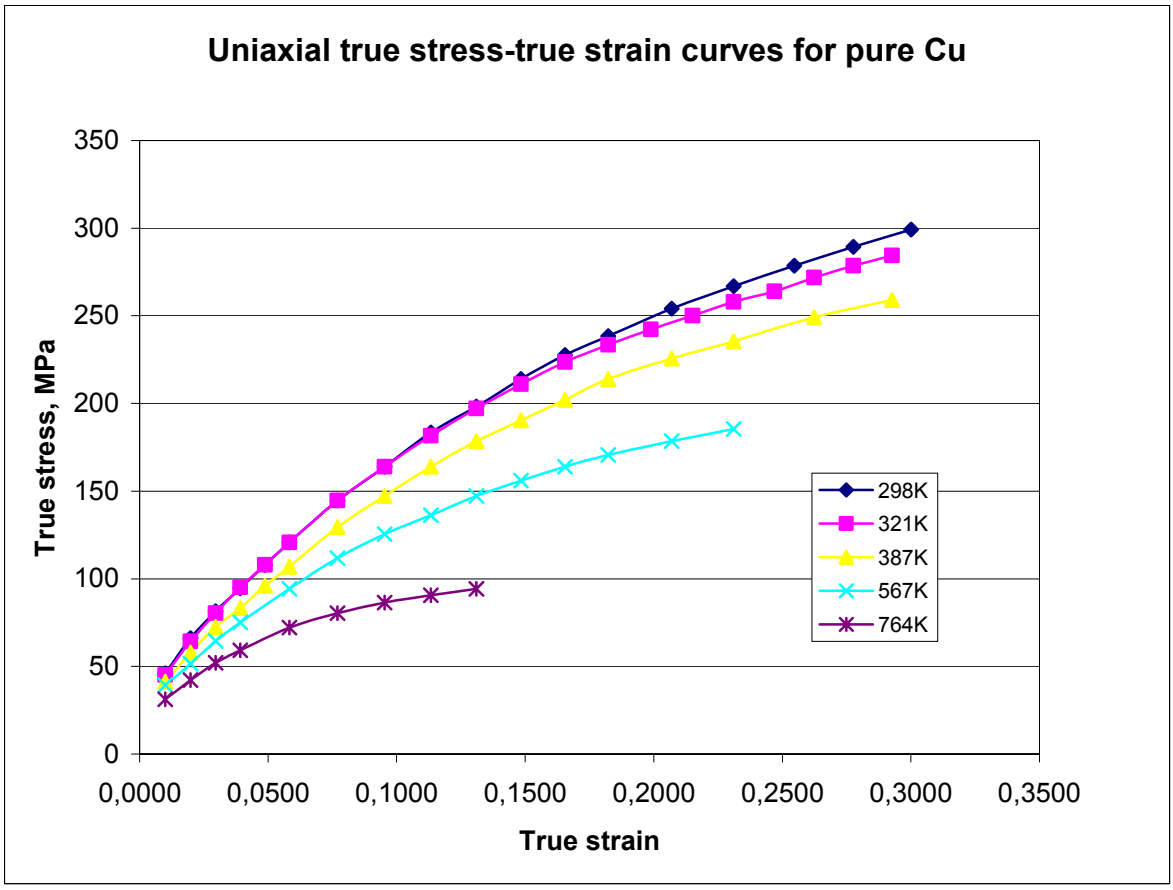

Fig. 1 Experimental true stress-true strain curves for pure copper uniaxially strained at various temperatures in the range 298K – 764K (3)

No dislocation density measurements have been carried out in this investigation since acceptable data are available in the literature which allows an estimate of the dislocation strengthening parameter α , see eqn(2).(4,5).

The latter results for pure copper at room temperature are plotted in Fig. 2 and from the slope of the fitted line the α-value is calculated to be ~1. Furthermore, the best straight line through the experimental σ - √ρ data passes near the origin indicating a near-zero friction stress.

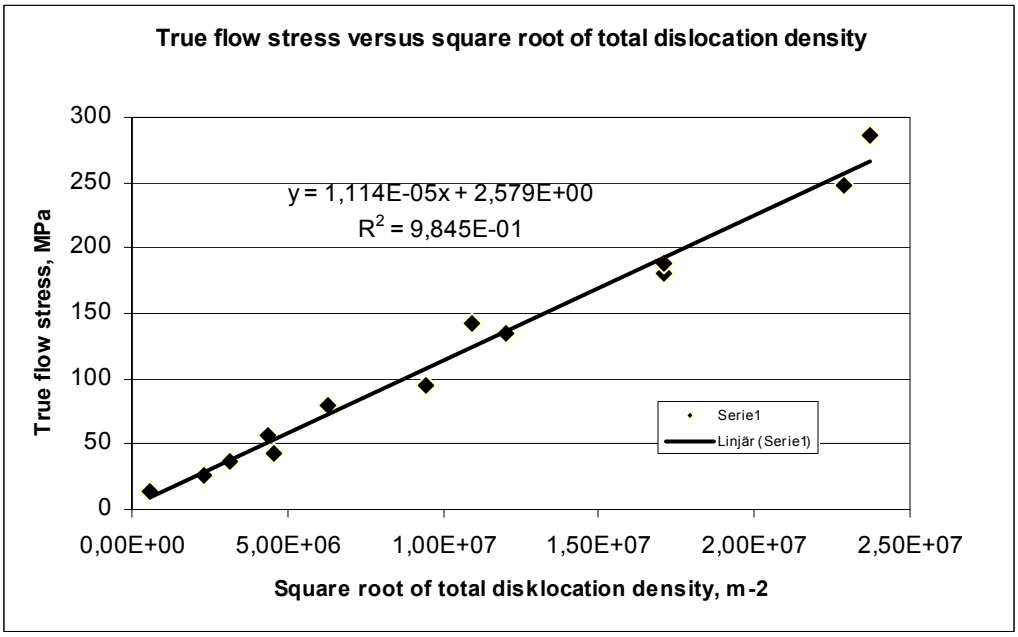

Fig. 2 Evaluation of the parameter α at RT for pure copper. The slope $1.114 \cdot 10^{-5}$ MNm^{-1} results in an α-value of ~1.

Fitting of eqns(2) and (7) to experimental σ-ε curves

A special Matlab subroutine, based on the Matlab Curve Fitting Toolbox, was designed for fitting the fcc-model to the experimental stress-strain curves. In the fitting procedure the following parameters were kept constant: α=1, b=$2.55 \cdot 10^{-10}$ m, m=3.1 and $\rho_0=2 \cdot 10^{12}$ m^{-2}. The temperature dependence of the shear modulus G was taken into account in the fitting process.

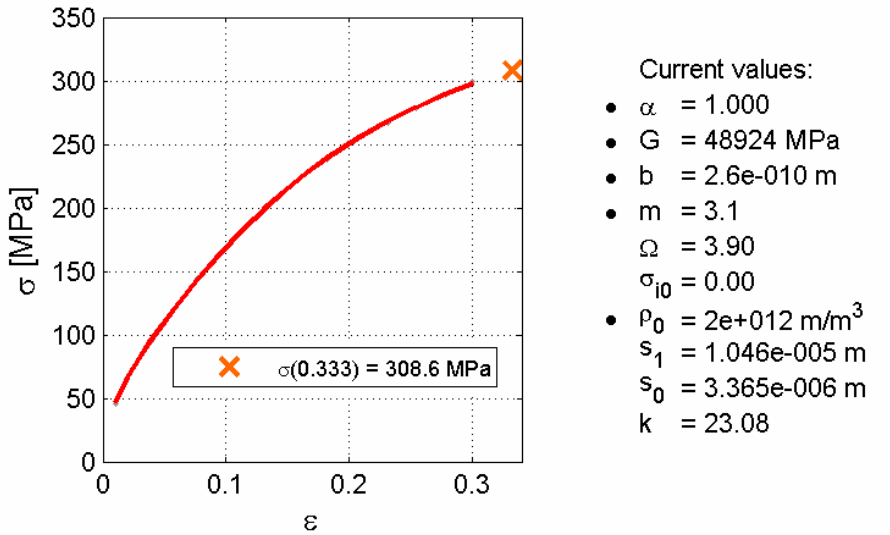

Fig. 3 Fitting of the fcc model to pure copper tensile test data. The experimental points are covered by the theoretical red curve. (Testing temperature RT, strain rate $7.4 \cdot 10^{-4}$ s^{-1}) about 20% of straining.

The parameters Ω, σ_{i0}, s_1, s_0 and k were allowed to vary freely until the best fit was achieved. The result obtained by fitting the model to a stress-strain curve recorded at room temperature is presented in Fig. 3. The strain dependence of the dislocation mean free path, s, is shown in Fig. 4 and it is observed that s decreases from a value of approximately 10 μm to 3.4 μm after ca 20% of strain. This decrease in s gives rise to the typical "s-shaped" $\rho(\varepsilon)$-behaviour of low stacking fault energy materials like copper, see Fig. 5. The experimental ρ-ε points inserted in the figure are taken from TEM-studies presented in the literature (4,5).

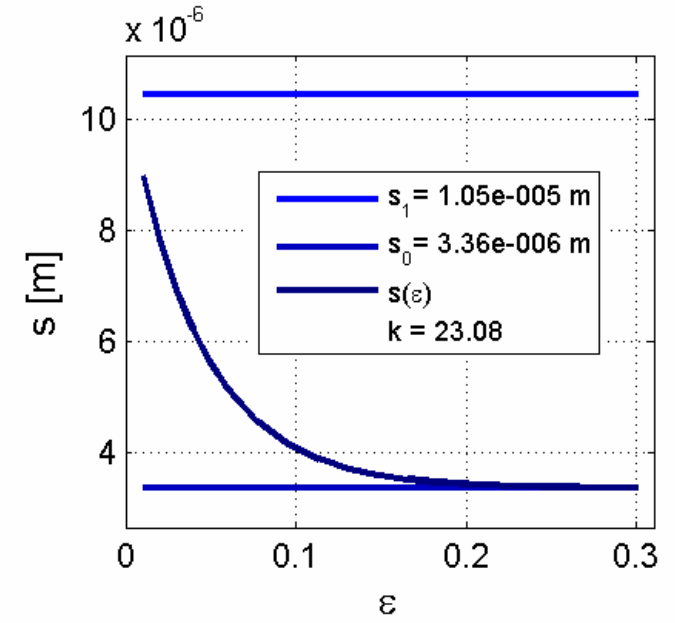

Fig. 4 Strain dependence of the mean free path of dislocation motion, s, in pure Cu tested at RT and at a strain rate of $7.4 \cdot 10^{-4}\ s^{-1}$.

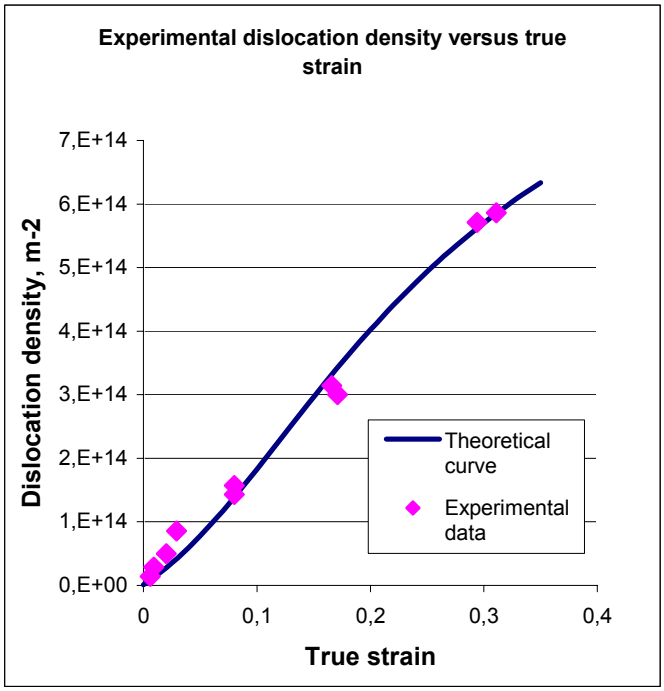

Fig. 5 Strain dependence of total dislocation density in Cu at RT according to theory and experiments(4,5). ($\dot{\varepsilon} = 7.4 \cdot 10^{-4}\ s^{-1}$)

The temperature dependence of the dislocation remobilisation parameter, Ω, is presented in Fig. 6 and it is obvious that Ω is strongly sensitive to variations in temperature.
In a previous paper (6) it has been demonstrated that Ω may be written

$$\Omega = \Omega_0 + \Omega(T, \dot{\varepsilon}) \qquad (10)$$

where Ω_0 is the athermal part and $\Omega(T, \dot{\varepsilon})$ the thermal part varying with temperature, T, and strain rate, $\dot{\varepsilon}$. An analysis of Fig. 6 indicates that $\Omega_0 \sim 3.9$.

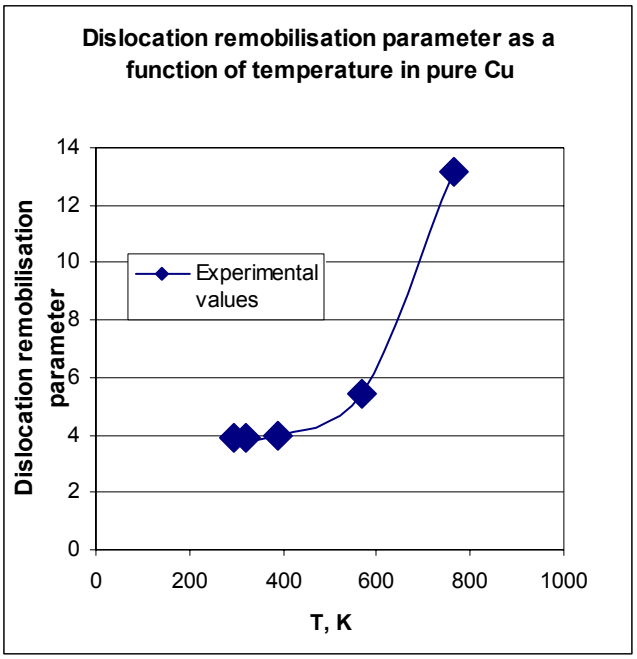

Fig. 6 Temperature dependence of the remobilisation parameter, Ω, in Cu ($\dot{\varepsilon} = 7.4 \cdot 10^{-4}\ s^{-1}$)

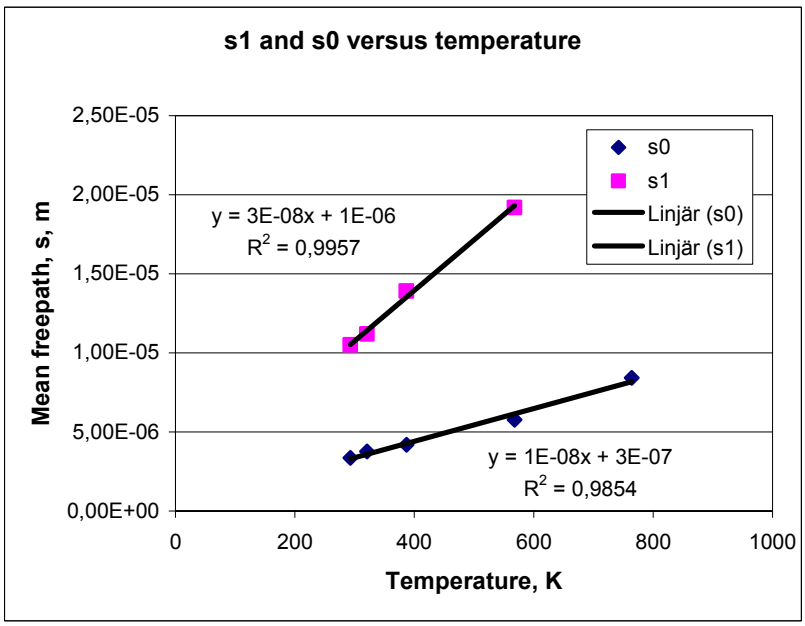

Fig. 7 The temperature dependences of s_1 and s_0.

The temperature dependences of s_1 and s_0 are presented in Fig. 7 and in the investigated temperature interval it seems that both these parameters vary linearly with T. The slope of the s_1-T graph is three times larger that of the s_0-graph indicating that s_1 is more T-sensitive than s_0. At 0K s_1~1μm while s_0~0.3μm. At the highest temperature, 764K, the bcc-model was used in the fit and therefore no s_1-value was recorded for this temperature.

The temperature and strain-rate dependences of pure Cu

Theory

It is demonstrated in (6)-Paper 1 that the dislocation remobilisation factor $\Omega(T,\dot{\varepsilon})$ can be written

$$\Omega(T,\dot{\varepsilon}) = K_1 \cdot D_0^{\frac{1}{3}} \cdot e^{-\frac{Q_m}{3 \cdot R \cdot T}} \cdot \dot{\varepsilon}^{-\frac{1}{3}} \qquad (11)$$

where K_1 is constant and D_0 and Qm are defined by vacancy migration according to the following expression for the diffusion constant D

$$D = D_0 \cdot e^{-\frac{Q_m}{R \cdot T}} \qquad (12)$$

where D_0 is a constant, Q_m, is the vacancy migration energy and R and T have their usual meaning. In eqn(11) it is assumed that a high enough concentration of vacancies is generated by the plastic deformation process and that therefore the thermally activated vacancy generation may be neglected.

By taking the logarithm of the expression in eqn(11) we obtain

$$\ln\left[\Omega(T,\dot{\varepsilon})\right] = \ln(K_1 \cdot D_0^{\frac{1}{3}}) - \frac{Q_m}{3 \cdot R \cdot T} - \frac{1}{3} \cdot \ln(\dot{\varepsilon}) \qquad (13)$$

According to this equation it holds that the activation energy, Q_m, for vacancy migration can be calculated from the slope of a $\ln(\Omega(T,\dot{\varepsilon}))$-1/T plot.

Estimation of the parameter values K_1, K_2, D_0 and Q_m in pure Cu

We will start by calculating the values of Q_m and D_0. For this purpose we will proceed from the values in Table 1 where testing temperature T (K), inverted testing temperature, 1/T, and the calculated values of Ω, Ω_0, $\Omega(T,\dot{\varepsilon})$ and $\ln(\Omega(T,\dot{\varepsilon}))$ are presented.

Table 1: Values used to calculate Q_m and D_0 for copper

T (K)	1/T	Ω	Ω_0	$\Omega(T,\dot{\varepsilon})$	$\ln(\Omega(T,\dot{\varepsilon}))$
293	0.003413	3.9	~3.9	0	-
321	0.003115	3.9	~3.9	0	-
387	0.002584	3.95	~3.9	0.05	-2.99573
568	0.001761	5.44	~3.9	1.54	0.43
764	0.001309	13.18	~3.9	9.28	2,227

In Fig.7 $\ln(\Omega(T,\dot{\varepsilon}))$ is plotted versus 1/T and the slope of the plot is approximately equal to -4104,7. According to eqn(13) it therefore holds that

$$-\frac{Q_m}{3\cdot R} = -\,4104{,}7 \qquad (14)$$

Since R=2 we have that Q_m~24630 cal/mole. An average value of D_0, based on calculations from the different test temperatures, is estimated to be ~0.85 cm^2/mole.

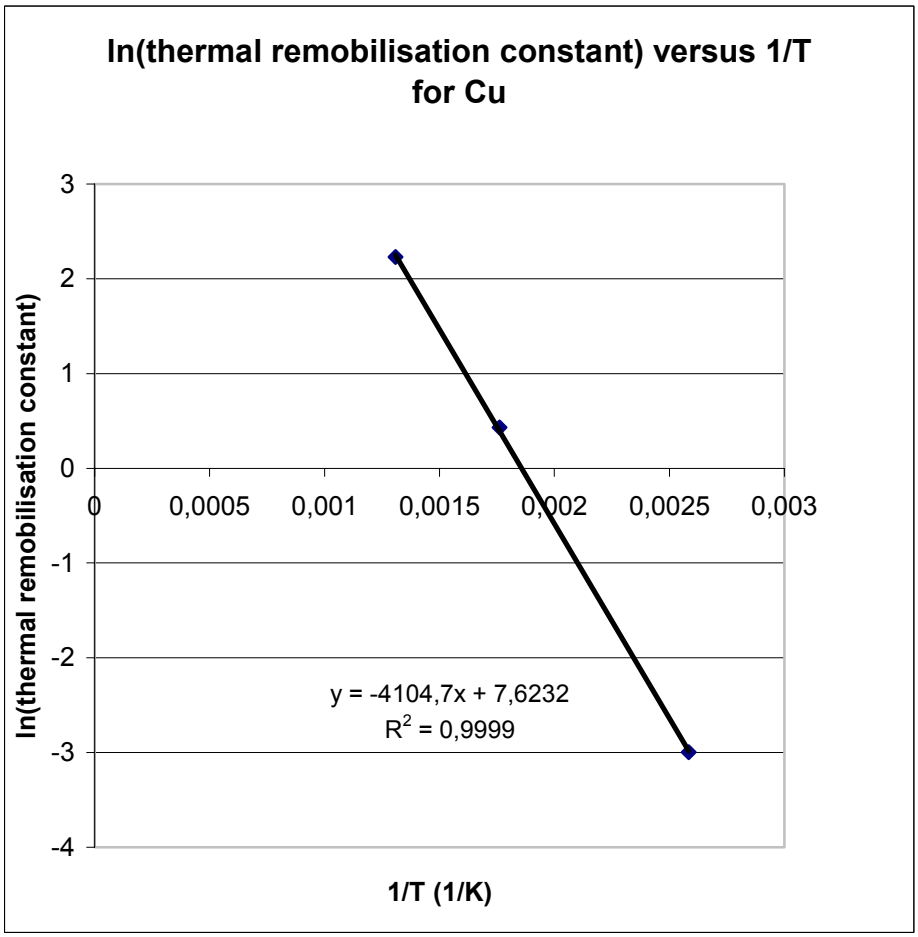

Fig. 7 Estimation of activation energy, Q_m, for vacancy migration in pure Cu

The diffusion constant D_m for vacancy migration in copper may therefore, according to the present investigation, be written

$$D_m = 0.85\cdot e^{-\frac{24630}{R\cdot T}} \ \text{cm}^2/\text{s}$$

where Q_m=24630 cal/mole. This is in good agreement with tabulated experimental data for vacancy diffusion in copper. It also holds according to this analysis that K_1~180 for copper.

Stainless steel – an analysis

It was mentioned above that austenitic steels usually have a low stacking fault energies and hence exhibit small rates of dislocation remobilisation. Below, we will present and discuss the stress-strain behaviour of a stainless steel exhibiting a zero dislocation remobilisation behaviour, that is $\Omega = 0$, see eqn(9).

Experiments

An austenitic stainless steel, AS, with the chemical composition presented in Table 2, and a grain diameter of 37 μm, is the next material to be analysed. Tensile testing is carried out at room temperature and at a strain rate of 0.001 s^{-1}.

Table 2: Chemical composition, wt%

C	Si	Mn	Cr	Ni	Mo	P	S	N	Al
0.017	0.39	1.72	17.5	13,2	2.8	0.11	0.011	0.0043	0.015

The average true stress – true strain curve at room temperature is presented in Fig. 8.

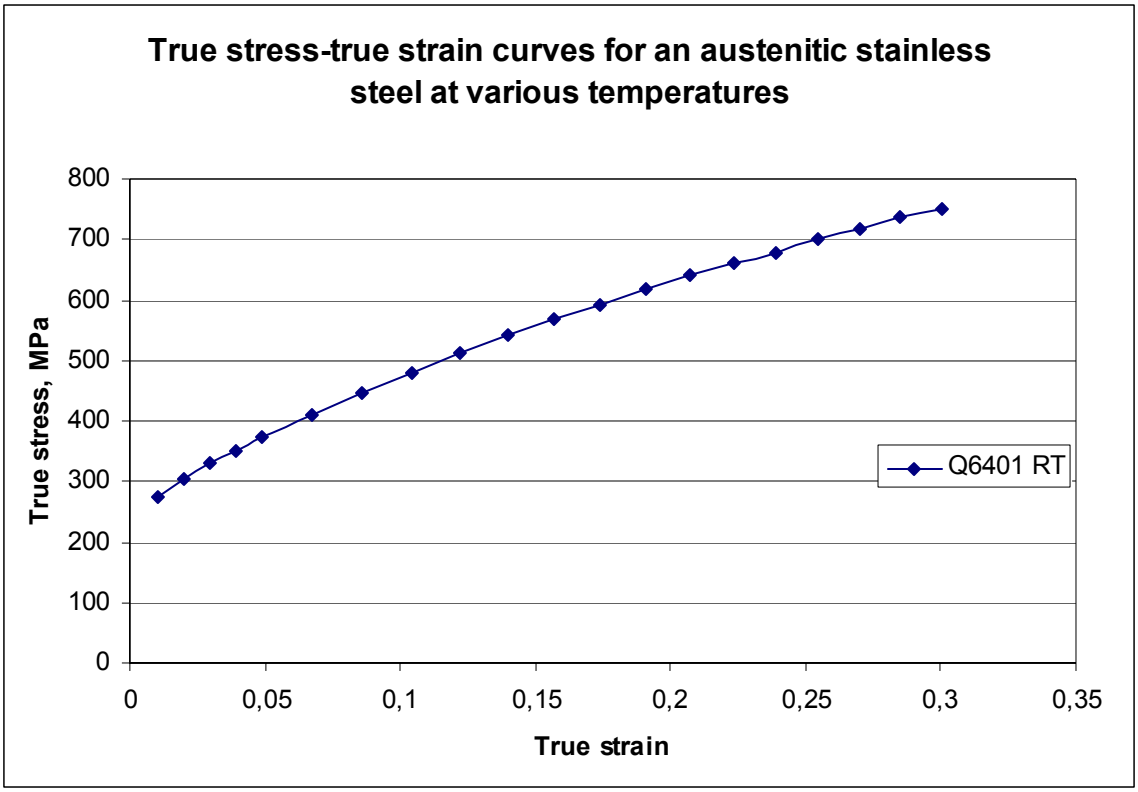

Fig.8. Experimental true stress-true strain curves recorded at RT and at a strain rate of 0.001 s^{-1}.

Fitting of eqns(2) and (7) to experimental σ-ε curves

General

A special Matlab subroutine, based on the Matlab Curve Fitting Toolbox, is designed for fitting the fcc-model to the experimental stress-strain curves at room temperature. In the fitting procedure the following parameters are kept constant: α=0.8, G=74917 MPa, $b=2.55\cdot10^{-10}$ m, m=3.1 and $\rho_0=1\cdot10^{13}$ m^{-2}.

Results from R.T. testing
The parameters Ω, σ_{i0}, s_1, s_0 and k are allowed to vary freely until the best fit is achieved. The result obtained by fitting the model to a stress-strain curve recorded at room temperature is presented in Fig. 9. The theoretical curve is covering the experimental σ-ε points and we can see that the theoretical strain to necking is 0.35 and that the corresponding stress is 803.6 MPa. It should also be noticed that the dislocation remobilisation constant Ω=0 indicating that eqn(9) alternatively can be used to describe the stress-strain curve at RT. (In this case, however, we have used the general procedure in the fitting procedure assuming a non-zero start value for Ω). This gives exactly the same result as if we had used eqn(9).

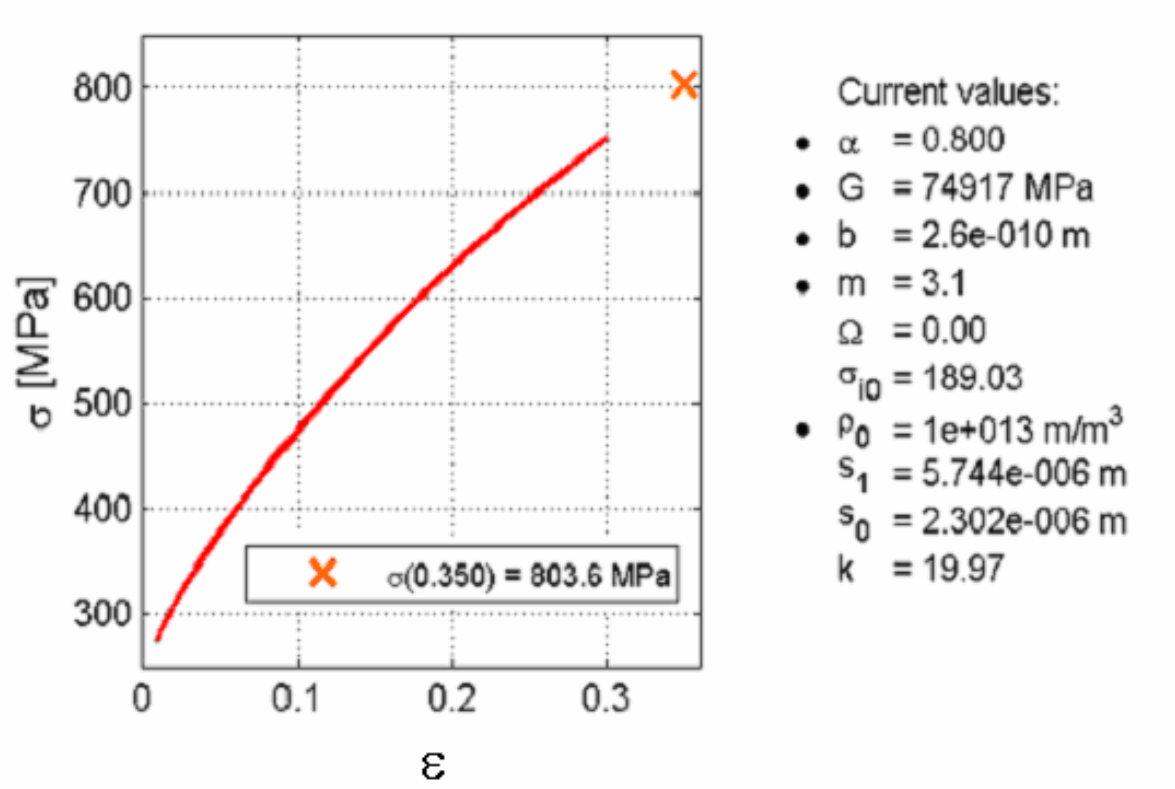

Fig.9. Fitting of the fcc-model to an austenitic stainless steel tested at RT at a strain rate of 0.001 s^{-1}. The current parameter values are presented to the right. The average error is less than 0.075 MPa while the running error is less than 0.03 MPa.

The strain dependence of the dislocation mean free path, s, is shown in Fig. 10 and it is observed that s decreases from a value of approximately 5.7 μm to 2.3 μm after about 20% of straining. The rate constant k for this strain dependence takes a value equal to approximately 20.

The corresponding strain dependence of the total dislocation density ρ is presented in Fig. 11 and it can be seen that the theoretical ρ – ε curve is slightly concave upwards which explains the high ductility of low stacking fault materials as stainless austenitic steels.

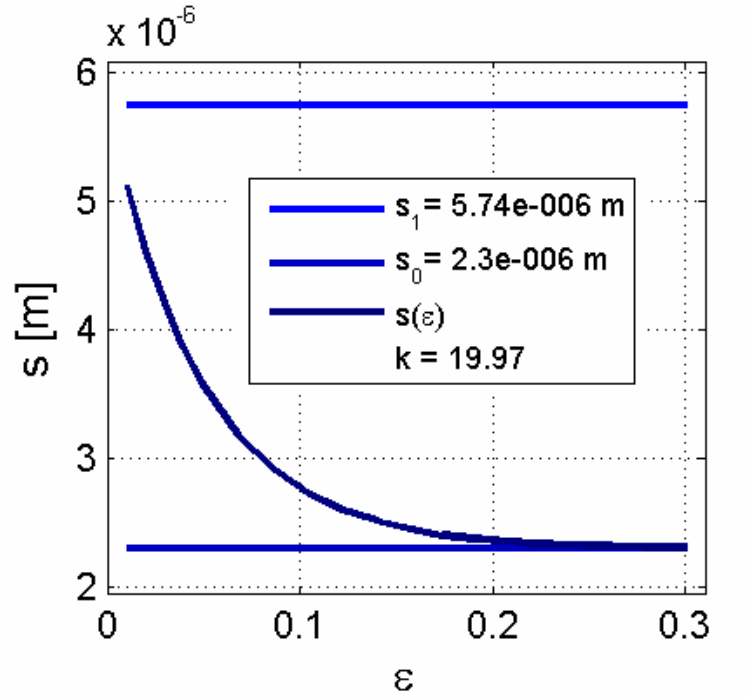

Fig.10. The strain dependence of the mean free path, s, of dislocation motion, corresponding to the σ-ε curve in Fig .9

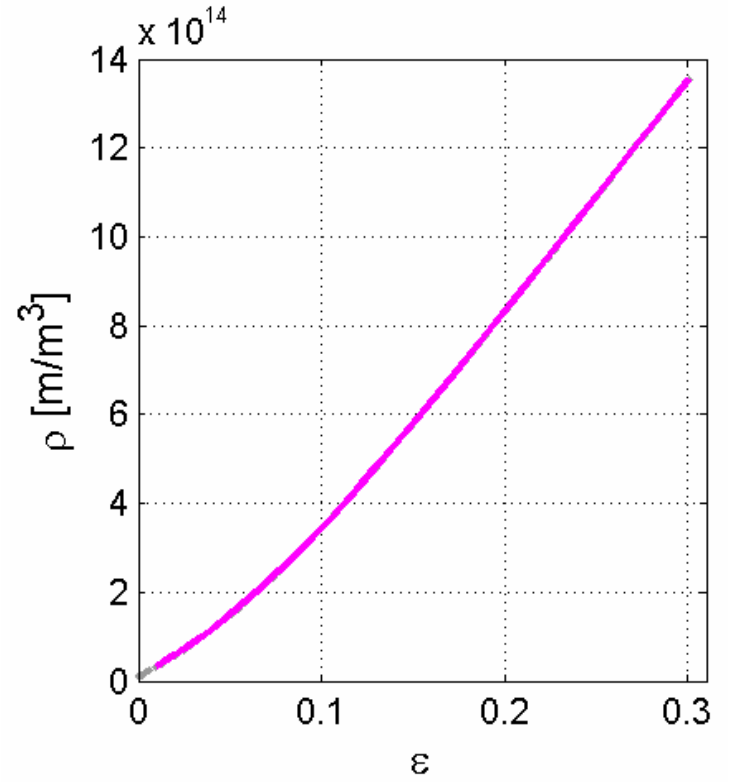

Fig. 11. Theoretically calculated R.T. strain dependence of ρ of the AS-steel

SUMMARY

A dislocation model for fcc metals, based on the following assumptions, is proposed:
- the mobile dislocation density is small and strain independent
- the increase in total dislocation density, ρ(ε), with increasing true strain, ε, is controlled by the creation, the immobilisation and the remobilisation of dislocations according to the following expression

$$\frac{d\rho(\varepsilon)}{d\varepsilon} = \frac{\bar{m}}{b \cdot s(\varepsilon)} - \Omega \cdot \rho(\varepsilon) \qquad \text{(S1)}$$

where Taylors factor $\bar{m}$ ~3.1 for fcc metals, b is the magnitude of Burgers vector, s(ε), is the mean free path of dislocation motion and, Ω, is the dislocation remobilisation constant. The mean free path, s(ε) of dislocation motion varies with strain according to the following expression

$$s(\varepsilon) = s_0 + (s_1 - s_0) \cdot e^{-k \cdot \varepsilon} \qquad \text{(S2)}$$

where s_1 is the initial mean free path of dislocation motion, s_0 the final mean free path and k is a rate constant. This implies that eqn(S1) may be written

$$\frac{d\rho(\varepsilon)}{d\varepsilon} = \frac{m}{b \cdot \left[s_0 + (s_1 - s_0) \cdot e^{-k \cdot \varepsilon} \right]} - \Omega \cdot \rho(\varepsilon) \qquad \text{(S3)}$$

In order to describe the true stress – true strain behaviour of fcc – metals the Tailor equation

$$\sigma(\varepsilon) = \sigma_{i0} + \alpha \cdot G \cdot b \cdot \sqrt{\rho(\varepsilon)} \qquad \text{(S4)}$$

is applied where σ_{i0} is the friction stress and α is a dislocation strengthening factor and G is the shear modulus

In the analysis a specially designed program based on the MATLAB Curve Fitting Toolbox has been used to fit eqn(S3) and eqn(S4) to experimental true stress – true strain data. In the fitting-procedure the parameter values used for respective material are presented in Fig. 3. and Fig. 8. The accuracy of fit is good.

The parameter values σ_{i0}, Ω, s_1, s_0 and k are allowed to vary freely until the best fit is obtained.

In the case of pure cupper the Ω-values obtained at various temperatures in the interval 300K – 765K are used to estimated the diffusion coefficient, D_m, for vacancy migration in cupper. The following result is obtained:

$$D_m = 0.85 \cdot e^{-\frac{24630}{R \cdot T}} \ \text{cm}^2/\text{s}$$

For pure cupper the dislocation remobilisation constant takes the value 3.9 at room temperature. For the stainless steel the corresponding value is estimated to 0. This is a reasonable result remembering that the stacking fault energy is much smaller in the steel.

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