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The Effect of Temperature on Cottrell Atmospheres

By N. LOUAT

Aeronautics Research Laboratory, Melbourne, Australia

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Abstract. The variation with temperature of solute atom density close to (within $\sim 10 \text{ \AA}$) an edge dislocation is examined. The results of this analysis are used to predict the effect of temperature on the yield point. Good agreement is found between theoretical prediction and three apparently dissimilar experimental results.

§ 1. INTRODUCTION

COTTRELL (1948) and his co-workers (1949) have shown that atmospheres of impurity atoms will tend to form around edge-type dislocations. On this basis they have given an explanation for yielding and strain ageing phenomena in iron and other metals. In formulating these theories it has been assumed that the atmosphere density follows the Maxwell-Boltzmann distribution

$$\theta(r, \phi) = \theta_0 \exp U(r, \phi) / kT$$

where θ_0 is the average solute density and $\theta(r, \phi)$ the density at a distance r and direction ϕ from the centre of the dislocation. Using this distribution, and values for $U(r, \phi)$ calculated on the basis that the impurity is carbon, Cottrell (1953) concludes that at equilibrium an atmosphere will be complete when iron is at a temperature less than about 700°K . That is to say, there will be a continuous line of carbon atoms close to the centre and directly beneath the extra half-plane of the edge dislocation.

However, the Maxwell-Boltzmann distribution is not valid close to the dislocation since Cottrell and Bilby (1949) have shown that only one solute atom per atom plane of dislocation should lie within about 10 \AA of the centre. The purpose of the present paper is to take some account of this fact and to examine its consequences.

§ 2. ATMOSPHERE DENSITIES

The treatment adopted here is essentially qualitative and a simplified model is used. It is supposed, considering one atom plane of dislocation, that the region near a dislocation may be divided into a number of discrete sub-regions of various sizes, each characterized by a unique solute atom-dislocation interaction energy, and that at most only one solute atom can occupy each sub-region at any instant. It is assumed further that the interaction between solute atoms in neighbouring sites along the length of the dislocation may be neglected. For an assembly of atom planes under these conditions it may be shown, either by setting up the appropriate partition functions, or more simply by considering

directly the thermally activated equilibrium interchange of atoms between adjoining energy levels, that the resultant distribution is

$$\frac{n_1}{n_0} = \frac{N_1 - n_1}{N_0 - n_0} \exp\left(\frac{U_1 - U_0}{kT}\right)$$

or

$$\frac{\theta_1}{\theta_0} = \frac{1 - \theta_1}{1 - \theta_0} \exp\left(\frac{U_1 - U_0}{kT}\right)$$

where N_1 and N_0 are the number of possible positions for a solute atom of free energy U_1 and U_0 respectively in a dislocation which is N atomic planes in length. $n_1 = N_1\theta_1$ and $n_0 = N_0\theta_0$ are the number of these positions which are occupied. It may be seen that this distribution reduces to the Maxwell-Boltzmann form when θ_1 is small. (Lomer has apparently reached similar conclusions (see Cottrell 1953 b).)

Further, for small θ_0 and with $U_0 = 0$, the density in the lowest energy level (energy V) is given by

$$\theta = \frac{\theta_0 \exp(V/kT)}{1 + \theta_0 \exp(V/kT)}$$

and θ tends to an equilibrium value of 1 when $\theta_0 \exp(V/kT) \rightarrow \infty$ and hence as $T \rightarrow 0$ provided $\Sigma N_i \theta_i \geq N$.

However, the time taken for a state of equilibrium to be reached depends on the rate of diffusion of solute atoms in the parent lattice. Since this rate is usually low at room temperature and below, it follows that atmosphere densities in material used in tests at low temperatures will have been determined by the temperature at which significant diffusion last took place. This fact can be expected to be of practical importance only when $\theta_0 \exp(V/kT) \sim 1$ or less where T is some elevated temperature, and the rate of cooling to the testing temperature is sufficiently rapid to prevent considerable diffusion during cooling. It is doubtful whether these conditions can be satisfied without special precautions. Finally, it should be noted that, under equilibrium conditions, θ_0 is determined by the solid solubility of the solvent and is, in general, a monotonic function of the temperature.

§ 3. THE EFFECT OF TEMPERATURE ON A PREDETERMINED COTTRELL ATMOSPHERE

We shall now investigate how such a predetermined atmosphere would behave with varying temperature, and the consequent effect on the mechanical properties of the metal.

Cottrell (1948) gives, with a change in sign, the interaction energy of a solute atom with an edge dislocation as

$$U(r, \phi) = -\Delta v \frac{\mu b}{3\pi} \frac{1+\nu}{1-\nu} \frac{\sin \phi}{r} = \frac{-A}{r} \sin \phi \quad \dots\dots(1)$$

where Δv is the dilatation produced by the solute atom, μ the shear modulus and ν Poisson's ratio for the lattice; b is the magnitude of the Burgers vector and ϕ the angle between the direction of the Burgers vector and a line joining the solute atom to the centre of the dislocation.

Cottrell and Bilby (1949) estimate for the case of carbon in iron that $A \approx 3 \times 10^{-20}$ dyn cm², but consider that such a value leads to a gross overestimate of the interaction energy when the solute atom is only a few angstrom units from the dislocation centre.

Now, since the expected error in A will be greater when r is small, we must anticipate that the curve $[U(r, \phi), r]$ will be appreciably flatter for small r than would be predicted from equation (1). To take account of this, we shall suppose that there exists a small region contiguous with the dislocation centre in which the interaction energy is sensibly constant. We suggest further that in this region, which in the case of interstitial solute atoms is one of extreme dilatation, the activation energy for movement of solute atoms from one site to another is much less than in the bulk of the crystal.

It is to be expected, then, that the equilibrium distribution of solute atoms within such a region would vary with temperature and that the time taken to reach equilibrium would be small, even at low temperatures. For simplicity we assume that each region (again one atomic distance in length) may be divided into two parts, each portion being characterized by a unique value of the interaction energy. Further, we consider that the portion remote from the dislocation centre contains β times as many solute sites as the central volume. Now, for temperatures at which diffusion is not important in the bulk of the crystal, we may, in accord with our earlier conclusions, consider that the total number of effective solute atoms in a length of dislocation is constant and equal to $N\theta_0 \leq N$ where N is the total number of atom planes in the dislocation under consideration. It may easily be shown then, that the density in the central portion is

$$\alpha = \frac{\theta_0 \exp(W/kT)}{\beta + \exp(W/kT)} \quad \dots\dots(2)$$

where W is the difference in energy of the two levels.

§ 4. EFFECT ON MECHANICAL PROPERTIES

4.1. Dislocation Locking

In accordance with the concept of an 'equipotential' region we cannot expect that equation (1) will be valid for small r . Therefore we cannot, without further examination, consider, as in effect do Cottrell and Bilby, that the restoring force on a dislocation displaced laterally a distance x , parallel to the Burgers vector, from the solute atom is given by

$$\frac{\partial}{\partial x} \frac{A \sin \phi}{r} = \frac{A \sin 2\phi}{r^2}$$

where r is small.

Further, we note from the work of Peierls (1940), Foreman, Jaswon and Wood (1951), and others, that a dislocation in a crystal lattice must be considered to have considerable lateral extent which in the case of the edge dislocation is parallel to its Burgers vector.

As a first step in determining the influence of solute atoms on mechanical properties we have to enquire what effect the presence of solute atoms will have on the dislocation distribution and, since we are mainly interested in condensed atmospheres, we have to consider the results of the presence of numbers of solute atoms arranged in what is approximately a straight line parallel to the dislocation. The shear stresses from such a line of solute atoms centred at a point $-\delta, y$ and lying parallel to the z axis are

$$\sigma_{xy} \simeq \frac{2\mu\Delta v}{\pi a} \frac{(x+\delta)y}{\{(x+\delta)^2 + y^2\}^2}$$

where Δv is the volume change in the crystal caused by the introduction of a solute atom and a is the atomic spacing along the line of the solute atoms. Following Peierls one may write an equation for the dislocation distribution when such shear stresses are present. We have

$$\frac{\mu}{2\pi(1-\nu)} \int_{-\infty}^{\infty} \frac{du}{dx} \frac{d\bar{x}}{\bar{x}-x} = \frac{-b\mu}{2\pi a} \sin\left(\frac{4\pi u}{b}\right) - \frac{2\mu\Delta v}{\pi a} \frac{(x+\delta)y}{\{(x+\delta)^2+y^2\}^2}$$

where u is the displacement of atoms on the surface of the upper half crystal from their normal positions. No solution has as yet been obtained for this equation but it seems reasonable to assume that the effect of the solute atoms when close to the dislocation centre, is to make the Peierls approximation very nearly correct since the maximum values of the two parts of the right-hand side of the above equation are of the same order of magnitude, supposing, as Cottrell and Bilby do, that $y=2\text{\AA}$ and that (for carbon in iron) $\Delta v=7.8 \times 10^{-24} \text{ cm}^3$. Adopting this view and restricting ourselves to those cases where x is small, we shall suppose that the dislocation width $\zeta(y)$, for small y , is some monotonic function of y only and consider (Leibfried and Lucke 1949) that the stresses in the lower half crystal behave as if the dislocation were a line singularity located at $x=0$, $y=\zeta$. We find that equation (1) becomes

$$u(\bar{r}, \bar{\phi}) = \frac{-A[y+\zeta(y)]}{x^2 + [y+\zeta(y)]^2}$$

where \bar{r} , $\bar{\phi}$ refer to the new centre of coordinates $(0, \zeta)$. Also, it may be seen that the elastic energy of the dislocation will increase as ζ decreases and it is found by evaluating the energy contained in two infinite regions bounded by planes normal to the y axis which pass through the points $y=\zeta_1$, and $y=\zeta_2$ in one case and $y=-\zeta_1$, $y=-\zeta_2$ in the other, that the increase in elastic energy per atomic length of dislocation due to a change in ζ from ζ_1 to ζ_2 is given by

$$\mu_{\zeta} \simeq \frac{\mu b^3}{4\pi(1-\nu)} \ln\left(\frac{\zeta_1}{\zeta_2}\right).$$

Substituting values suitable for iron one finds that $\mu_{\zeta} \sim 0.5 \text{ ev}$ per atom plane when $\zeta_1 \sim 1.6\zeta_2$, which seems a not unreasonable change in ζ to be caused by the movement of the solute atom (see Foreman, Jaswon and Wood 1951).

A tendency for the existence of an 'equipotential' region may then be inferred since the solute atom-dislocation interaction energy is the sum of two quantities $U(r, \phi) + \epsilon$ and U_{ζ} whose maxima are of similar magnitude but of opposite sign. Here ϵ represents the energy of other, apparently minor, interactions including electrical interaction (Cottrell, Hunter and Nabarro 1953), and those due to the presence of shear stresses (Crussard 1950).

We shall assume that such an 'equipotential' region does exist and also consider that the restoring force per atom plane is given by

$$\frac{\partial}{\partial x} \left[\frac{A \sin}{\bar{r}} \bar{\phi} + U_{\zeta} \right] \simeq 2Ax(\zeta+y)/\{(\zeta+y)^2+x^2\}$$

with the assumption that ζ does not change significantly with x for small values of x , which seems reasonable.

A result of the same form but differing by a numerical factor is obtained if we consider the interaction between the shear stresses due to a row of solute atoms and a dislocation distributed according to the Peierls relation, assuming

as before that ζ remains constant for the small displacements involved. In the former case the maximum restoring stress with $y=0$, $\zeta=2\text{ \AA}$ and $A=3 \times 10^{-20} \text{ dyn cm}^2$ (see Cottrell and Bilby 1949) is $2 \times 10^{11} \text{ dyn cm}^{-2}$. The second method gives $\sigma_0 \simeq 6 \times 10^{10} \text{ dyn cm}^{-2}$ with the same values for y and ζ . Of these, the latter result is perhaps to be preferred since in this case we have considered the effect of a row of solute atoms which is a better representation of condensed atmosphere than is a single solute atom.

Again, we see that the restraining stresses for the largest values of y , perhaps $2\text{--}3\text{ \AA}$, in the 'equipotential' region are likely to be markedly different from those for the smallest values of y since both y and ζ should increase together in this range. Thus, in accordance with the original approximation of dividing the 'equipotential' region into two discrete interaction energy levels, we may characterize these levels by two widely different values of the maximum restraining stress, e.g. σ_0 for $y=0$, $\zeta=2\text{ \AA}$, and $\sigma_0/16$ for $y=3\text{ \AA}$, $\zeta=5\text{ \AA}$.

Finally, it must be remarked that while little reliance can be placed on the quantitative results of this analysis, the qualitative information should indicate the trends in behaviour to be expected in real crystals and thus provide sufficient grounds to justify investigating the consequences of Cottrell atmospheres having the structure we have envisaged. Thus, in the next section we shall use this model to predict the variation of the yield stress with temperature.

4.2. Temperature Dependence of the Yield Stress

The behaviour under applied shear stresses of great lengths of dislocation may now be determined by finding the maximum expected length which contains solute atoms in an outer, but not in an inner position.

We shall neglect the effect of thermal stresses on 'bound' lengths of dislocation for several reasons. Thus, Cottrell and Bilby in their analysis of this question consider that the thermally supplied activation energy U varies in such a fashion that U/kT is a constant, and that this constant should not exceed about 50. To achieve this value they found it necessary to set the energy per atomic length of dislocation as 1 ev and their factor A as $3 \times 10^{-21} \text{ dyn cm}^{-2}$. But Cottrell's (1953 a) analysis of Dijkstra's experiments indicates that $V \simeq 0.5 \text{ ev}$, which, using the Cottrell-Bilby relation, gives $A = 1.5 \times 10^{-20} \text{ dyn cm}^{-2}$, which is in rather better agreement with their theoretically derived value ($A = 3 \times 10^{-20} \text{ dyn cm}^{-2}$). Again, it is felt that 1 ev per atom plane of dislocation is too small an estimate when it is remembered that μb^2 for iron is 8.75 ev. Thus, if $A = 1.5 \times 10^{-20} \text{ dyn cm}^{-2}$ and the energy per atom plane of dislocation is $x \text{ ev}$, Cottrell and Bilby's equation for U leads to $U/kT = 105\sqrt{x}$.

Further, Cottrell and Bilby in evaluating U take no account of the elastic strain energy associated with the thermal stress in the surrounding crystal which leads to the bending of the dislocation. This energy would appear to be appreciable (Becker 1925) if σ_0 , the stress equivalent of the maximum force exerted by the solute atoms, is as large as $6 \times 10^{10} \text{ dyn cm}^{-2}$, which is the most recent estimate (Cottrell 1953b).

These considerations are not sufficient to invalidate the Cottrell-Bilby mechanism, but it is considered that they raise sufficient doubts to justify separate consideration of another process.

Following Koehler (1952), and assuming random distribution, we have the probability of finding two locking points separated by l/b atoms in a great length

of N atoms is $p = \alpha(1-\alpha)^{1/b}$ where $\alpha = k/N$ is the concentration of locking points and k is the number of them. Hence, the number of lengths between l and $l + \delta l$ is

$$N(l) \delta l = N(1-\alpha)^{1/b} [\ln(1-\alpha)]^2 (1-\alpha) \frac{\delta l}{b}$$

and the number greater than or equal in length to a certain length L is

$$-N(1-\alpha) \ln(1-\alpha)(1-\alpha)^{L/b}.$$

Now, it is suggested that, for a sharp yield point to be observed, there need be only one such length greater than or equal to a certain critical length in a region of the crystal in which the maximum shear stresses occur. It is supposed that this region contains MN atomic lengths of dislocation. Hence it is required that

$$-MN(1-\alpha) \ln(1-\alpha)(1-\alpha)^{L/b} = 1$$

whence

$$\frac{b}{L} \simeq \frac{\ln[1/(1-\alpha)]}{\ln[MN(1-\alpha)]}. \quad \dots\dots(3)$$

Now, under the action of a sufficiently large stress, a length L will tear away from the restraining forces (principally) at its ends. Thereafter, the increased length of free dislocation will continue to grow longer until the entire length of dislocation is free and able to operate as a Frank-Read source. The condition for initial movement is approximately

$$\theta L b \frac{\sigma_0}{n} + 2\sigma_0 b^2 = L \sigma b \quad \dots\dots(4)$$

where σ_0 is the shear stress equivalent to the maximum restraining force, σ the applied shear stress and n a dimensionless constant whose value is the ratio between the maximum restraining forces of the lower and upper levels of the 'equipotential' region. The first term of this equation represents the effect of those atoms which lie in the upper level and which are considered to exert a uniform drag $\theta_0 \sigma_0 / n$ per unit length over the whole 'free' length, where θ_0 is the solute density over the 'free' length.

Equation (4) reduces to

$$\frac{\sigma}{\sigma_0} = \frac{2b}{L} + \frac{\theta_0}{n}$$

and combining this result with equations (2) and (3) we have

$$\frac{\sigma}{\sigma_0} = \left[2 \ln \left\{ \frac{\beta + e^{W/kT}}{\beta + (1-\theta_0)e^{W/kT}} \right\} / \ln[MN(1-\alpha)] \right] + \frac{\theta_0}{n} + \delta$$

where δ is a term, independent of temperature, added to allow for the internal stresses etc. which Cottrell (1950) has shown can cause an increase in the yield point.

§ 5. COMPARISON WITH EXPERIMENT

In view of the number of disposable constants available, it is not surprising that this function can be made to fit, with sufficient accuracy, the experimental observations of McAdam and Mebs (1943). These observations are compared in figure 1, with the equation

$$\sigma = 1.5 \times 10^9 \ln \left\{ \frac{3 + e^{5.90/T}}{3 + e^{-4.6e^{5.90/T}}} \right\} \text{ dyn cm}^{-2}.$$

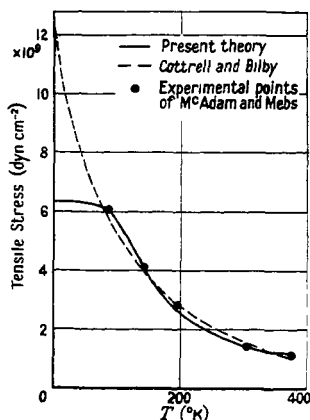


Figure 1.

Here, in order to obtain a solution in a reasonable time, the constant terms and the term in n , which appear to be small, were ignored. In view of this and other approximations made earlier, no particular significance can be attributed to the values obtained for the parameters. However, for the sake of clarity typical values are given in the following table.

T	L	α	β	θ
303	84 <i>b</i>	0.7	3	0.99
144	29 <i>b</i>	0.95	3	0.99

It may be seen that the shape of the predicted curve at temperatures below those employed by McAdam and Mebs differs from that suggested by Cottrell and Bilby (1949). This low temperature prediction is supported to some extent by other work. Thus, our general expression may be fitted, employing the values for β and W found from the data of McAdam and Mebs, to the results obtained by Eldin and Collins (1951) from hot rolled SAE 1020 steel.

The calculated curve and experimental points are shown in figure 2. The equation employed is

$$\sigma = 0.89 \times 10^9 \ln \left\{ \frac{3 + e^{590/T}}{3 + e^{-10} e^{590/T}} \right\} + 3.4 \times 10^9 \text{ dyn cm}^{-2}.$$

It may be seen that the factor $1 - \theta_0$ is considerably smaller here than is the case for the previous result, and it is apparent that, over much of the range of temperature represented, $(1 - \theta_0) \exp(W/kT) \ll \beta$ while at the same time $\exp W/kT \gg \beta$. Under these conditions we should expect that σ/σ_0 would be proportional to $1/T$. It was to illustrate that such a limited linear dependence does occur that the yield stresses were plotted against $1/T$. In addition it may be seen that flattening predicted at low temperatures does in fact occur. However, it must be remembered that Eldin and Collins did not observe a yield point at temperatures below 61°K and the points plotted in this range represent the onset of fracture. This is not a serious objection if one considers, as suggested by Zener (1948), that fracture occurs only after some plastic deformation involving substantial movement of dislocations.

It may be seen by comparing the equations for the two sets of experiments that the term $\ln MN(1-\alpha)$ varies by a factor of about 1.5 and that the constant term is not negligible in the second case. It cannot be claimed that these

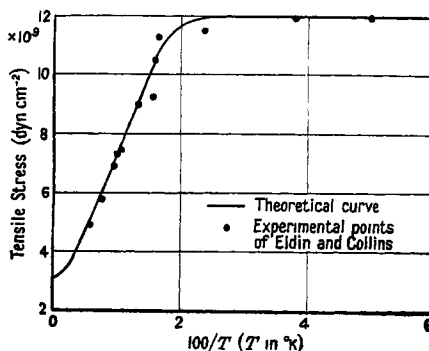


Figure 2.

differences are understood, but it is felt that they are not unreasonable in view of the different nature and history of the materials employed in the two cases.

Finally, one notes that if $\beta \gg \exp(W/kT)$ the general expression reduces to

$$\frac{\sigma}{\sigma_0} = \frac{2\theta_0 \exp(W/kT)}{\beta \ln[MN(1-\alpha)]} + \frac{\theta}{n} + \text{constant.}$$

This expression is to be compared with the results of Rosi and Mathewson (1950) for 99.996% aluminium tested in tension. These workers found that $\sigma \approx 6.1 \times 10^6 \exp(150/T)$ dyn cm⁻² where σ is the stress at which plastic deformation first became appreciable. A similar temperature dependence has been found by Schmid (1931) for the same property in zinc.

It is apparent that, unless β is much greater than the value (~ 3) found for the case of steel, no such exponential dependence on $1/T$ can be expected. But it is possible that β may satisfy the required condition. Thus, in a face-centred cubic or hexagonal-close-packed metal, Cottrell locking will, in the absence of interaction between solute atoms and shear stress fields of the dislocation, be least for screw dislocations and will require the dissociation of complete dislocations as described by Heidenreich and Shockley (1948). In the case of an originally pure screw dislocation, each partial dislocation has a Burgers vector whose edge component has a magnitude b .

Now Cottrell's quantity A is proportional to the product of the Burgers vector and the shear modulus so that, for the case of a screw dislocation in aluminium, A and hence V have only about one-tenth of their values in iron for the same solute dilatation of the lattice. It is likely, therefore, that the magnitude of β will be determined by the size of the region within which diffusion processes can occur easily. β may, on this account, be considerably greater than is the case for carbon atoms in iron.

§ 6. CONCLUSIONS

It has been found that the atmosphere density is characterized by a particular equilibrium value determined by the density of solute and the ambient temperature. In general, when a metal containing solute atoms which interact with dislocations has been cooled to a temperature at which the solute diffuses

slowly, this equilibrium will not be attained. Consequently, those mechanical properties which depend on the atmosphere density will also depend to some extent on the temperature history of the material.

Again, it has been seen that the 'structure' of an atmosphere is temperature-dependent and leads to a relation between the yield strength and the testing temperature.

The predictions of the theory have shown qualitative and to some extent quantitative agreement with three apparently different types of experimental results.

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