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The influence of crystal anisotropy on mechanical behaviour

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Anisotropy of crystal structure leads to complications in mechanical behaviour. Robert Cahn, 50 years ago, made valuable contributions through determination of crystallographic features of plastic deformation in large crystals in polycrystalline α-uranium. This research area has become increasingly linked with the effects of internal and external stresses on many materials in polycrystalline form comprised of grains with anisotropic crystal structure. The extent of irreversibility of deformation when such materials are subjected to thermal cycles leads to the significance of crystallographic textures but major effects on mechanical behaviour are often apparent where grains are randomly aligned without preferred crystal orientation when small external stresses are imposed. The importance of these features, their main characteristics and their analysis are briefly reviewed

1. Introduction

The crystallographic nature of slip and twinning has long been recognised [1]. Extensive knowledge has accumulated firstly through surface observations on single crystals coupled with X-ray determinations of their crystal structure and orientation. For more complex structures such work becomes more difficult, especially in materials subject to solid-state phase transformations when single crystals of widely varying orientations are difficult to grow [2]. The latter situation is typified by studies on α uranium. Only a short time after the crystal structure of this element (Fig. 1) at room temperature was finally agreed upon, Cahn [3, 4] presented impressive results from his studies of its deformation modes. His work, in fact, relied on observations on large grains within polycrystalline samples but his conclusions were substantially supported by studies on single crystal material [5].

A feature of Cahn's work was his noting that extensive slip could be induced by repeated thermal cycling of the large grain material between room temperature and 635°C. This arose through the stresses caused by differential thermal expansion between the adjacent grains. Though this aspect was not central to the work that Cahn was then undertaking, it has subsequently proved to be of major significance. The phenomenon can be linked with earlier surface observations by Boas and Honeycombe on several other thermally cycled materials with anisotropic crystal structures that provided evidence that slip had been induced [6–8].

Through such studies, it has become apparent that crystal anisotropy must be linked to the generation of internal stresses and, in consequence, opened up new areas of concern.

2. Thermally induced stresses

When the thermal expansion of each grain is orientation dependent then a change of temperature must lead to the development of internal stresses in the polycrystalline material if adjacent grains are to remain in contact without any separation. Crystals of cubic symmetry are immune from this situation for, although their atom spacing varies along different non-axial directions, their thermal expansion coefficients are independent of orientation. This can readily be seen because each of the 3 orthogonal axes is identical and so the precise cubic shape is retained as the lattice expands or contracts.

In mathematical terms, the thermal expansion coefficient is defined by a second rank tensor α_{ij} such that the strain ε_{ij} induced by a temperature change ΔT is given by $\varepsilon_{ij} = \alpha_{ij}\Delta T$. It follows [9], for any crystals whose unit cell axes are unequal or non-orthogonal, that their thermal expansion will be orientation dependent.

The extent of the variation of thermal expansion with orientation differs substantially between different materials [6]. This is important in determining the level of internal stress that may be induced. Here, we are also concerned with the values of the elastic moduli that are themselves orientation dependent. Their orientation dependence is of different character from that of the thermal expansion coefficients for they are governed by the strength of directional bonding without geometrical constraint. This implies that even for cubic crystals with 3 equal and orthogonal unit cell axes, their elastic moduli, but not their thermal expansion coefficients, can vary in the intermediate directions. Such polycrystals are thus immune to thermal stresses and so do not come under consideration here. Mathematically, in the general case, the elastic moduli must be defined by

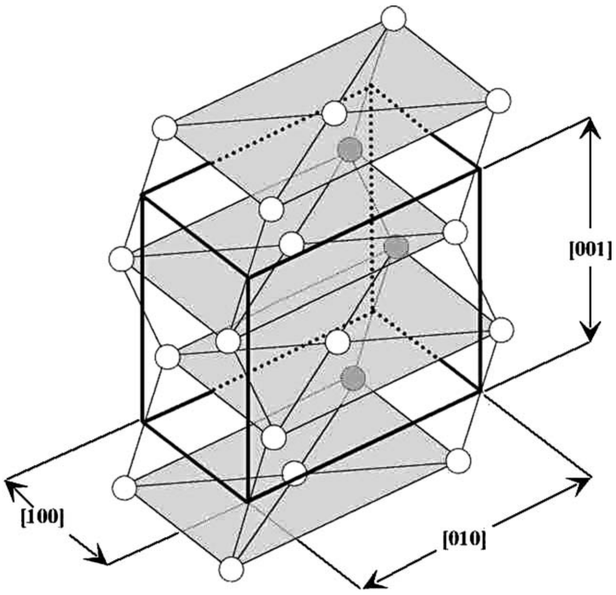

Figure 1 The crystal structure of α-uranium. The unit cell, marked with bold lines, is orthorhombic and the crystallographic directions are indicated.

fourth rank tensors E_{ijkl} such that the generalised elastic stress-strain relationship takes the form $\sigma_{\mathrm{ij}} = E_{\mathrm{ijkl}}\, \varepsilon_{\mathrm{kl}}$. We shall not explore further the detailed significance of these features but it is important to appreciate that, for complete analysis, extensive experimental data that has provided values of these parameters must be taken into account. The full application of such an approach still presents formidable difficulties. The crystallographic dependence of deformation modes and of temperature dependent stress relaxation add further complications.

Nevertheless, it is possible to gain some impression of the magnitude of internal stress generation by taking a value for $\Delta\alpha$ that is some fraction, typically about 0.5, of the difference between the largest and smallest thermal expansion coefficients. An averaged value of Young's modulus E over the temperature range in question is a further simplification that may be made, providing, the inaccuracies of such an approach through the factors previously mentioned are born in mind. In applying these simplified considerations, α-uranium (Fig. 1) forms an example. There are temperature dependent and relatively large thermal expansion coefficients in the [100] and [001] directions, each of average value about 3×10^{-5} per deg · K and a smaller, but negative thermal expansion coefficient of about -6×10^{-6} per deg · K in the [010] direction.

Taking approximate values of $\Delta\alpha \approx 2 \times 10^{-5}$ per $\deg \cdot K$ and $E \approx 2 \times 10^{11}$ Pa, then a temperature cycle of only ± 10 degs · K will induce a stress of $\approx$80 MPa. The induction of such a stress level may exceed the elastic limit of the material thus causing plastic deformation to occur within the grains. It must be noted further that the magnitude of the elastic limit is not easy to define, for it may be time dependent as well as influenced by the precise form of the stress that is generated.

Where the material has preferred orientation, temperature cycling may cause significant permanent change of shape because the plastic deformation that is caused in each individual grain is not entirely reversible [10]. Thus a form of ratchetting takes place with each thermal cycle inducing a particular increment of distortion. With many repeated thermal cycles this distortion can be considerable as illustrated in Fig. 2, but its extent can be modified by heat treatments that alter the crystallographic texture.

In a purely randomly oriented polycrystalline material not externally stressed, thermal cycling may have only a small external manifestation if the grains have sufficient plasticity under the complex internal stress system. The principal observation is the wrinking of the surface grains, effectively creating surface oscillations with a wavelength similar to the grain size [11]. The origin of this process lies in the occurrence of slip and of twinning, as Cahn identified [3], in the free exposed surfaces of the grains that eventually leads to their distortion.

So far we have only considered material that is unstressed externally. Highly important additional aspects arise if the material is subjected to external loading and the main features of these will next be considered.

3. The effects of external stress

If we consider a randomly oriented polycrystal under a small tensile load at constant temperature, the stress will initially be resisted by purely elastic deformation. With a sufficiently large change ΔT in temperature a situation will be reached when $E\Delta\alpha\Delta T$ induces an internal stress level that exceeds the yield stress σ_{y} of the material. Then the stress resistance will no longer be accommodated elastically so the initial increment of elastic strain is converted into a plastic strain of similar magnitude. A reversal of temperature will have a comparable effect. Clearly, a precise analysis of this phenomenon would be highly complex but results derived from the simple analysis outlined have proved remarkably close to practical observations. The origins of this approach lay in Cottrell's far-sighted perception [12] and interpretation of the enhanced creep (more appropriately referred to as "pseudo creep" because it is not directly related to time) of α uranium subject to neutron irradiation. In the original analysis, the internal stresses are not caused by temperature changes but by the crystallographic dependence of the precipitation of vacancies and intersticials created during the fission process. A thermal neutron flux causes an irradiation growth rate $\dot{\varepsilon}_{\mathrm{g}}$ in the [010] direction of an unrestrained α-uranium single crystal [13] leading to a strain $\dot{\varepsilon}_{\mathrm{g}}t$ in time *t*, where the grain is contained within a polycrystal this results in an internal stress $E\dot{\varepsilon}_{\mathrm{g}}t$ so the time taken to reach the yield stress σ_{y} is $\sigma_{\mathrm{y}}/E\dot{\varepsilon}_{\mathrm{g}}$. In this interval, the initial elastic strain σ/E produced by an external stress σ becomes a plastic strain $\dot{\varepsilon}_{\mathrm{p}}$. This strain increment is continually reproduced as long as the irradiation is maintained so inducing a pseudo creep process at a rate $\dot{\varepsilon}_{\mathrm{p}} \approx (\sigma/E)/(\sigma_{\mathrm{y}}/E\dot{\varepsilon}_{\mathrm{g}}) \approx \dot{\varepsilon}_{\mathrm{g}}\sigma/\sigma_{\mathrm{y}}$. The rate of strain produced by this mechanism can substantially exceed the normal creep rate of the material at a similar temperature and stress and this enhancement is greater at lower stresses and mean temperatures.

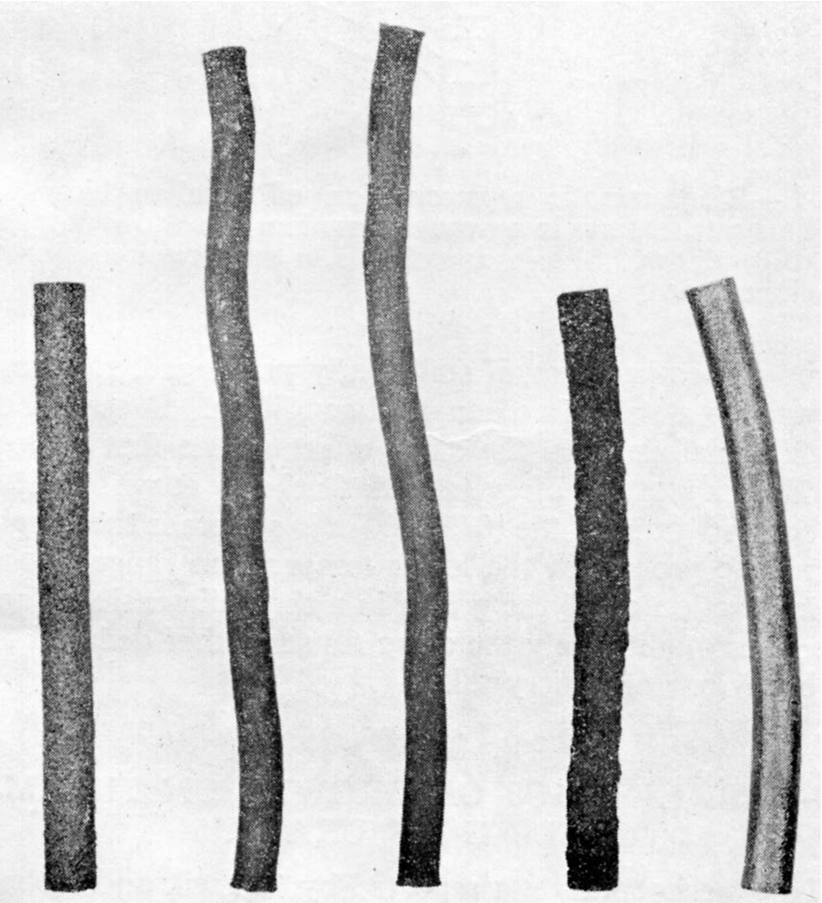

Figure 2 The effect of 850 thermal cycles between 50° and 600°C on α-uranium bars 25 mm in diameter, originally smooth and of equal length [10]. The different extent of their distortion is due to differences in preferred orientation arising from their mode of fabrication and heat treatment. From left to right, the bars were respectively, (1) as cast, (2) hot rolled, (3) cold swaged, (4) annealed in the β phase at 700°C and (5) quenched from the β-phase.

There is a close analogy between the process described and the effect of internal stress arising from thermal cycling. If the yield stress σ_y is reached by a change of temperature ΔT such that $\Delta\alpha\Delta T \approx \sigma_y/E$, the increment of strain caused by an external stress σ becomes a plastic strain $\dot\varepsilon_p$ so that $\dot\varepsilon_p \approx \Delta\alpha\Delta T\sigma/\sigma_{y.}$

Considerations of this kind have raised further questions. One of these concerns the influence of thermal cycles sufficient only to cause intergranular stresses that are below the yield stress. Fortunately, this situation has proved amenable to analysis that has again been supported by experimental results [14–16].

In the foregoing discussion, a specific value of the yield stress σ_y has been presumed Its magnitude, however, becomes less definite at elevated temperatures where relaxation processes occur at increasing rates. It is then more appropriate to consider the effect of conventional creep processes in which the creep rate generally varies with stress raised to some power n. Under multi-axial stresses, this can be coupled with the Levy-von Mises equation [17] to take the form

$$\dot\varepsilon_{xx}/\sigma'_{xx} = \dot\varepsilon_{yy}/\sigma'_{yy} = \dot\varepsilon_{zz}/\sigma'_{zz} = \gamma_{yz}/\tau_{yz} = \dot\gamma_{zx}/\dot\tau_{zx}$$
$$= \dot\gamma_{xy}/\tau_{xy} = AI^{n-1}. \qquad (1)$$

where $\dot\varepsilon_{xx}$, etc. are the tensile creep rates in the directions indicated and $\dot\gamma_{yz}$, etc. are the shear components of the creep rates under the shear stress components τ_{yz} etc. σ'_{xx}, σ'_{yy} and σ'_{zz} are the deviatoric stresses, that is, the tensile stresses $\sigma_{xx,}\sigma_{yy}$ and σ_{zz} in the respective directions minus the hydrostatic component of stress such that

$$\sigma'_{xx} = \sigma_{xx} - (\sigma_{xx} + \sigma_{yy} + \sigma_{zz})/3$$
$$= (2/3)[\sigma_{xx} - (\sigma_{yy} + \sigma_{zz})/2]$$

I is the internal stress given [17] by

$$(2/3)I^2 = (\sigma'_{xx})^2 + (\sigma'_{yy})^2 + (\sigma'_{zz})^2 + 2(\tau_{yz})^2$$
$$+ 2(\tau_{zx})^2 + 2(\tau_{xy})^2$$

Complete analyses have not been attempted for the application of these equations to the simultaneous presence of internal and externally applied stresses, though satisfactory approximate solutions have been given [15] for the case where an externally applied stress $\sigma_{ex} \ll I$. To illustrate the situation, a simplified analysis can be presented as follows. If, in the x direction, a small external stress σ_{ex} is applied at a level much less than an internal stress σ_{xx}, then the first term of Equation 1 is written $\dot\varepsilon_{xx}/(\sigma_{xx} + \sigma_{ex})'$. Now the internal stress in each individual grain is such that $\sigma_{xx} \neq \sigma_{yy} \neq \sigma_{zz}$ but for the material as a whole, over all the grains, the internal stresses must have no orientation dependence so that for their average values $\sigma_{yy} = \sigma_{zz} = \sigma_{zz}$. Thus

$$(\sigma_{xx} + \sigma_{ex})' = \sigma_{xx} + \sigma_{ex} - (\sigma_{xx} + \sigma_{ex} + \sigma_{yy} + \sigma_{zz})/3$$
$$= 2\sigma_{ex}/3$$

It follows that $\sigma'_{yy} = -\sigma_{ex}/3$ and also $\sigma'_{zz} = -\sigma_{ex}/3$.

It is further noted that, making these substitutions in Equation 1, that $\dot{\varepsilon}_{xx} + \dot{\varepsilon}_{yy} + \dot{\varepsilon}_{zz} = 0$ so matching the requirement that volume is conserved during plastic deformation.

The unit axial creep equation for the creep rate $\dot{\varepsilon}_{xx}$ subjected to a tensile stress σ_{ex} in the presence of internal stresses now takes the form

$$\dot{\varepsilon}_{xx} = (3/2)I^{n-1}\sigma_{ex} \qquad (2)$$

In a more extensive analysis [15], the numerical factor is found to be slightly influenced by the values of n but differing from the above by no more than a few percent.

More serious uncertainties arise from a lack of knowledge of the effects of frequency and of wave form of the temperature cycles. Nevertheless, if some average value of the internal stress I can be evaluated, it is apparent from this that the acceleration of creep caused by the temperature cycles is proportional to $(I/\sigma_{ex})^{n-1}$ and is greatest when the external stress is small. For example, when $n = 3$ and the external stress is 6 MPa, frequent temperature fluctuations of only ±3 deg·K can cause an acceleration of creep rate [16] which is more than an order of magnitude greater than the creep rate at constant temperature.

4. The effects of crystal anisotropy on ductility

Our discussion so far has dealt with essentially pure single-phase materials. Different phases have different properties that can substantially influence behaviour. Small particles, even at low concentrations, can cause problems. The degree of cleanliness of a material, the number, size and shape of inclusions can be influential. Even in materials without preferred textures these can be responsible for thermally induced stresses but where grain anisotropy also exists, the overall effects can be much enhanced. An early manifestation of damage to a material on thermal cycling lies in the internal stress generated nucleation of voids around the inclusions [18]. This can be non-destructively detected at an early stage by determinations of changes in density. Further , thermal cycling can cause these voids to grow, eventually linking up to form cracks, seriously deteriorating the mechanical properties.

In complete contrast to such effects however, it is significant that some beneficial features of the generation of internal stresses have been noted [19]. These arise essentially from the modified form of the relationship that is generated between the strain rate and the external stress applied. Where there is a low dependence of strain rate on applied stress, that is when n is small, then it has long been known that there is only very slow development of a neck during tensile deformation with consequent enhancement of ductility. This can easily be appreciated by noting that the tensile stress $\sigma = F/A$ where F is the force perpendicular to an area A. It has become conventional [20] in this case to write the Norton equation as $\dot{\varepsilon} = K(F/A)^{1/m}$ and, to preserve constant volume, $\dot{\varepsilon} = -\mathrm{d}A/A\ \mathrm{d}t$ so $-\mathrm{d}A/\mathrm{d}t \propto A^{1-1/m}$. It follows that $\mathrm{d}A/\mathrm{d}t$ is independent of A when $m = 1$. This implies that the rate of reduction of cross sectional area is independent of the size of the area. Thus, deformation is not concentrated in the region of smallest cross section with the consequence that necking is delayed and ductility enhanced [20]. A dramatic early demonstration [21] of this effect is illustrated in Fig. 3.

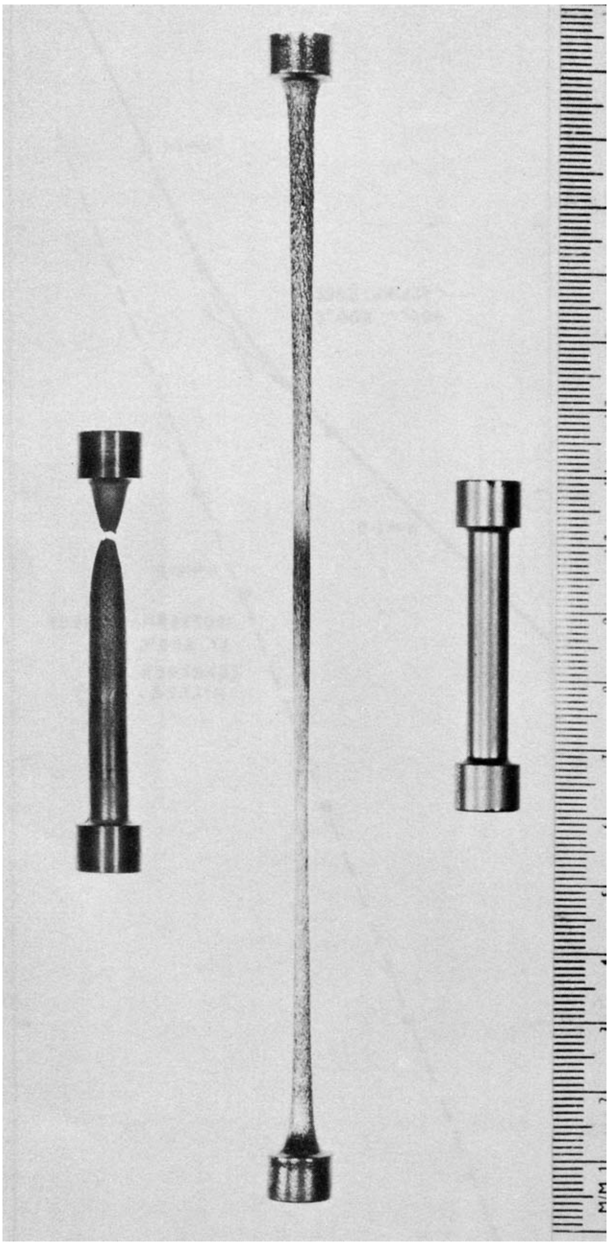

Figure 3 The superplastic behaviour of α-uranium (without preferred crystal orientation) with and without thermal cycling under external stress is illustrated. The specimen on the left, under a tensile stress of 16 MPa at 600°C, fractured after 55% elongation. In contrast the centre specimen has been subjected to the same stress but with thermal cycles between 400° and 600°C superimposed at a rate of one cycle per hour. A tensile ductility of 430% has been achieved [21]. The original specimen size is illustrated on the right.

It has been noted earlier that the presence of internally generated stresses simultaneously with the application of an external stress at elevated temperatures leads to a linear dependence of strain rate $\dot{\varepsilon}_{xx}$ on the applied stress σ_{ex} as in Equation 2. Thus the superimposition of thermal cycles during mechanical working under low stresses enhances the ductility of material with crystallograhically anisotropic grains [22]. This feature can be utilised in superplastic forming to create specific shapes by relatively simple mechanical operations. The potential opportunities for such practical applications have been extensively reported.

5. Conclusions

Anisotropy of crystal structure in polycrystalline materials leads to a features that are absent in materials with isotropic structures. α-uranium typifies an anisotropic structure with notably large difference in its thermal expansion coefficients between the [001] and [100] and the [010] directions. Thermal cycling induces large internal stresses in polycrystals, sufficient to cause deformation that is manifest as slip and twinning on free surfaces, that enabled Cahn [3, 4] to elucidate the crystallographic features of the deformation modes. Linking these with the earlier observations of Boas and Honeycombe [6–8] on different materials has led to increasing realisation of the importance of crystal anisotropy in the generation of internal stresses. With these, the significance of preferred orientation in influencing distortion in materials without external stress becomes apparent. When external stresses are superimposed mechanical behaviour is greatly affected, especially in materials without preferred texture. The analysis of such situations is facilitated by the approach first proposed by Cottrell [12] to explain the enhancement of creep rate by the internal stresses generated by neutron irradiation. Temperature fluctuations produce analogous effects and the enhancement is greatest when the external stress is small in comparison to the internal stresses. This feature is connected with the reduction of stress sensitivity of the strain rate that can reach the situation where these two parameters are linearly related. The ductility of the material is then substantially increased because of the delay in necking and this has opened up potential areas for practical exploitation [22].

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