CONSTRUCTION OF DEFORMATION – MECHANISM MAPS FOR METALS AND SOLID SOLUTION ALLOYS: A NEW APPROACH

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Abstract A new approach has been introduced to construct deformation-mechanism maps for metals and solid solution alloys. For this purpose two computer programs named DEFOR and GRAPH have been written in BASIC to be run on IBM compatible personal computers. Using these programs, deformation - mechanism maps for a number of pure metals and a solid solution alloy (Ti-6wt% Al) have been plotted and effects of grain size and alloying element have been studied.

چکیده   نقشه‌های تغییر فرم خزشی فلزات و آلیاژهای محلول جامد با ارائه روش جدید و ساده‌ای در رسم آنها معرفی شده است بدین منظور دو برنامه کامپیوتری به نامهای DEFOR و GRAPH به زبان بیسیک نوشته شده است که قابل اجراء با ریز کامپیوترهای منطبق با IBM بوده و تهیه نقشه‌های مذکور را برای همگان میسر مینماید. با استفاده از این برنامه‌ها نقشه‌های تعدادی از فلزات خالص و یک آلیاژ محلول جامد (Al ٪ wt ۶ ـ Ti) برای اولین بار تهیه گردیده است و اثرات اندازه دانه و عنصر آلیازی مورد مطالعه قرار گرفته است.

INTRODUCTION

Polycrystalline materials can deform plastically by a number of different mechanisms. In studying the mechanical behavior of solids, one of the most important considerations is to identify the dominant deformation process. Deformation - mechanism mapping is a special way of summarizing information about the range of dominance of each of the mechanisms of plasticity and the rate of flow they produce. These maps depict normalized shear stress, σ_s/G, versus homolgous temperature, T/Tm, where σ_s is the shear stress, G is the shear modulus, T is the temperature and Tm is the melting temperature in $^{\circ}$K. They show different regions of stress and temperature over which each of the deformation mechanisms is dominant. Contours of constant strain rates, $\dot{\gamma}$, are superimposed on the maps.

The purpose of this paper is to introduce computer programs which have been developed in order to construct the deformation - mechanism maps for metals and substitutional solid solution alloys. The programs named DEFOR and GRAPH are written in BASIC. They are versatile and can be run very easily on IBM compatible microcomputers. DEFOR does all computations and finds the points of boundary lines, separating different fields and strain rate contours. The position of the points on the map are stored in a file which is used as a data file in running GRAPH to plot the map.

RATE EQUATIONS

In the present work we have considered the following deformation mechanisms:
1) defect-less flow
2) dislocation glide
   a) limited by discrete obstacles
   b) limited by Peierls resistance
3) dislocation creep
   a) lattice diffusion controlled
   b) core diffusion controlled
4) diffusional creep
   a) Nabbaro - Herring creep
   b) Coble creep
5) Harper- Dorn creep

Deformation processes such as phonon or electron drag and adiabatic shear are not included in our maps.

They need more knowledge and data to be formulated and included in this program*.

1) Defect-less Flow

A stress which exceeds the theoretical shear strength causes flow even in a defect - free crystal. The strain rate due to this process, $\dot{\gamma}_1$, can be described as follows [2]:

$$\begin{cases} \dot{\gamma}_1 & \infty & \text{when } \sigma_s \geq \alpha G \\ \dot{\gamma}_1 & 0 & \text{when } \sigma_s < \alpha G \end{cases} \quad (1)$$

where α is a constant value between 0.05 and 0.1 depending on the crystal structure [2].

2) Dislocation Glide

Below the ideal shear strength, flow by the glide motion of dislocations is possible when an adequate number of independent slip systems is available. This motion is controlled by the presence of certain barriers. For the strain rate produced by this motion, we have used rate equations based on thermal activation of dislocations over discrete obstacles or Peierls resistance. Examples of discrete obstacles are strong dispersoids or precipitates, solute atoms, forest dislocations and weak precipitates. Peierls resistance is lattice frictional force which acts as a barrier to dislocation motion.

a) Dislocation glide limited by discrete obstacles

The shear strain rate produced by this deformation mechanism, $\dot{\gamma}_2$, is calculated as follows [2]:

$$\dot{\gamma}_2 \quad \dot{\gamma}_0 \exp\left[-\frac{\Delta F}{kT} (1 - \frac{\sigma_s}{t_s}) \right] \quad (2)$$

where $\dot{\gamma}_0$ is a pre-exponential constant, ΔF is the total free energy required to overcome the obstacle without any use of external stress, k is the Boltzman constant and t_0 is the Peierls controlled flow stress 0°K.

b) Dislocation glide limited by Peierls resistance

The rate equation which is used to calculate the shear strain rate for this process, is as follows [2]:

$$\dot{\gamma}_3 \quad \dot{\gamma}_0 (\frac{\sigma_s}{G})^2 \cdot \exp\left\{ -\frac{\Delta F_p}{KT} [1 - (\frac{\sigma_s}{---})^{3/4}]^{4/3} \right\} \quad (3)$$

where $\dot{\gamma}_0$ is the pre-exponential constant, ΔF_p is the Helmholtz free energy of an isolated pair of kinks and t_{op} is the flow stress at 0°K.

* Attempts have been made to show the field of dominance of these mechanisms for some metals and alloys. For this purpose a more suitable kind of deformation map with the axes of $\dot{\gamma}$ and T Tm has been introduced [1].

3) Dislocation Creep

At temperatures above 0.5 Tm, dislocations can climb as well as glide. This is possible due to the sufficient mobility of vacancies. Thus deformation takes place at lower stresses than would be needed for glide alone. At high temperatures dislocation climb is generally lattice diffusion controlled but at lower temperatures the transport of matter through the dislocation core is more feasible. The steady state strain rate is related to the stress by a power form relationship [2]:

$$\dot{\gamma} \alpha (\frac{\sigma_s}{G})^n \quad (4)$$

where n, a material property constant, has a value between 3 and 10. This is the reason that the corresponding process is called «power - law creep».

At high stresses (above about $10^{-3}G$) the simple power law breaks down i. e., the measured strain rates are greater than the value predicted by the equations in the form of relation (4) [2]. Thus, to describe the process, other forms of rate equations which are in better fit to the experiment are used.

a) Lattice diffusion controlled dislocation creep

The power - law rate equation for the process is [1]:

$$\dot{\gamma}_4 \quad A \cdot \frac{D_{cr} G b}{kT} (\frac{\sigma_s}{G})^n \quad (5)$$

$$\text{where } D_{cr} \quad D_{ocr} \exp (-Q_{cr} / R T) \quad (6)$$

A' and n are material constants, D_{cr} is the lattice diffusion coefficient, b is the Burgers vector, D_{ocr} is a pre - exponential constant, Q_{cr} is the activation energy for creep and R is the universal gas constant.

In power - law breakdown region the rate equation used will be [1]:

$$\dot{\gamma}_4 \quad A \cdot \frac{D_{cr} G b}{kT} [\beta \text{ Sinh} (\frac{\sigma_s}{G\beta})]^n \quad (7)$$

where β is the normalized stress above which the power - law breaks down.

b) Dislocation core diffusion controlled creep

The power - law rate equation governing this mechanism is [1]

$$\gamma_{5} = A \cdot \frac{(D_c f_c)G b}{kT} (\frac{\sigma_s}{G})^n \quad (8)$$

$$\text{where } f_c \quad \frac{10 a_c}{b^2} (\frac{\sigma_s}{G})^2 \quad (9)$$

$$D_c = D_{oc} \exp(-Q_c / RT) \qquad (10)$$

a_c is the cross sectional area of the dislocation core. D_{oc} is the pre - exponential constant and Q_c is the activation energy for this diffusion process.

At high stresses when power-law breaks down the proper rate equation is [1]:

$$\dot{\gamma}_5 \quad A^{\cdot} \frac{(D_c f_c)G\, b}{kT}[\beta\, \text{Sinh}\, (\frac{\sigma_s}{G\beta})]^n \qquad (11)$$

4) Diffusional Creep

Diffusional flow of atoms either by volume diffusion or by boundary diffusion leads to the Newtonian - viscous creep of a polycrystal.

a) Nabbarro - Herring creep

At higher temperatures diffusion of atoms through grains is the dominant diffusion mechanism. The resultant creep is called Nabbarro - Herring creep. The strain rate produced by this process is found as follows [2]:

$$\dot{\gamma}_6 \quad 42\frac{\sigma_s \Omega}{kTd^2}D_v \qquad (12)$$

$$\text{where} \quad D_v \quad D_{ov} \exp(-Q_v\, RT) \qquad (13)$$

Ω is the atomic volume, d is the grain size, D_{ov} is the pre - exponential constant and Q_v is the activation energy of the volume diffusion.

b) Coble creep

At lower temperatures diffusion of atoms along grain boundaries is faster. The resultant creep process is called Coble creep. The governing rate equation is [2]:

$$\dot{\gamma}_7 = 42\,\pi\cdot\frac{\sigma_s \Omega}{kTd^3}\delta D_1 \qquad (14)$$

$$D_1 \quad D_{ob} \exp(-Q_1\, RT) \qquad (15)$$

δ is the effective thickness of the boundary, D_{ob} is the pre - exponential constant and Q_b is the activation energy for diffusion through grain boundary.

5) Harper - Dorn Creep

Some metals and alloys show a special type of creep process at sufficiently low stresses. This phenomenon was first noted by Harper and Dorn [3] in pure aluminum with large grain sizes and at high tempera-

tures. Similar behavior has been detected in some other metals and alloys including lead and tin [4], aluminum alloys [5] and α - titanium [6]. The most plausible explanation for the mechanism is that of climb controlled creep under conditions such that the dislocation density does not change. In this process $\dot{\gamma}$ is proportional to σ_s [2], i. e:

$$\dot{\gamma}_{HD} = A^{\cdot}_{HD}\frac{D_v\, b\, \sigma_s}{kT} \qquad (16)$$

where $A^{\cdot}_{HD}$ is the proportionality constant.*

The Effect of Alloying on the Diffusion Coefficent

If the solid solution binary alloy is M type (metal type with n=4 to 7) the volume or lattice diffusion coefficient for the alloy will be estimated as follows:

$$D_{allo} \quad D_A\, D_B / (D_A\, X_B + D_B\, X_A) \qquad 17)$$

where D_A and D_B are diffusion coefficients of the solute and solvent atoms and X_A and X_B are their atomic fractions, respectively. When the alloy is A type (alloy type n $\approx$ 3), the volume of lattice diffusion coefficient will be found using the following relation:

$$D_{allo} \quad (D_A\, X_B + D_B\, X_A)(1 + \frac{\delta_{ln}\, \gamma_A}{\delta_{ln}\, X_A}) \qquad (18)$$

where γ_A is the activity coefficient of the solute atom. γ_A for dilute solutions usually obeys Henry's law [7]. Then Equation 18 will be simplified yielding:

$$D_{allo} = (D_A\, X_B + D_B\, X_A) \qquad (19)$$

Construction of the Maps

The rate equations relate the shear strain rate to the shear stress and temperature for each deformation mechanism that appears as a field on the map. A field boundary is the loci of points of stress and temperature at which the dominant mechanism changes. Superimposed on the maps are the contours of constant shear strain rate, which are found by calculating net shear strain rate value, $\dot{\gamma}_{net}$, as follows:

$$\dot{\gamma}_{plas} \quad \text{Least of}\, \{\dot{\gamma}_2\, \text{and}\, \dot{\gamma}_3 \qquad 20)$$

* $A^{\cdot}_{HD}= 3\, A_{HD}$ where A_{HD} is the proportionality constant when tensile strain- rate- tensile stress relationship is used.

$$\dot{\gamma}_k = \text{Greatest of } \{\dot{\gamma}_6 \text{ and } \dot{\gamma}_{11D}\} \quad (21)$$

$$\dot{\gamma}_{net} \quad \text{Greatest of } \{\dot{\gamma}_{plas} \text{ and } (\dot{\gamma}_4 + \dot{\gamma}_5)\} + \dot{\gamma}_7 + \dot{\gamma}_8 \quad (22)$$

The above mentioned logic has been formulated in the program DEFOR. We have used DEFOR and GRAPH to construct the maps for fcc metals like Al and Ni (Figures 1 and 2), bcc metals like V and W (Figures 3 and 4), hcp metals like Ti (Figure 5 and 6) and Ti - 6wt% Al alloy (Figure 7). Data for plotting these maps can be found in references [2] and [8].

DESCRIPTION OF COMPUTER PROGRAMS

In the program DEFOR there are three subroutines. The first finds the points of boundary lines by searching over temperature increments for a stress increment at which the dominant mechanism changes. The dominant mechanism at a point is the one with the maximum value of shear strain rate. The second subroutine finds the contours of constant strain rate by searching over temperature increments for a stress increment at which $\dot{\gamma}_{net}$ becomes less than the contour value. The temperature increments are optional. A smaller increment causes the position of the points on the boundary lines and contours to be closer to each other. The third subroutine finds the shear strain rate values for each mechanism at each increment of temperature and stress used in the first and second subroutines.

The positions of all the points of field boundaries and strain rate contours on the map are stored in a file called MAP. This file is the input data file for the program GRAPH which plots the maps.
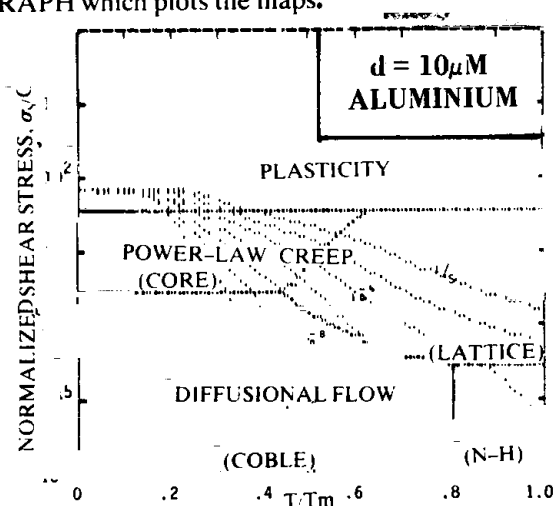

Figure 1. Deformation - Mechanism Map for Aluminum with a Grain Size of 10 μm.

DISCUSSION

The package is versatile and can be run to print out the maps for pure metals and solid solution alloys with different grain sizes and takes into consideration possible allotropic transformations. We have avoided to complicate the construction of the maps by choosing those deformation mechanisms which are experimentally developed. The method that we have chosen for the superposition of the rate equations has been found to be in better agreement with the experimental results reported by a number of researchers especially in considering the Harper - Dorn creep [8, 9, 10].

The effect of the alloying element on the deformation mechanisms can be studied by comparing the maps for the pure metal and the alloy with identical grain sizes. Figures 5 and 7 can be used to compare the effect of Al as an alloying element on Ti [8]. When there is not enough diffusion data for M type or dilute A type binary solid solution alloy, the program is capable of plotting the map for the alloy by having the diffusion data for the solute and the matrix while it distinguishes between the two types of alloys (M type or A type) in calculating dislocation creep strain rates.

Any change in grain size may alter the deformation behavior of a metal or an alloy. This change can be studied by plotting the maps for different grain sizes. Figures 5 and 6 show the map for pure Ti with grain sizes of 100 μm. In the latter, it is clear that Harper - Dorn creep replaces Nabbarro - Herring creep at high temperatures and low stresses.

ACKNOWLEDGMENT

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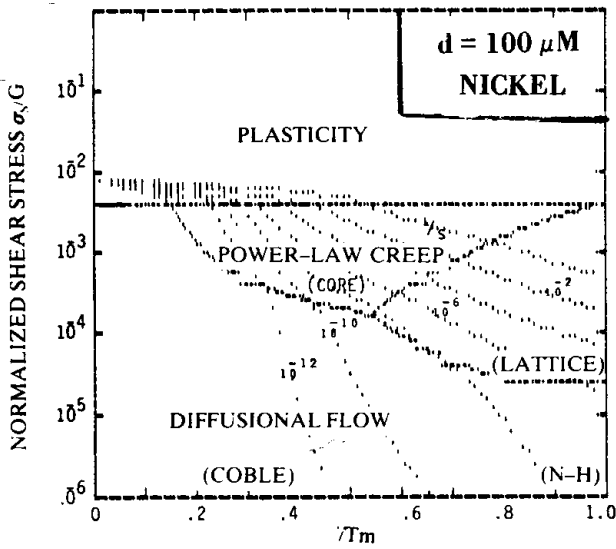10. G. Malakondaiah and P. Rama Rao, Acta Met. 29, 1981, p. 1263.

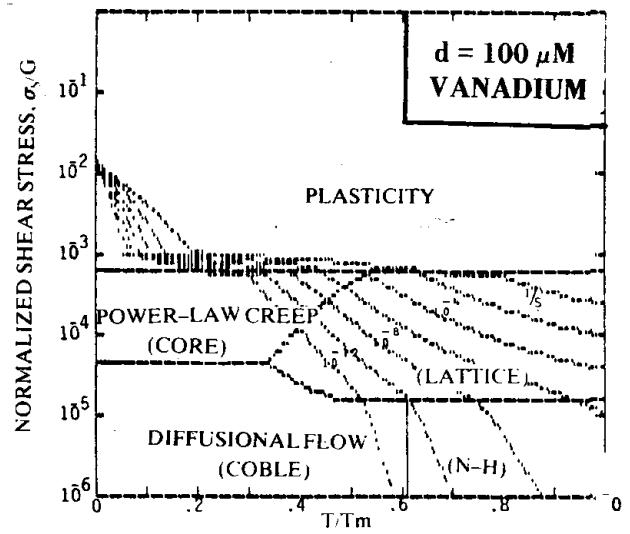**Figure 2.** Deformation- Mechanism Map for Nickel with a Grain Size of 100 μm.

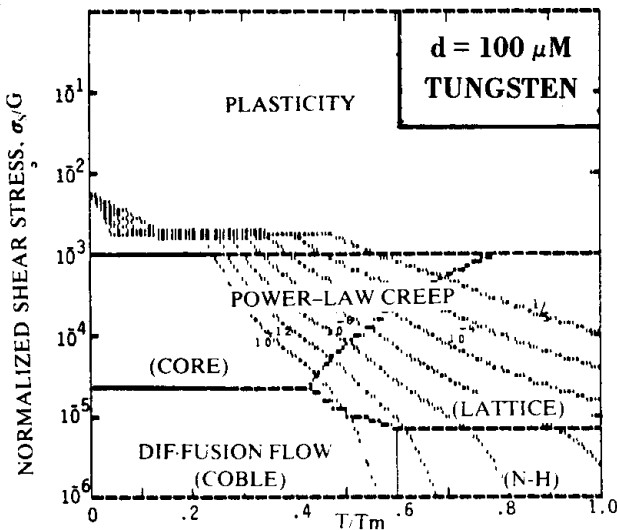**Figure 3.** Deformation- Mechanism Map for Vanadium with a Grain Size of 100 μm.

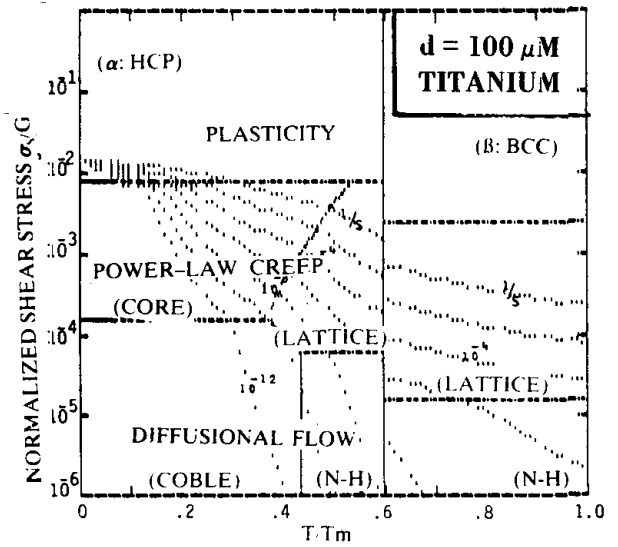**Figure 4.** Deformation- Mechanism Map for Tungsten with a Grain Size of 100 μm.

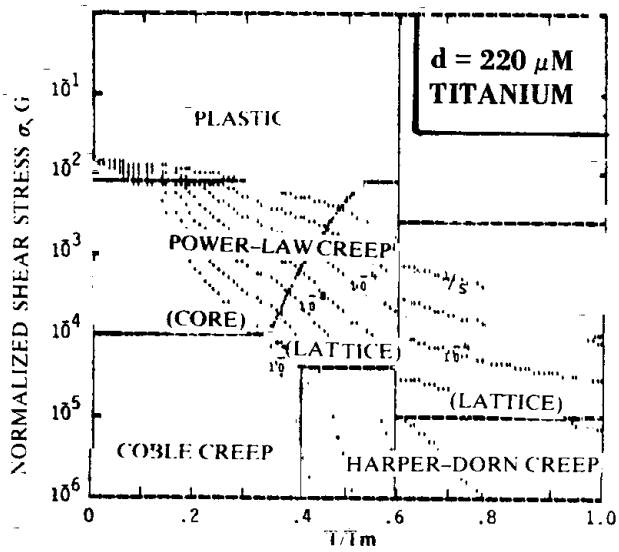**Figure 5.** Deformation- Mechanism Map for Ti with a Grain Size of 100 μm.

Figure 6 (left):

NORMALIZED SHEAR STRESS σ_s/G

10^1
10^2
10^3
10^4
10^5
10^6

d = 220 μM
TITANIUM

PLASTIC

POWER-LAW CREEP

(CORE)

(LATTICE)

(LATTICE)

COBLE CREEP

HARPER-DORN CREEP

0 .2 .4 .6 .8 1.0

T/Tm

Figure 6. Deformation- Mechanism Map for Titanium with a Grain Size of 220 μm.

Figure 7 (right):

NORMALIZED SHEAR STRESS σ_s/G

10^1
10^{-2}
10^3
10^4
10^5
10^6

(α: HCP)

d = 100 μM
TI–6AL

(B: BCC)

PLASTICITY

POWER-LAW CREEP

(CORE)

(LATTICE)

(LATTICE)

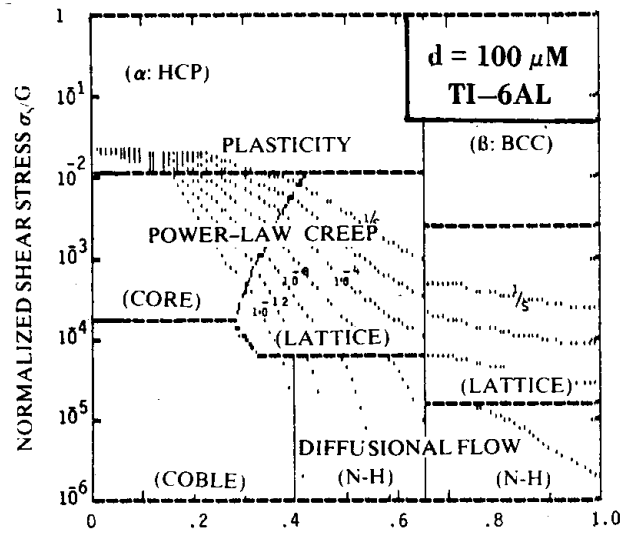DIFFUSIONAL FLOW

(COBLE) (N-H) (N-H)

0 .2 .4 .6 .8 1.0

Figure 7. Deformation- Mechanism Map for Ti-6 Al with a Grain Size of 100 μm.