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Influence of orientation, temperature, and strain-rate on the yield strength of Fe_2B single crystals

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The deformation behaviour of Fe_2B single crystals with different orientations has been studied by the compression test over the temperature range 800 to 1100° C. Three slip systems (1 1 0) [0 0 1], (1 1 0) [1 $\bar{1}$ 1], and ($h\,k\,l$) [1 $\bar{1}$ 1] have been found to be active in the present work. The operation of ($h\,k\,l$) [1 $\bar{1}$ 1] slip system appears to require about ten times higher stress than those of (1 1 0) [0 0 1] and (1 1 0) [1 $\bar{1}$ 1] slip systems. The temperature and strain-rate dependence of the yield stress suggests that the Peierls mechanism controls the plastic deformation of Fe_2B crystals. The activation energy for the thermally activated deformation of Fe_2B varies between 6 and 10 eV and the activation volume between $10b^3$ and $160b^3$. The remarkably high activation energies have been discussed in connection with the large Burgers vectors of Fe_2B.

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1. Introduction

Fe_2B has a body-centred tetragonal structure of the $CuAl_2$ type. The $CuAl_2$ type structure is crystallographically more complicated and has larger Burgers vector than a number of ordinary cubic or hexagonal close packed structures. Only a few works have been reported on the mechanical properties of intermetallic compounds with $CuAl_2$ structure [1–4]. Kirsten stated that a slip system of $CuAl_2$ was (1 1 0)[0 0 1] [4]. Dey and Tyson showed that polycrystals of $CuAl_2$ were fairly ductile around temperatures of $0.8\,T_m$ and, moreover, that the activation energies for the deformation of $CuAl_2$ indicated rather high values of 3 to 4 eV [2]. Alternatively, the previous report by the present authors described that the single crystals of Fe_2B exhibited some ductility around temperatures of $0.5\,T_m$ [1], which were lower than those in $CuAl_2$ polycrystals. The difference probably comes from the fact that the plastic deformation of the intermetallic compounds with $CuAl_2$ type structure depends markedly on the crystal orientation. Although the authors have confirmed that one of the slip systems in Fe_2B is (1 1 0)[0 0 1], detailed investigations on the other slip systems have not been conducted. The purpose of the present work is to clarify the operative slip systems in Fe_2B and to obtain more informations on the deformation behaviours.

2. Experimental procedures

The method of preparation of Fe_2B single crystals has been described in a previous paper [1]. Single crystals included small amounts of FeB particles as a second phase. Compression tests were carried out over a temperature range 800 to 1100° C under an atmosphere of mixed gas Ar + 10% H_2.

Four kinds of compression axes were selected so that each of probable slip systems (1 1 0) [0 0 1], (1 1 0)[1 $\bar{1}$ 1], (1 0 $\bar{1}$)[1 $\bar{1}$ 1], and (1 0 0)[0 1 0] can be activated with the most preference. The orientations of compression axes and the Schmid factors for the probable slip systems are shown in Table I. The [2 1 1] orientated specimen is most favourable for (1 1 0)[0 0 1] slip to occur. Because Fe_2B has a tetragonal symmetry, atomic configurations in (1 1 0) and (1 0 1) planes are different to each other. Thus, the [1 0 0] and [0 0 1] compression axes were chosen in order to study the difference between two expected slip systems

TABLE I Compression axes and Schmid factors for expected slip systems

Compression axis	Slip system			
	$(1\,1\,0)[0\,0\,1]$	$(1\,1\,0)[1\,\bar{1}\,1]$	$(1\,0\,1)[1\,1\,1]$	$(1\,0\,0)[0\,1\,0]$
2 1 1	0.440	0.417	0.350	0.258
1 0 0	0.062	0.462	0.406	0.017
0 0 1	0.026	0.013	0.400	0.001
1 1 0	0.035	0.035	0.424	0.498

$(1\,1\,0)[1\,\bar{1}\,1]$ and $(1\,0\,\bar{1})[1\,\bar{1}\,1]$. Finally, the $[1\,1\,0]$ specimen is most favourable for $(1\,0\,0)$ $[0\,1\,0]$ slip system to operate.

The standard strain-rate of $4 \times 10^{-4}\,\mathrm{sec}^{-1}$ was adopted, and in most cases the strain-rate change tests, where the strain-rate was abruptly changed among 4×10^{-5}, 1×10^{-4}, 4×10^{-4}, and 1×10^{-3} sec^{-1}, were performed after specimens were compressed about 6% at the standard strain-rate.

3. Results

Typical examples of stress–strain curves obtained at various temperatures are shown in Fig. 1. For the $[0\,0\,1]$ specimen compressed at 1000° C, the brittle-fracture occurred around the upper yield point of $1200\,\mathrm{MN\,m^{-2}}$. Since slip lines were, in general, very fine and occasionally could not be observed at high temperatures, a two surface analysis method was not able to successfully apply to determine the slip system.

The yield strength rapidly decreased with increasing temperature. In such cases as specimens deformed at high temperature without showing definite yield points, the yield strengths were determined from the intersections between the prolongations of the elastic regions and the early stage of plastic regions. The results are shown in Fig. 2 where log σ_y is plotted against temperature T. The yield strength σ_y, as found in TiC [5], NiAl [6], Ge and Si [7], is expressed by an empirical equation of the form

$$\sigma_y = A \exp(-BT)$$

where A and B are constants. The strain-rate sensitivity of the flow stress was determined by the method of the strain-rate change. A linear relationship between $\ln\dot{\epsilon}$ and σ was obtained over a range of tested strain rate $\dot{\epsilon}$ from 4×10^{-5} to 1×10^{-3} sec^{-1}. The activation volume v^* in a thermal activation process is associated with the strain-rate sensitivity by the relation

$$v^* = kT(\partial \ln \dot{\epsilon}/\partial \tau^*)$$

where k is a Boltzmann constant. The activation

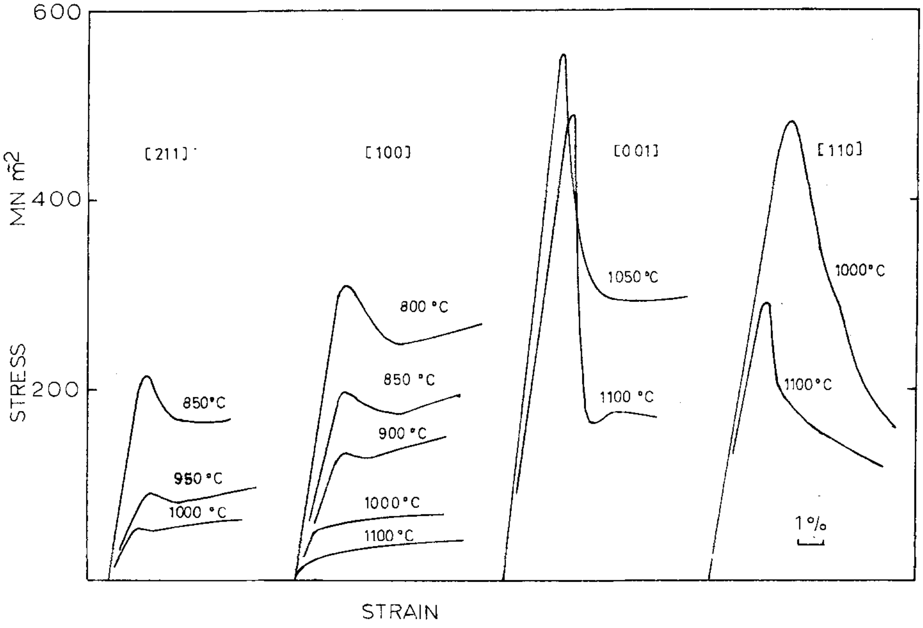

Figure 1 Stress–strain curves for Fe_2B single crystals with various compression axes.

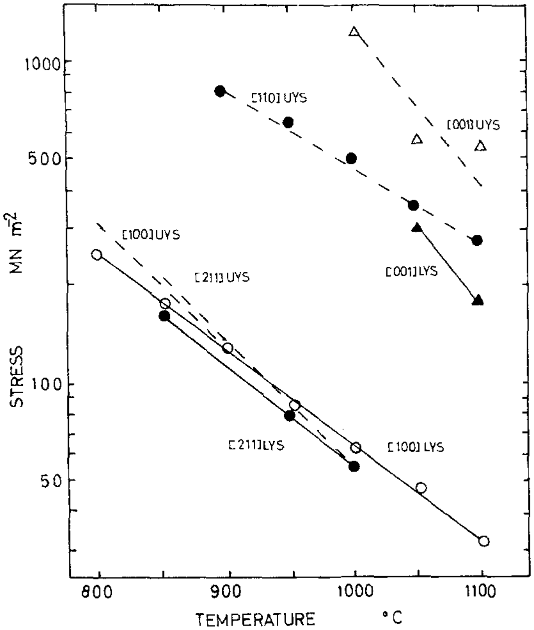

Figure 2 Temperature dependence of the upper yield stress (UYS) and lower yield stress (LYS).

energy H is determined from the theory derived by Conrad [9]:

$$H = -kT^2(\partial\tau^*/\partial T)_{\dot{\epsilon}}(\partial \ln \dot{\epsilon}/\partial\tau^*)_T.$$

The effective stress τ^* is given by $\tau^* = \tau - \tau_\mu$, where τ is the applied shear stress and τ_μ is the athermal stress component which depends on the temperature only through the shear modulus μ. Since the variation of shear modulus with temperature was unknown in Fe_2B, it was assumed that τ_μ was constant over the investigated temperature range. Consequently, $\partial\tau^*/\partial T = \partial\tau/\partial T$ and $\partial \ln \dot{\epsilon}/\partial\tau^* = \partial \ln \dot{\epsilon}/\partial\tau$; The calculated values of the activation energy and volume are shown as a function of τ in Figs. 3 and 4 respectively.

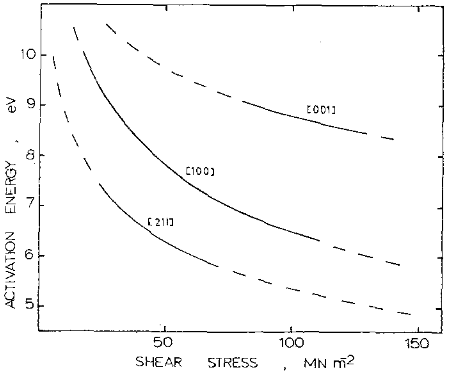

Figure 3 Effect of stress on the activation energy for the deformation of Fe_2B.

4. Discussion

4.1. [2 1 1] compression

Referring to the previous work [1], it is obvious that the deformation of [2 1 1] oriented specimen is due to the (1 1 0) [0 0 1] slip system.

4.2. [1 0 0] compression

The yield behaviours of [1 0 0] oriented crystals were very similar to those of [2 1 1] crystals. However, the Schmid factor for the (1 1 0) [0 0 1] slip is very small. If the (1 1 0) [0 0 1] slip would operate, the yield stresses of these crystals should be larger about ten times than those of [2 1 1] crystals. This was not the case of the present work. Therefore, it is reasonable to deduce that the (1 1 0) $[1\,\bar{1}\,1]$ slip operated in these crystals.

4.3. [0 0 1] compression

The extremely sharp yield points are observed in [0 0 1] compression test; the yield drop amounts to 67% of the upper yield stress at 1100° C. On the other hand, the upper yield points in [2 1 1] and [1 0 0] compressions are much smaller or disappear above 1000° C. There is another additional result which supports that the (1 1 0) [0 0 1] and (1 1 0) $[1\,\bar{1}\,1]$ slips did not take place in these crystals. The slope of $\log \sigma - T$ curve in [0 0 1] compression is steeper than in [2 1 1] and [1 0 0] compressions. These results suggest that $(h\,k\,l)$ $[1\,\bar{1}\,1]$ slip might have activated in [0 0 1] compression. Unfortunately, there lack the experimental data to conclude that the slip planes $(h\,k\,l)$ intersecting [0 0 1] compression axis are (1 0 1) planes.

4.4. [1 1 0] compression

The shape of specimens in [1 1 0] became rhombic after compression. The such shape change of specimens caused the monotonous decrease of load after the upper yield points in their stress–strain

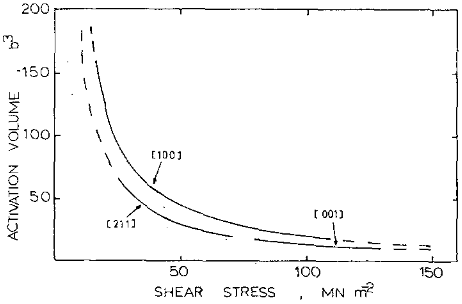

Figure 4 Effect of stress on the activation volume for the deformation of Fe_2B.

curves. Since the log σ–T curve in [1 1 0] compression is nearly parallel to that in [2 1 1] or [1 0 0] compression, the slip system (1 1 0) [0 0 1] or (1 1 0) $[1\bar{1}1]$ must have operated in this case. Where the Schmid factor is nearly zero, a tiny error of orientation affects severely the calculation of the critical resolved shear stress. The calculated critical resolved shear stress for (1 1 0) [0 0 1] or (1 1 0) $[1\bar{1}1]$ in [1 1 0] compression is about 0.7 times of that in [2 1 1] or [1 0 0] compression. The difference is within the setting error of 1 degree. Therefore, the unusual deformation mode in [1 1 0] compression will be explained as a consequence of the rotation of crystal due to the active (1 1 0) [0 0 1] or (1 1 0) $[1\bar{1}1]$ slip system with a very small Schmid factor.

4.5. (1 0 0) [0 1 0] slip system

The difficulty to activate the (1 0 0) [0 1 0] slip system is quite reasonable because the Burgers vector 5.109 Å of this system is very large in comparison with 4.192 Å of the $[1\bar{1}1]$ slip systems and 4.248 Å of the [0 0 1].

4.6. (1 1 0) [0 0 1] and (1 1 0) $[1\bar{1}1]$ slip systems

The slip systems of (1 1 0) [0 0 1] and (1 1 0) $[1\bar{1}1]$ show very similar deformation behaviours, i.e. the stress level, the temperature dependence of the yield stress, and the deformation curve. The similarity can be explained in terms of the atomic arrangements in the (1 1 0) planes of Fe_2B shown in Fig. 5. The stacking sequence of the atomic planes, which are constituted by Fe atoms only, is ... 1234321 .... The atomic planes of B atoms are situated between Fe atomic planes 2 and 3. Hence, a slip motion between planes 2 and 3 requires higher energy owing to smaller distances of interatomic planes. On the other hand, the shear displacement between planes 1 and 2 (or 3 and 4) is energetically more favourable. Therefore, we will now consider only the slip between planes 1 and 2. The Fe atoms on plane 1 constitute an approximate hexagonal network shown in Fig. 5b. The Fe atoms on plane 2 are located above the centre positions of the hexagonal network of plane 1. The slip directions [0 0 1] and $[1\bar{1}1]$ are almost equivalent. Thus, the $[1\bar{1}1]$ slip direction on (1 1 0) plane would be preferable in almost the same degree as [0 0 1] slip direction.

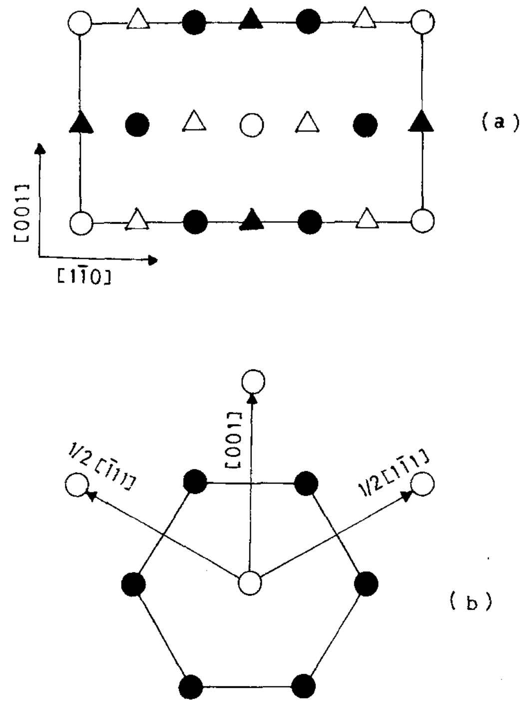

Figure 5 Atomic arrangement of Fe atoms in (1 1 0) planes of Fe_2B. The stacking sequence of (1 1 0) planes is such as ... 1 (closed circle) 2 (open circle) 3 (closed triangle) 4 (open triangle) 321 ....

4.7. (hkl) $[1\bar{1}1]$ slip system

The $[1\bar{1}1]$ slip on (hkl), where $l \neq 0$, is by about ten times more difficult to operate than on (1 1 0). If the B atoms in the Fe_2B structure would form chains along [0 0 1], the slips on such planes as to cut the B–B bonds, $l \neq 0$, would be difficult. However, the B atoms in Fe_2B have been reported to be isolated from each other [8]. Consequently, the effect of the B–B bonds, if any, might be minor. Another reason of the difficulty of slip on (hkl) is connected with the comparatively complex atomic arrangements of the slip plane. An atomic arrangement on (1 1 0) have a hexagonal symmetry as shown in Fig. 5, but this symmetry disappears on the other planes.

4.8. Temperature and strain-rate dependence

The strong temperature dependence of the yield stress in b c c transition metals have been reported as a stress assisted thermal activation process [9–11]. The similar analysis has been conducted for Fe_2B in the present work. The activation volumes from $10b^3$ to $160b^3$ are in the same order as those predicted from the Peierls process [11]. The calculated activation energies, 6 to 10 eV, are extraordinarily high compared with the values reported for b c c metals from 0.5 to 1.8 eV. The high activation energies, 3 to 4 eV, have been also reported for the $CuAl_2$ polycrystals [2]. Thus, the high activation energies for Fe_2B could be mainly attributed to the complex structure. The Burgers vectors of Fe_2B are about 4.2 Å, which is remarkably large compared with those of b c c metals of about 2.5 Å. Conrad and Hayes have reported that the activation energy is approximately equal to $0.1\mu \boldsymbol{b}^3$ [10]. Using the values of 1.24×10^{11} $N m^{-2}$ for μ [12] and 4.248 Å for $\boldsymbol{b}$, one can obtain 6 eV, which is lower limit of the values obtained from the present experiment, as the activation energy for (1 1 0) [0 0 1] slip in Fe_2B.

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