THE CRYSTALLOGRAPHY OF CLEAVAGE FRACTURE IN Al_3Sc

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ABSTRACT

The intermetallic compound Al_3Sc is a trialuminide with the $L1_2$ structure, which deforms easily in compression at room temperature, with yield stresses around 100 MPa. In tension Al_3Sc fractures transgranularly in a brittle manner. The predominant cleavage plane is {011}. Regions, which are flat within experimental resolution are only occasionally observed. Numerous cleavage steps, which are aligned in 3 major crystallographic directions, are found. Some of these steps consist of {111} or {001} planes, but others are not distinctly crystallographic. Plastic deformation involving dislocation motion or twinning may have occurred at some of these steps. Reactions between different types of steps are also observed. One type of cleavage patterns found is strikingly similar to the typical appearance of fracture surfaces of fcc brass and Cu_3Au after stress corrosion cracking. However, this particular pattern is only rarely observed in Al_3Sc. Our observations indicate that an interpretation of cleavage fracture in Al_3Sc in terms of surface energies alone is unlikely to be successful. A full understanding of the fracture morphology of Al_3Sc will require detailed atomistic simulations taking dislocation motion and twinning into account.

INTRODUCTION

Intermetallic compounds based on trialuminides (e.g. Al_3Ti, Al_3Zr, Al_3Nb, Al_3Sc) are of interest owing to their high melting points in the 1600 to 1850 K range, their low densities (as low as 3 Mg/m^3) and their potential oxydation resistance. One disadvantage of Al_3Ti and Al_3Zr are their tetragonal structures (DO_{22} and DO_{23}, respectively). However, substitution of approximately 7 a/o of the aluminium by elements like V, Cr, Mn, Fe, Co, Ni, Cu, and Zn changes their structure to the cubic ordered $L1_2$ structure [1,2,3,4]. In contrast to ductile $L1_2$ compounds like Cu_3Au or Ni_3Al, trialuminides are brittle in tension. Whereas brittleness in some other $L1_2$ systems (e.g. Pt_3Al, Ref. [5]) is plausible in view of their high yield stresses, the brittleness of trialuminides is more difficult to understand. Al_3Sc, for example, has a lower yield stress than Ni_3Al, yet it is brittle in spite of its cubic structure [6]. It tends to cleave on {011} planes, and not on {111} planes, which generally exhibit the lowest surface energy in fcc materials [6,7].

In the present work we present detailed observations of fracture surfaces in Al_3Sc. The full interpretation of these surfaces will require future theoretical work. Our measurements serve as a basis, against which such future calculations can be checked.

EXPERIMENTAL PROCEDURE

Small buttons of Al_3Sc (typically a few g) were prepared from high-purity materials by arc-melting in argon. In order to minimize inhomogeneities they were remelted several times and subsequently annealed in vacuum for 2 hours at 1473 K. Approximately 1 mm thick slices were prepared with a slow speed saw and broken in bending. A particularly large cleavage facet was oriented by optical reflection parallel to the sample holder of

JEOL 840 scanning electron microscope (SEM). This facet was indexed by means of selected area channeling patterns (SACP's). Detailed observations involving tilting around specific crystallographic directions were carried out in a high resolution Hitachi S-800 SEM. From measurements of projected widths as a function of tilt angle the inclinations of cleavage step planes with respect to the main fracture plane were determined.

An Al_3Sc single crystal was grown in a cone-shaped Al_2O_3 crucible by the Czochralski method and homogenized for 16 hours at 1423 K. Two perpendicular faces of a compression sample fabricated from the crystal were mechanically polished to a mirror finish. The crystallographic orientation was determined by the Laue technique. After compression by approximately 2% a two-surface trace analysis was performed in order to determine the slip plane.

EXPERIMENTAL RESULTS AND DISCUSSION

Slip trace analysis showed that slip in Al_3Sc occurs on {111} planes. Also, since the Burgers vector is <011> [7], Al_3Sc has 5 independent slip systems. Compression experiments with polycrystalline samples [6] indicate that the critical resolved shear stress is less then 100 MPa. Al_3Sc thus is easily deformed in compression, yet it is brittle in tension. The {011} cleavage surface examined in this work exhibits numerous cleavage steps in 3 different crystallographic directions. If the cleavage steps themselves are produced by cleavage, they are, by definition, low index planes. We consider here, somewhat arbitrarily, planes with indices up to 2. The possible cleavage step planes are then found from the condition that the step plane normals [ijk] are normal to the directions [hkl] of the steps, i.e., $[i,j,k]\cdot[h,k,l]=0$. If we exclude step angles > 90 degrees, then for steps aligned in the $[01\bar{1}]$ direction the following angles with respect to the (011) plane are possible:
19.5°, 35.3°, 54.7°, and 90°. For steps aligned along $[21\bar{1}]$ we have angles of 50.8° and 90°, and for steps aligned along [100] we have 18.4°, 45°, 71.6° and 90°. In the following we will compare the measured step angles to

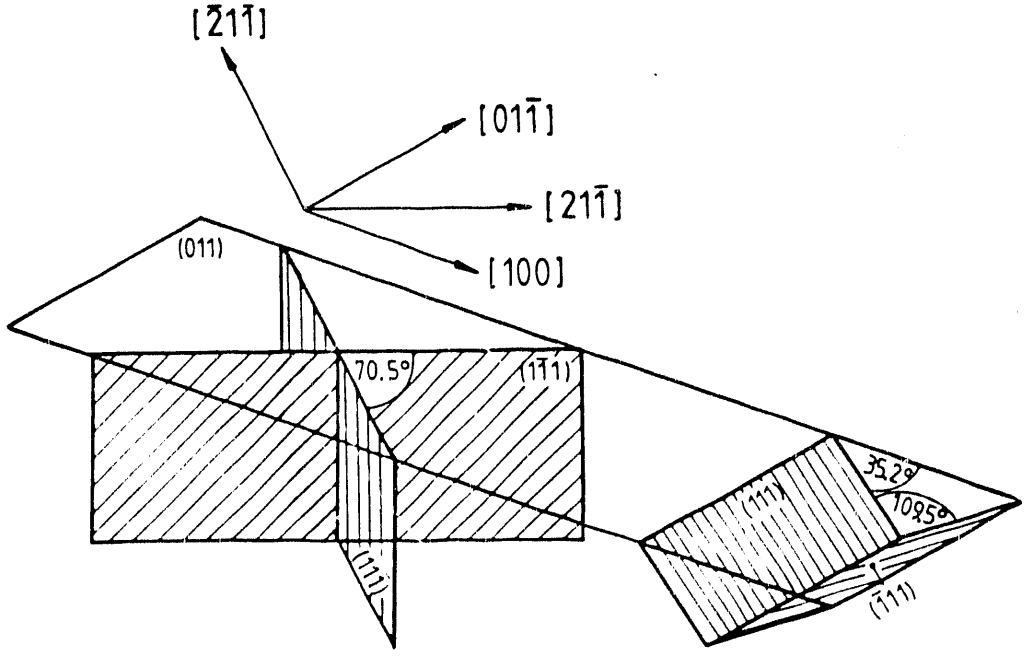

Fig. 1. Schematic of {111} planes in relation to (011) cleavage plane.

those listed above. To this purpose it is useful to visualize the possible slip planes in relation to the (011) cleavage plane (Fig. 1).

A. Steps aligned in the [01$\bar{1}$] direction

The cleavage step shown in Fig. 2 is aligned approximately in the [01$\bar{1}$] direction. From an analysis of the projected widths for several tilt angles (tilt axis [01$\bar{1}$]) and assuming that the step consists of a planar surface, a cross section through the fracture surface, perpendicular to the step direction, was found. This cross-section is shown in the lower part of Fig. 2. The step angle (31°) is very close to the 35° angle expected for {111} planes, i.e., the step planes are {111} planes. The secondary steps (triangular features) seen in Fig. 2 correspond to the traces of (1$\bar{1}$1) and (11$\bar{1}$) planes perpendicular to the main (011) cleavage plane (compare Fig. 1). The striations in the vicinity of, and parallel to, the [01$\bar{1}$] steps, correspond to the traces of (111) and ($\bar{1}$11) planes. The striations may indicate some localized dislocation activity.

B. Steps aligned in the [21$\bar{1}$] direction:

In Fig. 3 we show a cleavage step aligned in the [21$\bar{1}$] direction. This step consists of three differently inclined planes which are indicated in the lower part of the figure. Except for the 48° step, a comparison between crystallographically possible, and experimental step angles does not reveal any similarities, i.e., these steps are not completely crystallographic. Their [21$\bar{1}$] direction is the only distinctly crystallographic feature. The fine striations along this direction correspond, by reference to Fig. 1, to the traces of (1$\bar{1}$1) planes perpendicular to the main cleavage plane. The [01$\bar{1}$] striations in the vicinity of the steps correspond to the traces of (111) or ($\bar{1}$11) planes. These striations continue sometimes into features on the steps which look like secondary cleavage steps.

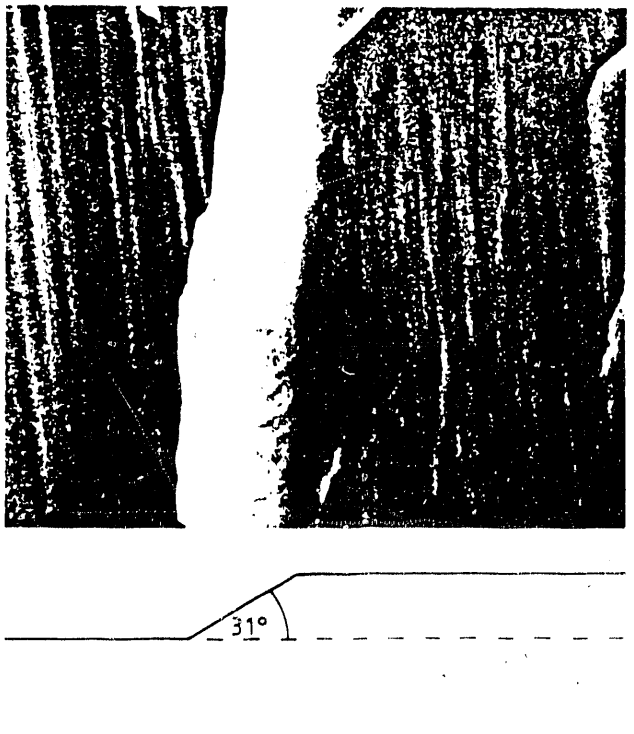

Fig. 2. SEM micrograph of [01$\bar{1}$] cleavage step on (011) facet. Tilt angle = 0°.

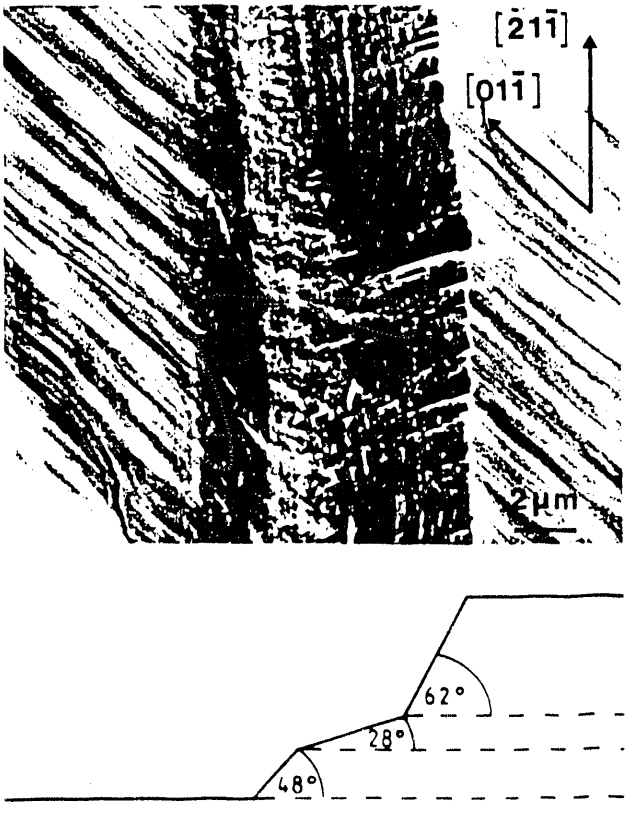

Fig. 3. SEM micrograph of [21$\bar{1}$] cleavage step on (011) facet. Tilt axis = [21$\bar{1}$], tilt = 45°, right-hand side tilted down.

Occasionally [21$\bar{1}$] steps much smaller than those in Fig. 3 are found. Their heights vary from approximately 20 to 200 nm (Fig. 4). Equivalent steps are also oriented along the [$\bar{2}$1$\bar{1}$] direction. These steps form 90° angles with the main (011) cleavage plane. Identical fracture patterns have been reported for the stress corrosion cracking of Cu_3Au [8] and fcc brass [9]. Figure 4 also shows some evidence for twinning as indicated by the zig-zag line near its center.

C. Steps aligned in the [100] direction:

A typical step aligned in the [100] direction is shown in Fig. 5. The steeply inclined main step is 1 to 2 μm wide. On either side are fairly wide, slightly inclined regions. They exhibit striations along [01$\bar{1}$]. Only occasionally were smooth regions seen near such steps (smooth within the experimental resolution, approximately 10 nm). Several measurements of the steep parts of [100] aligned steps indicated usually angles close to 45°, i.e., these steps are {001} cleavage planes. The [01$\bar{1}$] striations perpendicular to the main step which correspond to the traces of (111) and ($\bar{1}$11) planes, curve into the structure of the steep part of the step. The straight striations on the steep part (36° in Fig. 5) may also be the traces of [1$\bar{1}$1) and (11$\bar{1}$) planes. Fig. 5 thus suggests that localized slip may have occurred on {111} planes. Of course the possibility of microtwins too small to be resolved by SEM, as they have been observed in fractured gold by Wilsdorf [10] cannot be ruled out.

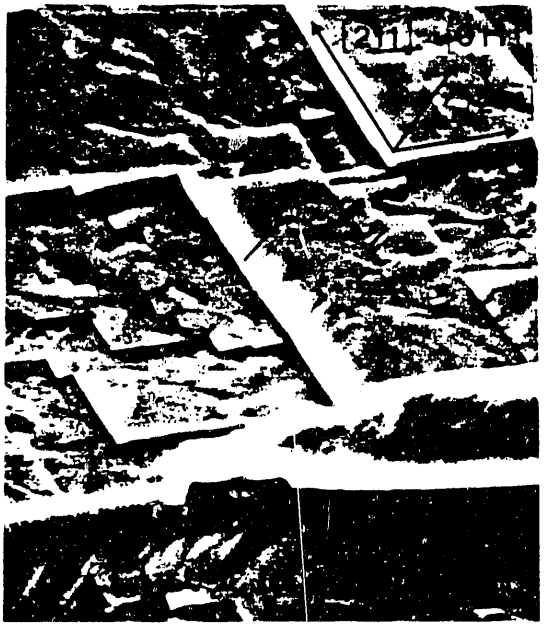

Fig. 4. SEM micrograph of [21$\bar{1}$] and [$\bar{2}$1$\bar{1}$] cleavage steps. Tilt axis = [21$\bar{1}$],45° tilt, top side tilted down.

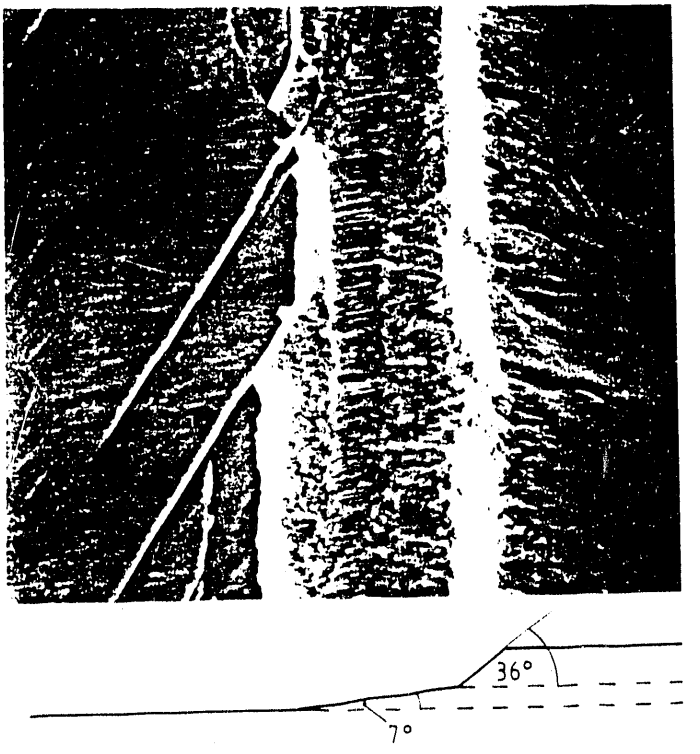

Fig. 5. SEM micrograph of [100] cleavage step on (011) facet. Tilt = 0°.

D. Cleavage step reactions

In Fig. 5 we note <211> and [100] steps, which react with each other. For example, if the crack propagation direction was [100], [100] steps dissociated into <211> steps. In the case of [$\bar{1}$00] crack propagation, <211> steps recombined. Since the crack growth direction was not determined in our experiments, the sequence of this reaction is not known.

F. General discussion

Our fracture surface observations indicate some slip or twinning activity on {111} planes. It is not conclusively possible to distinguish between slip and twinning. However, in view of the low yield stress of Al_3Sc, some localized slip during fracture is quite likely. In particular in the case of [100] steps several slip systems may have been involved. The 90° steps in Fig. 4 also indicate {111} slip in the stress field of a crack propagating on {011}.

Fig. 6. Reaction between [100], [21$\bar{1}$] and [2$\bar{1}$1] steps.

As we have seen, cleavage fracture in Al_3Sc is quite complicated. Perfect cleavage (i.e., atomically smooth fracture along low index planes), if it exists, is the exception rather than the rule. It may occur occasionally in the vicinity of [100] steps and, in a highly localized way, on all three step types. This means that an explanation of brittle failure based exclusively on surface free energies would be of doubtful value. In fcc and $L1_2$ materials {111} is commonly the plane with the lowest surface energy, but {011} is clearly the preferred cleavage plane in our case. The low cleavage strength on {011} for Al_3Sc and other trialuminides [7] is difficult to understand in the framework of such models. In order to understand the fracture behavior in full detail, surface energy as well as plasticity and fracture mechanics arguments are therefore required. Environmental effects as the major cause for embrittlement are not very likely, since they usually require slow crack propagation [8,9]. Consistent with this features like those in Fig. 4, which are typical for fracture surfaces produced by SCC, are the exception rather than the rule in Al_3Sc.

Recently, Kohlhoff et al. [11] have made substantial progress in the atomistic simulation of cleavage fracture in bcc materials, in wich a similar dilemma exists. Kohlhoff et al. have indentified reasons why cleavage does not occur on the surface with the lowest energy, {01$\bar{1}$}, but rather on the {001} surface which exhibits a slightly higher energy. On {011} planes crack propagation is easy only in one direction. In all other directions plastic mechanisms like twinning or dislocation nucleation and motion become important. On {001} planes, on the other hand, crack propagation is relatively easy in all directions. Therefore, fracture on these planes is preferred, although the surface energy is not a minimum. Calculations of this type are required for Al_3Sc. The present experiments provide a base line against which such calculations can be compared.

CONCLUSIONS

Al_3Sc is soft and exhibits 5 independent slip systems, yet it is brittle.

The main fracture surface of Al_3Sc is {011}. {001} and {111} surfaces are only occasionally found and are usually highly localized.

The fracture surfaces exhibit features indicating slip and/or twinning. Only occasionally are small regions found which may be atomically flat, i.e., which may have been formed by perfect cleavage.

Cleavage steps are oriented in 3 major crystallographic directions. Each step type exhibits its own distinct morphology.

Although fracture in Al_3Sc is not thought to be primarily an environmental effect, certain fractographic similarities with the stress corrosion cracking of fcc and $L1_2$ materials are found.

An explanation of brittle fracture in Al_3Sc based exclusively on surface energy arguments is unlikely to be successful. Detailed atomistic modelling will be required for a fuller understanding.

ACKNOWLEDGEMENTS

We would like to thank C.A. Carmichael for preparing and testing the Al_3Sc single crystal and V. Bacher for the preparation of the manuscript. This research was sponsored by the Division of Materials Sciences, United States Department of Energy under contract DE-AC05-84OR21400 with Maria Marietta Energy Systems, Inc.

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