A MECHANISTIC STUDY OF THE BRITTLE TO DUCTILE TRANSITION IN HIGH MELTING POINT INTERMETALLIC COMPOUNDS

A Report on a Program of Research Conducted at
The University of Illinois
Department of Materials Science and Engineering

Principal Investigator:
Hamish L. Fraser

Preamble

This report describe the work done on an ONR grant involving a study of high melting point intermetallic compounds. This grant was supposed to be of a three year duration, but lasted only approximately nine months because the Principal Investigator accepted a position on the faculty of the Ohio State University. The program was transferred to the Ohio State University, and was eventually renewed and enlarged in scope - a successful program.

Aims of the Program

The previous program of research was aimed at developing a fundamental understanding of the mechanisms of plastic deformation in certain high melting point intermetallic compounds. The results of this study were to have lead in part to a more detailed understanding of the factors that influence the lack of ductility exhibited at ambient temperatures by these types of compound.

In order to study the deformation mechanisms of these materials at ambient temperatures, where they exhibit brittle behavior, it was proposed that ductile phase toughening should be employed so that some degree of plastic deformation might be induced in the brittle compounds. It was hoped that from a detailed analysis of defects in the deformed samples the various factors influencing the deformation mechanisms would become apparent. In the case of the higher temperature deformation experiments, a determination of the contribution of diffusive mechanisms to plastic deformation was to be made.
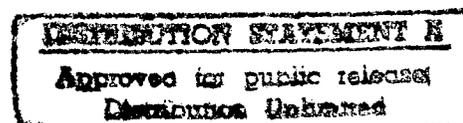
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Scientific Officer Code: 1131M
Dr. Donald E. Polk
800 North Quincy Street
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SUBJECT: ONR Grant N00014-89-J-1233 - Final Report

Dear Dr. Polk:

In accordance with the terms of the subject grant, enclosed are three (3) copies
of the final technical report that have been prepared by Professor Hamish
Fraser, the principal investigator.   Please accept our apologies for the lateness
of this report. I trust this will allow for the official close-out of the subject
grant to be completed. Additional copies of the final report have been
distributed as indicated below.

Should you have any questions concerning the technical content of the
report, please contact Professor Fraser at Ohio State University at (614)292-
2708. If I can be of assistance, please feel free to contact me at (217)244-6422.

Very truly yours,
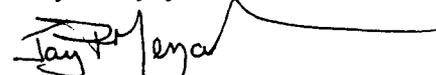
Jay P. Menacher
Assistant to the Head

enclosures

cc: ONR/Administrative Grants Officer/Chicago (1)
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       Defense Technical Information Center (12)
       UIUC Grants & Contracts (1)
       H. Fraser

The effect of extrinsic factors such as the possible detrimental rôle of interstitial impurities and the influence of alloying elements on microstructure was to be examined. Alloying additions were to be made in response to the results of the work aimed at determining the mechanisms of plastic deformation; the specific additions were to be chosen on the basis of their intended rôle (e.g. modification of crystal structure) and the results of calculations being performed elsewhere concerning the influence of electronic structure on crystal structure and mechanical properties.

Finally, the creep properties of two types of alloy samples were to be determined.

2.2 *Summary of Results*

The original proposal called for studies of Al_3Nb, $RuTi$, V_3Si, Ti_5Si_3 and Nb_3Al. Work for the nine month program was initiated on Al_3NB, Ti_5Si_3, V_3Si and Nb_3Al.

In the case of the compound Al_3Nb, There appears to be a tendency for the compound Al_3Ti to tolerate ribbons of anti-phase boundaries (APB's) on (001), whereas the opposite trend for is observed in Al_3V, and also ordered microtwinning occurs commonly in Al_3Ti, whereas this deformation mechanism is absent in Al_3V. The difference in this behavior may be accounted for as follows. Thus, the formation of ribbons of APB on (001), is consistent with a significant difference in the APB energy between the two compounds. Careful consideration of the stacking sequences about these faults in DO_{22} crystals shows that the formation of an APB on the (001) plane produces a thin ribbon of DO_{23} structure. It is proposed here that the difference in the APB energy on the (001) planes is due to the relative stability of the DO_{22} structure compared to that of the DO_{23} structure for these compounds. Thus, Carlsson and Meschter (1989) have performed calculations, based on the augmented spherical wave method, of the variation in energy of these two structures compared with the $L1_2$ structure for several Al_3X compounds. These results have been used here to deduce the energy differences between the DO_{22} and DO_{23} structures for the various compounds, shown in Table 1. As can be seen, for Al_3Ti the energy difference between the two crystal structures is rather small, and so it seems reasonable to assume that the APB energy would be rather low. However, for the case of Al_3V this difference in energy of the two structures is relatively large, and so therefore the apparently high value for the APB on (001) for this compound may be understood. It is, of course, tempting to interpret the difference in the twinning behavior in the same way. In the case of the twinning shear provided by glide of dislocations with $b=1/6<111>$ on {112} in the DO_{22} structure, ribbons of material with the Cu_3Ti-type structure are produced. The differences in energy between the two structures DO_{22} and Cu_3Ti-type for these two compounds have not been computed. However, it is significant that the compound Al_3Ti with

the DO_{22} structure appears to be less stable relative to several other structures, such as $L1_2$ or DO_{23}, as suggested by the results of calculations (Carlsson and Meschter 1989). If it is assumed that this trend concerning relative phase stability applies also to a comparison of the Cu_3Ti-type and DO_{22} structures for these two compounds, then it follows that the energy associated with the formation of a twin will be significantly lower in Al_3Ti than in Al_3V.

	Ti	V
$E(DO_{22})-E(L1_2)$	-0.059	-0.175
$E(DO_{23})-E(L1_2)$	-0.026	-0.067
$E(DO_{22})-E(DO_{23})$	-0.033	-0.108

Table 1. The energy differences (in eV/atom plane) between the various structures listed for Al_3X (where X is Ti or V). The data in the first two rows have been obtained from the results of Carlsson and Meschter (1989), whereas the final row contains values deduced from these latter rows. Note that the DO_{22} structure is the most stable from the point of view of free energy.

It is proposed then that the occurrence of order twinning in compounds with the DO_{22} crystal structure is influenced by the difference in energy between this structure and the Cu_3Ti-type structure, and so for compounds where the deformation mechanisms are dominated by twinning it is expected that there would be a relatively small difference in energy between these two structure types. One such compound is Ni_3V which is relatively ductile and where plastic deformation is effected in the main by twinning (e.g. Liu 1984). The energy differences between the two structure types (DO_{22} and Cu_3Ti-type) have not been calculated for this compound, but the fact that this difference may be relatively small may be deduced by reference to the *structure map* proposed by Pettifor (1986 and 1988) for the AB_3 compounds. There are a number of compounds exhibiting the Cu_3Ti-type structure adjacent to the group of compounds having the DO_{22} structure. This is consistent with there being a small energy difference between these two structures in the case of Ni_3V.

We have determined that the compound Al_3Nb deforms in similar manner to Al_3V, and therefore it is reasonable to assume that this compound is reasonably stable in the DO_{22} form. It has been a popular thesis that, to increase ductility, alloying should be used to effect changes in crystal structures of compounds, such as those with the DO_{22} structure, to ones of higher

symmetry, e.g. cubic L1$_2$. The present results suggest that rather than attempting to cause a change in structure, it may be more profitable in terms of ductility to add alloying elements that result in a reduction in the relative energies of the DO$_{22}$ and Cu$_3$Ti-type structures, and so promote the degree of twinning during plastic deformation in the DO$_{22}$ structure. However, despite this conjecture, it has not been possible to alloy Al$_3$Nb such that these changes have occurred!

A part of the study which has proven to be the most tedious involves the compound Ti$_5$Si$_3$ since it has been almost impossible to cause plastic deformation. Thus, our scheme has been to produce the compound in the presence of α-Ti, where this latter phase was added to provide ductile phase toughening. It was hoped that the total strain experience by samples during compression testing might be increased by the presence of such a phase so that some deformation might occur in the harder, more brittle, phase. However, we have no evidence that in our experiments plastic strain has been produced in Ti$_5$Si$_3$. These experiments were terminated in view of the very exciting results obtained in the case of our studies of Nb$_3$Al, described below. Samples of V$_3$Si were also found to be rather brittle.

A very exciting set of results have been obtained from experiments involving the compound Nb$_3$Al; these are summarized briefly here. Nb$_3$Al was chosen for study on the basis of its melting point (≈2000°C), the range of composition over which the compound is stable, and because of a relatively low density (for example when compared to Ni-base superalloys). However, the binary compound in its stable form has the A15 crystal structure, and in common with many other compounds with this structure, it is very brittle at ambient temperatures. The brittle to ductile transition temperature is ≈1000°C. The exciting result of the present work is that we have been able to form a metastable form of Nb$_3$Al, having the B2 crystal structure, in rapidly solidified ribbons of Nb-Al alloys. On thermal cycling between room temperature and either 800°C or 1100°C, the grains of the B2 phase become more heavily dislocated, presumably because of the mismatch in coefficients of thermal expansion between the A15 and B2 phases. This is a very exciting result because it shows that the B2 phase can be readily deformed. This fact is to be exploited in a subsequent ONR program.

References

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Pettifor, D.G., 1988, Mat. Sci. and Tech., **4**, 675.

Papers Published as a Result of this Program

"Factors Influencing the Deformation Mechanisms in the Intermetallic Compounds Al_3Ti and Al_3V", Phil. Mag. Letts, 1990, **6 2**,143.

Students Supported by this Porgram

Robert Wheeler
Piu Chaudhuri