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UNIVERSITY OF SOUTHERN CALIFORNIA

University Park • Los Angeles, California 90089-0241

DOE/ER/ 45346--T1

DE93 002879

Professor Edward Goo
Materials Science & Engineering Department
School of Engineering
(213) 740-4426 phone
(213) 740-7797 fax
e-mail ekgoo@mizar.usc.edu

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Dr. Joseph B. Darby
Department of Energy
Division of Materials Sciences
ER-131, G-236, GTN
Washington D.C., 20545

Dear Dr. Darby:

Enclosed is a the Final Technical Report for grant DE-FG03-88ER45346.

Sincerely yours,

Edward Goo

Associate Professor

ccr/darby 9/15

**Final Technical Report for DOE Grant Entitled:
Deformation Twinning in Ordered Alloys
Transformation Induced Ductility in Intermetallics
DE-FG03-88ER45346**

**Edward Goo
Department of Materials Science and Engineering
University of Southern California
Los Angeles, CA 90089-0241
September 1992**

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I. Introduction

Intermetallics, which are ordered alloys, have excellent high temperature strength. Unfortunately a universal problem facing intermetallics is the lack of ductility. The research performed under this grant attempts to look at some novel solutions for enhancing ductility in intermetallics.

Deformation twinning has been demonstrated in TiNi to be responsible for its ductility. This was a surprising result since twinning was not believed to occur readily in ordered alloys. Furthermore the twinning occurred on a {114} plane which had not been previously observed.¹ Research into determining the mechanisms for twinning in ordered alloy and understanding how twinning enhances the ductility of intermetallic was funded by this grant.

Martensitic transformations in many intermetallics also provides a possible means of enhancing ductility. The detwinning of martensite twins or transformation induced martensite provides a mechanism for accommodating large strains. It is known that a metastable martensitic phase may be created by quenching a non-stoichiometric NiAl alloy. This presents the potential of substantial ductility in NiAl. Investigation of the martensitic phase transformation and its effect on the ductility of NiAl alloys was investigated under this grant.

II. Research Results

Much of research results has been published or submitted for publication. I have included the reprints and preprints as an appendix to this report. This section will summarize the results and the details are given in the papers in the appendix.

A. Deformation Twinning in Ordered Alloys

In our research we are only concern with deformation twinning as opposed to growth or transformation twinning, therefore the word "twinning" in this report always refers to deformation twinning. To understand why NiTi twins on the $\{114\}$ planes all possible twinning modes were calculated for the B2 structure. For crystal structures with a one atom basis, twinning generally occurs by a shear mechanism and this is referred to as a simple twinning mechanism. For crystal structures with more than one atom in the basis, such as ordered alloys, twinning often occurs by a mechanism requiring a shuffle in addition to a shear and this type of twinning mechanism is referred to as a complex twinning mechanism. For simple twinning mechanisms the operative twinning mechanism is one that minimizes the magnitude of the shear. For complex twinning mechanisms that require a shear and a shuffle it is necessary quantify the "difficulty" of the shuffle to determine which twinning mechanism is expected to be favored. The shuffle is characterized by the fraction of atoms and the average distance the atoms have to be shuffled. For twinning mechanisms that require a shear and a shuffle the operative mechanism is one that minimizes the magnitude of the shear, the fraction of atoms shuffled and average distance shuffled. When this approach was applied to the B2 structure it becomes evident why $\{114\}$ twinning is an observed twinning mode.²

Qualitatively it is understood that twinning will enhance the ductility of materials by providing alternate modes for strain accommodation. In cases where the slip systems do not satisfy the von Mises Criterion, the presence to twin systems adds additional degrees of freedom to allow ductility in polycrystalline alloys. However it has been known for some time

that the von Mises Criterion as applied to slip is not valid for twinning due to the fact that twinning is unidirectional while slip is bidirectional. Reversing the twin direction does not produce an equivalent twin as opposed to slip where reversing the slip direction does produce an equivalent slip system.³ It is possible to determine if a set of twinning systems satisfy the von Mises Criterion. The problem reduces to a mathematical problem of determining if a set of vectors span all space under the restriction that only positive values of the vector be used. This is a well known problem in convex analysis and occurs quite often in optimization problems. The solution not only allows one to determine if the von Mises Criterion is satisfied by a set of twinning systems, it also applies to situations where both slip and twinning are present. Therefore this is a general method for applying the von Mises Criterion to slip and/or twinning.⁴ The method has been applied to {114} twinning and it was determined that {114} twinning does satisfy the von Mises Criterion. It was also applied to twinning systems often observed in hexagonal close-packed(HCP) metals and the results are consistent with ductility observed in HCP metals.

Twinning has also been observed in DO_3 ordered Fe_3Al alloys. A theoretical analysis of possible twinning modes for the DO_3 structure was done and the results agree with the experimental observations.⁵ We have also done some work on $L1_0$ ordered Ni_3Al . Theoretical analysis of twinning modes in $L1_0$ structure has been done. The $L1_0$ work is in the process of being written up as a paper.

B. Transformation Induced Ductility in Ordered Alloys

Many intermetallics undergo a martensitic transformation at low temperatures. There are several methods by which martensitic transformations may be used to enhance ductility in intermetallics. We have attempted to create a ductile alloy by creating an intermetallic that is fully martensitic and therefore would be extremely ductile. This martensitic alloy could be deformed to the desired shape and subsequent heat treatment would revert the martensitic phase to the parent phase and restore the excellent high temperature property.

An alternative approach is to form precipitates of the martensitic phase which would toughen the intermetallic by a mechanism similar to zirconia dispersed ceramics. This method is being tried with Ni_3Al alloys.⁶

It is well known that Ni-rich B2 NiAl alloys created by quenching undergo a martensitic transformation. We have shown at USC that a fully martensitic, polycrystalline Ni-rich NiAl alloy may be fabricated by quenching and the alloy yields below 100 MPa and has a plastic strain of 4% when deformed in compression.⁷ Subsequent heat treatment after deformation does transform the alloy back to a B2 NiAl phase with Ni_3Al precipitates. There are two problems with this approach. It is difficult to scale up the process because when sample dimension exceeds 5mm quenching cracks develop during the water quench from 1200° C. The second problem is that upon heat treating the alloy to form the B2 phase after deformation the shape memory effect causes the alloy to partially revert back to original shape. We believe both problems are solvable. Indications are that water quenching is not necessary to form the martensitic phase and substitutional alloying elements may enhance the formation of the martensitic phase. The shape memory effect may be avoided by a low temperature heat treatment to form the metastable Ni_2Al phase which would prevent the shape memory effect. We have studied the formation of the Ni_2Al phase and have submitted a paper for publication.⁸

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*preprints & reprints
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