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Marc Heggen, M. Feuerbacher. Metadislocation arrangements in the complex metallic alloy ξ' -Al-Pd-Mn. Philosophical Magazine, 2006, 86 (06-08), pp.985-990. 10.1080/14786430500259726 . hal-00513579

HAL Id: hal-00513579

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Submitted on 1 Sep 2010

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| Journal: | <i>Philosophical Magazine & Philosophical Magazine Letters</i> |
| Manuscript ID: | TPHM-05-May-0180.R1 |
| Journal Selection: | Philosophical Magazine |
| Date Submitted by the Author: | 06-Jul-2005 |
| Complete List of Authors: | Heggen, Marc; Forschungszentrum Juelich GmbH, Institut fuer Festkoerperforschung Feuerbacher, M.; Forschungszentrum Jülich, Institut für Festkörperforschung |
| Keywords: | plasticity, metallic alloys, dislocations |
| Keywords (user supplied): | |
| | |



Metadislocation arrangements in the complex metallic alloy ξ' -Al-Pd-Mn

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Abstract

In the present work different types of metadislocation arrangement are studied. It is shown that metadislocations can form dipoles or dissociate into partials, which leads to a decrease of the elastic line energy. Connected groups of metadislocations can assume large and complex network structures. Although the local elastic strain at the individual metadislocation cores remains small, they possess large total Burgers vectors and are highly effective means of plastic deformation. Furthermore, we present a characterization of phase boundaries built up by regular Metadislocation arrays and show that these metadislocations almost fully compensate the lattice mismatch.

Keywords: complex metallic alloy, metadislocations, metadislocation networks, ξ' -Al-Pd-Mn

1. Introduction

Metadislocations (MDs) are novel structural defects firstly observed in the complex metallic alloys (CMAs) ξ' - and ψ -Al-Pd-Mn [1]. They provide a physically useful principle of the plasticity of large-unit-cell materials. MDs comprise structural elements of both phases, ξ' - as well as ψ -Al-Pd-Mn. Both phases are structurally closely related and possess the same a and b cell parameters. However, the cell parameters in the c -direction are related by a factor $(\tau+3)$ where $\tau \approx 1.618$ is the irrational number of the golden mean. The lattice parameters are $a = 23.89 \text{ \AA}$, $b = 16.56 \text{ \AA}$, $c_{\xi'} = 12.56 \text{ \AA}$, and $c_{\psi} = (\tau+3) c_{\xi'} = 58.00 \text{ \AA}$ [2].

The core of a MD is a line defect which ideally extends along the $[0 1 0]$ direction. It is associated to a certain number of planar defects, so-called phason planes, which are ideally $(0 0 1)$ oriented. The term phason plane refers to the analogy to phason defects in Quasicrystals, although ξ' - and ψ -Al-Pd-Mn are crystalline phases processing translational symmetry.

Different types of MDs associated with 16, 10, 6, and 4 phason planes have been observed [3]. Recently MDs associated with 2 phason half-planes were observed [4]. Different types of

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3 MDs possess different Burgers vectors. They can be determined either by a Burgers circuit
4 around the MD core [1], by a modified Volterra process [5], or by calculating the lattice
5 mismatch at the interface between the ξ' - and the ψ -phase [6,7]. The Burgers vectors and
6 numbers of phason planes of different types of MDs are compiled in Table 1. The Burgers
7 vector moduli and the numbers of phason half-planes follow opposite sequences: a MD with a
8 high number of phason planes possesses a small Burgers vector and vice versa. The MD
9 associated with two phason planes possesses the largest Burgers vector of 4.80 Å. Hence, the
10 Burgers vectors of all MDs are small fractions of the lattice parameters $c_{\xi'}$ and c_{ψ} and their
11 local elastic strain energy is small. Therefore, in these materials, Metadislocations are
12 energetically more favourable than perfect dislocations.
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22 To date, the investigation of defects in ξ' -Al-Pd-Mn is limited to the structure and
23 properties of single MDs and their associated phason planes [1,3,8,9]. However, frequently
24 complex, network-like MD arrangements are observed. In this work the properties of MD
25 arrangements are analyzed.
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30 2. Experiments

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32 A ξ' -Al-Pd-Mn single crystal was grown by means of the Bridgman technique. A sample
33 of approximately $5 \times 2 \times 2 \text{ mm}^3$ in size was cut with the long axis inclined 45° to the [0 1 0]
34 axis. The sample was uniaxially deformed in compression to 0.5 % strain. Like icosahedral
35 Al-Pd-Mn the ξ' phase is brittle at room temperature [10,11]. Therefore deformation
36 experiments were performed at an elevated temperature of 700 °C.
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42 After plastic deformation the sample was quenched on a cold metal plate and prepared for
43 transmission electron microscopy (TEM) by standard techniques. The microstructural
44 investigation was performed in a JEOL 4000EX electron microscope. MDs are imaged with
45 the TEM sample oriented along the [0 1 0]-direction under bright-field Laue conditions, i.e.
46 applying a central aperture around a symmetric arrangement of spots.
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52 3. Results and Discussion

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54 Figure 1 shows two examples of interacting MDs. Arrows 1 and 2 point at two inversely
55 oriented MDs sharing six phason planes. Their Burgers vectors are 1.83 and -1.83 Å,
56 respectively (cf. Table 1). Hence this defect can be interpreted as a MD dipole or as part of a
57 prismatic loop. Arrows 3 and 4 indicate a dipole of MDs associated with ten phason planes.
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Figure 2 a shows a MD associated with ten phason planes (arrow 1) which is connected to a MD with six phason planes (arrow 2). They are mutually connected by six phason planes. Four phason planes are remaining, three on the right hand side and one on the bottom part of the micrograph. This situation can be interpreted in terms of MD splitting. A MD with 4 phason planes has split into an equally oriented MD with ten phason planes and an inversely oriented MD with 6 phason planes. Using Table 1 it can be shown that the Burgers vector of a MD associated with four phason planes is exactly equal to the Burgers vectors of the MD arrangement in Figure 2 a, i.e. $1.13 \text{ \AA} - (-1.83 \text{ \AA}) = 2.96 \text{ \AA}$. During the process of MD splitting, the local elastic strains at the MD cores is reduced. On the other hand, the creation of six additional phason planes introduces additional fault plane energy. Hence the process of MD splitting has to be treated similarly as splitting of dislocations into partials in structurally simple materials. The total energy balance of all defects involved has to be considered.

MD splitting is a phenomenon which is often observed in plastically deformed ξ' -Al-Pd-Mn. Figures 2 b and c show two more examples. Figure 2 b shows a MD with six phason planes (1) which is connected to a MD with four phason planes (2). It can be interpreted as splitting of a MD associated with two phason planes. The Burgers vector yields $-1.83 \text{ \AA} - 2.96 \text{ \AA} = -4.80 \text{ \AA}$. Figure 2 c shows a MD with ten phason planes (1) connected with two MDs with each six phason planes (2 and 3). Two phason planes leave the MDs at the right hand side (4 and 5). Two additional phason planes (6 and 7) are not connected to the MD arrangement. The Burgers vector yields $-1.13 \text{ \AA} - 2 \times 1.83 \text{ \AA} = -4.80 \text{ \AA}$ which is again equal to the Burgers vector of a MD associated with two phason planes. Hence, Figure 2 c shows splitting of a MD associated with two phason planes into three MDs. Splitting of a MD into even more partials is possible. For example a MD associated with two phason planes may split into two MDs with 16 phason planes and three inversely oriented MDs with 10 phason planes, hence two phason planes are left. The Burgers vectors add up to $2 \times -0.70 \text{ \AA} - 3 \times 1.13 \text{ \AA} = -4.80 \text{ \AA}$

Figure 3 shows a complex MD network, formed by the mutual interconnection of MDs via their associated phason planes. The creation of networks is possible, because a single MD can connect to more than one MDs by separating its phason planes. For the sake of clarity, the location and orientation of MDs are indicated by triangles. Furthermore, the numbers and the arrows indicate the number of associated phason planes and the direction and length of the Burgers vector, respectively. Remarkably, the Burgers vectors of almost all MDs are oriented in the same direction and add up to a large amount of 27.61 \AA . For MD networks can create objects with large total Burgers vectors, the movement of these objects through the structure

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3 leads to strong straining of the sample. Therefore they are highly effective means of plastic
4 deformation.
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8 Figure 4 shows a phase boundary between the ξ' -phase (upper left part of Figure 4) and the
9 ψ -phase (lower right part of Figure 4), which appears darker than the ξ' -phase. The presence
10 of both phases was confirmed by selected area electron diffraction patterns. The micrograph
11 shows five MDs associated with 10, and six MDs associated with 16 phason planes,
12 respectively. The total lattice mismatch at the phase boundary is $(5 \times 1.13 \text{ \AA}) + (6 \times -0.70 \text{ \AA})$
13 $= 1.45 \text{ \AA}$. The extension of the phase boundary in $[0\ 0\ 1]$ direction is 450 nm, hence the mean
14 residual elastic strain at the interface is 0.03 %. This is a remarkably small value. Especially,
15 since the lattice parameters in c direction are incommensurate - they are related by a factor of
16 $(3 + \tau)$.
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24 MDs forming a phase boundary possess low local strain at the individual MD cores,
25 especially when MDs with high numbers of phason planes are used. Mixing different kinds of
26 MDs creates a phase boundary with a low mean elastic strain at the interface, while adding up
27 MDs of the same type and hence the same Burgers vector, adds up lattice mismatch at the
28 phase boundary. A phase boundary with a perfect mean lattice mismatch can be created if
29 MDs with opposite Burgers vector direction are present in the right proportion. The Burgers
30 vectors of MDs subsequent in the series of MD types (cf. Table 1), for example MDs with 10
31 and 16 phason planes, are related by a factor of $-\tau$. Hence a perfect mean lattice mismatch at
32 the interface can be created, if these MDs are present in a proportion $1 : \tau$.
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41 **4. Conclusion**

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43 In the present work it is shown that MDs can, like dislocations in structurally simple
44 materials, form dipoles or dissociate into partials with smaller Burgers vectors. The formation
45 of partials leads to a decrease of the local elastic line energy and an increase of the fault plane
46 energy, which have to be balanced in order to find the energetically most favourable
47 configuration and geometry. Splitting of a MD into more than two partials is possible.
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53 MDs can create large and complex networks by the mutual interconnection of MDs via
54 their associated phason planes. MD networks with large total Burgers vectors are high
55 effective means of plastic deformation.
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59 Furthermore, MDs can form phase boundaries between the ξ' - and ψ -phase with low mean
60 elastic strain at the interface. These two examples stress that simply by the combination and

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arrangement of different types of MDs, structures with completely different properties are created.

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FIGURE CAPTIONS

Fig. 1: Metadislocation dipoles. Two MDs associated with six (arrow 1 and 2) and two MDs associated with ten phason planes (arrows 3 and 4) are indicated.

Fig. 2: Three examples of Metadislocation splitting. Arrows indicate a) a MD with ten (1) and a MD with six (2) phason planes, b) a MD with six (1) and a MD with four (2) phason planes, and c) a MD with ten (1) and two MDs with six (2 and 3) phason planes (additional numbers: see text).

Fig. 3: Metadislocation network. The orientation of MDs is indicated by triangles. Furthermore, the numbers and the arrows indicate the number of associated phason planes and the direction and length of the Burgers vector, respectively.

Fig. 4: Phase boundary between ξ' - (upper left part) and ψ -Al-Pd-Mn (lower right part). The interface is created by a stack of metadislocations.

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3 **TABLE / TABLE CAPTION**
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| Number of phason planes | Burgers vector |
|-------------------------|----------------|
| 16 | -0.70 Å |
| 10 | 1.13 Å |
| 6 | -1.83 Å |
| 4 | 2.96 Å |
| 2 | -4.80 Å |

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25 Table 1: Number of phason planes and Burgers vectors of all experimentally observed MDs.
26 The Burgers vector direction is related to MDs with phason planes oriented parallel to the
27 [1 0 0] direction [7]. Analogously, MDs with phason planes oriented parallel to the $[\bar{1} 0 0]$
28 direction possess inverse Burgers vectors.
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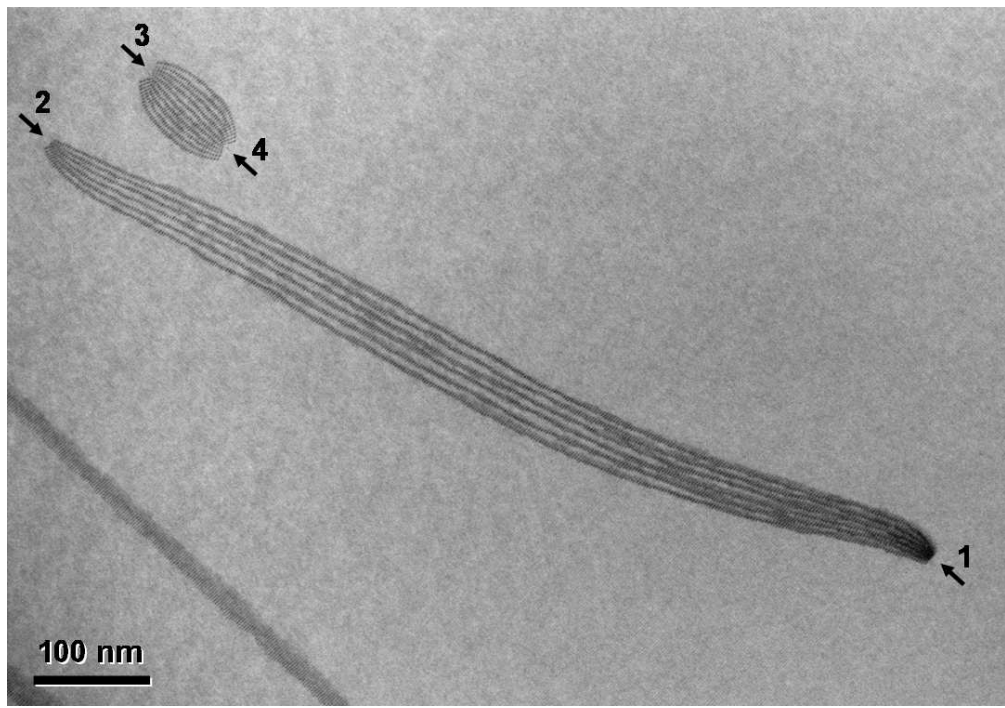


Figure 1
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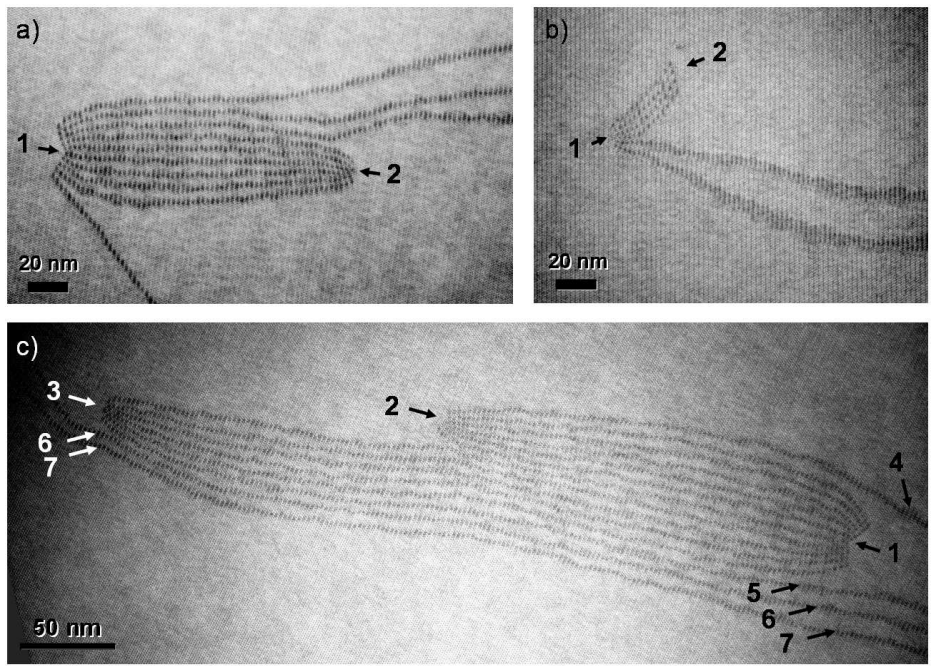


Figure 2
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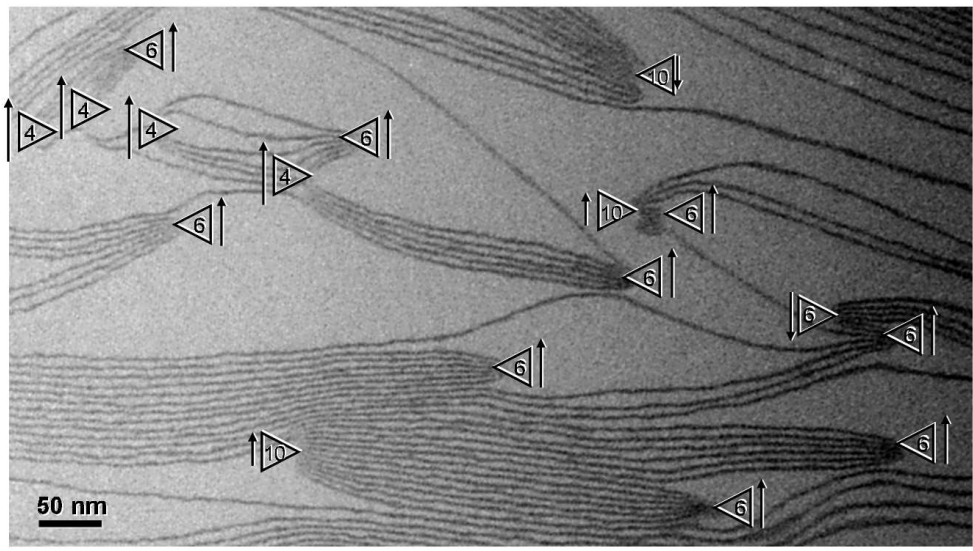
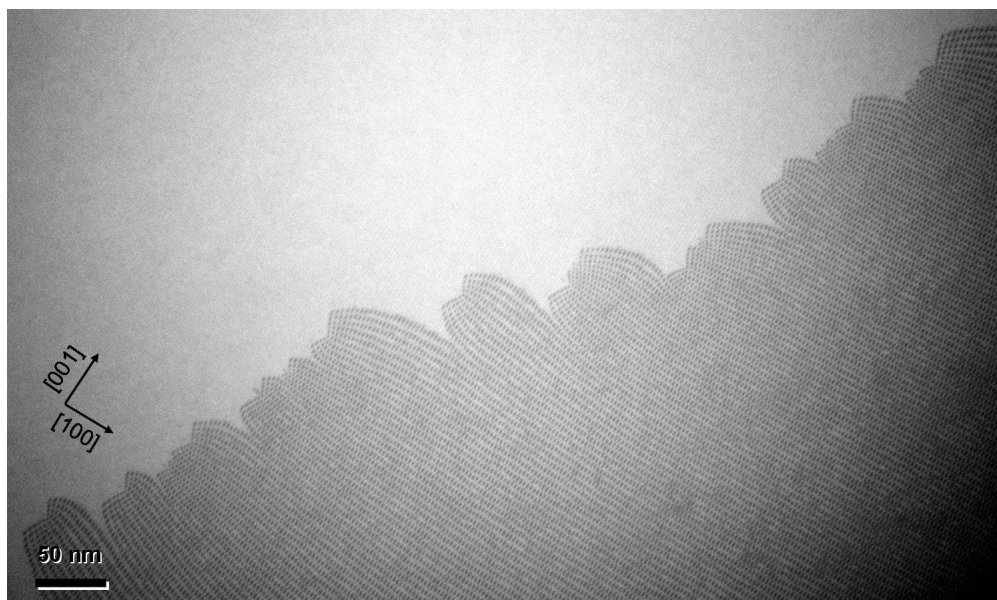


Figure 3
230x130mm (150 x 150 DPI)

Review Only



28 Figure 4
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