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STAR-LISCLINATION IN A FERRO-ELASTIC MATERIAL B19 MgCd ALLOY

Y. KITANO, K. KIFUNE and Y. KOMURA

Department of Materials Science, Faculty of Science, Hiroshima University, Higashi-senda-machi, Naka-ku, Hiroshima 730, Japan

Disclinations in thin crystals of MgCd alloy are demonstrated by high resolution electron microscopy. The disclinations appear along the intersection lines of twin boundaries which occur due to spontaneous lattice deformations at the phase transition temperature. A star-disclination which is not an intersection line comes out to compensate the strain field of the disclinations. A single disclination is seldom observed but dipoles, tripoles, quadrupoles and multiples of disclinations are found in stable crystals.

I. INTRODUCTION

In this paper particular arrangements of crystal domains observed in the B19 MgCd alloy explained by the special distribution of linear defects called disclinations. The B19 MgCd alloy shows a spontaneous lattice deformation and exhibits a typical behaviour of the ferro-elastic materials\cite{1,2,3} at the phase transition temperature, where the hcp structure (P6\textsubscript{3}/mmc) with \(a_0 = 0.31473\), \(c_0 = 0.51616\) nm of the higher temperature phase transforms into the B19 orthorhombic structure (Pcmm) with \(a_0 = 0.52700\), \(b_0 = 0.32217\), \(c_0 = 0.50051\) nm of the lower temperature phase.

Details on crystal structures of the alloy were described in the previous paper\cite{4} which will be called Paper I. In Paper I it was confirmed that crystallographic planes of the domain boundary are \((310)\) and \((110)\) of the orthorhombic indices. The former is called a reflection twin boundary, and the latter a rotation twin boundary. Sample preparation and other experimental details were also described in Paper I.

We have also pointed out in a short report\cite{5} which will be called Paper II that intersections of two or more boundary planes are linear defects called disclination and all possible disclinations were tabulated. In the present paper we demonstrate the existence of various types of disclinations in the MgCd alloy as well as the special distribution of them such as dipoles, tripoles, quadrupoles and multiples of disclinations.

In Chapter II we will describe the definition of the wedge type disclinations, and in Chapter III the twin boundaries which occur owing to lattice deformation are defined as disclinations. In Chapter IV we will discuss forty-three disclinations which occur in the alloy. Especially we will show a brief explanation of the star-pattern being a disclination. In Chapter V several examples of the characteristic domains are presented and they are explained with special arrangements of the disclinations.

II. DEFINITION OF WEDGE TYPE DISCLINATIONS

A disclination is one of the linear defects in crystals and is approximately specified with a vector \(\Theta\) which is defined as \(\Theta = \omega \Theta_0\) where \(\omega = 360 - \phi\), \(\Theta_0\) is a unit vector in a direction of a rotation axis, and \(\phi\) a rotation angle of a given circuit around a disclination line in an unstrained reference crystal. This circuit corresponds to a reference

\begin{figure}[h]
  \centering
  \includegraphics[width=0.5\textwidth]{wedge_type_disclination}
  \caption{Wedge type disclination.}
\end{figure}
circuit which is used for the determination of a Burgers vector of a dislocation. If a wedge type of gap appears in a reference crystal as shown in Fig. 1, the disclination is defined as a positive vector. To the contrary, if a wedge type of overlap appears in a reference crystal, the disclination is a negative vector.

III. TWIN BOUNDARY AS A DISCLINATION

In this chapter the twin boundaries which spontaneously occur due to the crystal deformation will be defined as disclinations. As shown in Figs. 2(a) and 2(b) we assume a deformation of a rectangle from LKGF to L2K2GF on the left side of the boundary and deformation from LHED to L1H1ED on the right side. Supposing Point 0 is only a point which is fixed on the boundary, then two crystals would produce a gap at a boundary in the upper side of Point O, but would produce an overlap in the lower side of Point O.

If we give a polarity to the twin boundary and assume the boundary OL to be positive and the boundary OT to be negative, we can reasonably assign a positive boundary OL a positive disclination, because a wedge type of gap L1OL2 is produced if Point O is fixed. On the other hand we can assign a negative boundary OT a negative disclination, because a wedge type of overlap T1OT2 is produced. Here we use the abbreviations m- or m-boundary to a positive or a negative reflection twin boundary on the (310) plane, and r- or r-boundary to a positive or a negative rotation twin one on (110). Therefore the boundary OL in Fig. 2(a) or 2(b) is a disclination with a positive vector and is abbreviated to m- or r-boundary, respectively. The boundary OT in Fig. 2(a) or 2(b) is also a disclination with a negative vector and is abbreviated to m- or r-boundary. If we use the lattice parameters mentioned in Chapter I, the m-boundary is a disclination of 2.80° and the m-boundary of -2.80°, and the r- and r-boundary are those of 2.88° and -2.88°. We summarize the definition of the boundary in Fig. 3.

Fig. 3. Definition of the polarity of boundaries. A mark O denotes intersection.

We, however, must note that any type of twin boundary is not itself a disclination and have no strain field. This is easily verified as follows; drawing a reference circuit around the fixed point such as Point O in Fig. 2, a boundary crossing the circuit at the upper side of Point O is a positive disclination but the other boundary crossing the circuit at the lower side of Point O is a negative one. As the magnitude is the same for both, the twin boundary is a zero disclination in total. It is very natural that the twin boundary is not a disclination.
IV. FORTY-THREE DISCLINATIONS

Out of 43 disclinations, 42's are intersections of two or more boundary planes which appear during phase transition. The 43rd disclination is the star-pattern which consists of special arrangement of disclination No.1.

IV-1. Intersections

It has been found that the 42 types of intersections are possible. [2,4] These intersections are all recognized to be disclinations if the strain field around them is not released by creation or annihilation of dislocations. These disclinations were listed in Paper II. In Paper II the polarities of the boundary were defined contrary to this paper. Therefore $m$ and $r$ in Table I and Fig. 2 of Paper II must be replaced by $\bar{m}$ and $\bar{r}$, and $m$ and $r$ by $\bar{m}$ and $\bar{r}$.

Out of 42 disclinations, schematic drawing of smaller twenty-four ones are presented in Fig. 4. Below each, a sequence number named in Paper II and an angle $\omega$ are attached. In the parentheses net numbers of the twin boundaries which cross the reference circuit are written; the former and the latter correspond to the net numbers of the reflection and rotation boundaries. For example of No.9, the reference circuit will meet with two $\bar{m}$-, two $r$- and one $\bar{r}$-boundaries. Therefore, the circuit effectively meets with two $\bar{m}$- and one $r$-boundaries. From these numbers disclination angles can be estimated.

Fig. 4. Twenty-four intersections appearing in MgCd.
IV-2. Star-disclination

The 43rd disclination (No.43) is not an intersection of the boundary planes but a special arrangement of several crystal domains with a similar shape. This is illustrated in Fig. 5. The star-pattern is found to be a disclination with \(-0.24^\circ\) and was cited as No.3 at the bottom of Table I of Paper II. In order to explain that the star pattern is a disclination we draw a circuit around its center and sum up the vectors for all the boundary disclinations which cross the circuit. From Fig.5, we easily find that the circuit meets three \(m\)-boundaries and three \(\tilde{r}\)-boundaries. Since an \(m\)-boundary is equal to a disclination with \(2.80^\circ\) and an \(\tilde{r}\)-boundary to a disclination with \(-2.88^\circ\), the total becomes equal to \(-0.24^\circ\). This means that the star-pattern is itself a disclination having \(-0.24^\circ\).

V. DISTRIBUTION OF THE DISCLINATION LINES

V-1. General Observations and Dipoles of Disclinations

As shown in Photo. 1, we have observed very artistic domain structures of the B19 MgCd alloy below the structural phase transition temperature. Above the phase transition temperature this area was a single domain of the hcp structure. Decreasing the temperature the domain structures such as in Photo. 1 appear. All the boundary planes are either \(r\)-boundary on (110) or \(m\)-boundary on (310). From the high resolution images such as Photo. 1, we have the information of not only the type of the boundary, i.e. \(r\)- or \(m\)-boundary, but also the polarity. Many intersections of the boundary planes are observed in Photo. 1. Each intersection corresponds to one of the 42 disclinations. All the intersections in the image are identified and several intersections are named by referring to the sequence numbers.
of Fig. 4. Near the center of the photograph we find star-patterns. As verified in Chapter IV this pattern is itself a disclination with -0.24° and is called a star-disclination in this paper.

It is easily recognized that the disclinations with an opposite direction are likely to come together in a short distance and to produce a disclination dipole. In Photo. 1 examples of the disclination dipole consisting of No.6 and No.8, and No.8 and No.11 are indicated by D1 and D2, respectively.

V-2. Tripoles, Quadrupoles and Multipoles of Disclinations

We can find not only dipoles, but also tripoles and quadrupoles of disclinations in the real crystals of the B19 MgCd alloy. An example of quadruple is given by Q in Photo. 2, which consists of four disclinations, Nos. 6, 8, 15 and 12.

A typical example of the multipole is found in Fig. 6 by a schematic drawing. This is one of the most typical domain structures which were exhibited by the MgCd alloy. A set of dark field images of this area was reported in Paper I. This pattern is the best example for demonstrating the distribution of the disclinations. It has been found that so far as all the disclinations in this area are concerned, the center of the positive disclinations indicated by P is almost the same position of the center of the negative disclinations indicated by N in Fig. 6.

An example of a triple of the disclinations is seen in the schematic drawing Fig. 6 and indicated by 4 in the right lower corner. This disclination is identical with No.4 disclination if all the twin boundary planes meet at one point, but the meeting point separates into three points corresponding to three intersections Nos.9, 24, 9 or 13, 18, 13, respectively.

VI. DISCUSSION

VI-1. Role of Star-disclination

It is important to remark that there are three disclinations of the intersection with small positive values less than 1° such as Nos. 2, 3 or 4 of Fig. 4, but there is no disclination of intersection with a small negative value. In order to compensate the strain fields of disclinations of No.2, 3 or 4, the star-disclination which is a small negative one is necessarily produced maybe at the last stage of the domain growth. Some examples of high resolution images of the center of the star-disclination were given in Paper I.
VI-2. Boundary Steps near Intersections

As shown in Photo. 3, some boundaries curve near the intersection or the center of the disclination. Many steps of the boundary occur accompanying the boundary dislocations. These dislocations may have the role to release the remaining strain field around the disclinations dipoles, tripoles, quadrupoles or multipoles which mainly release the strain fields in the crystals.

Photo. 3. A high resolution image showing the curves of the boundaries near the intersections, i.e. the disclinations.

VII. CONCLUSION

Grain boundary structures observed in the B19 MgCd alloy were explained by dipoles, tripoles, quadrupoles and multipoles of various type of disclinations which are not released by crystal dislocations. The star-pattern is verified to be one of disclinations having $-0.24^\circ$ and may be necessarily produced to compensate the strain fields of the disclinations having the same magnitude but being opposite in sign.

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