Orientation relationship and structure of lithium precipitates in MgO single crystals

M. Treilleux, G. Chassagne

► To cite this version:

M. Treilleux, G. Chassagne. Orientation relationship and structure of lithium precipitates in MgO single crystals. Journal de Physique Lettres, 1979, 40 (13), pp.283-286. 10.1051/jphyslet:019790040013028300 . jpa-00231625

HAL Id: jpa-00231625

<https://hal.science/jpa-00231625>

Submitted on 1 Jan 1979

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Classification

Physics Abstracts

61.50C — 61.16D

Orientation relationship and structure of lithium precipitates in MgO single crystals^(*)

M. Treilleux and G. Chassagne

Département de Physique des Matériaux (*), Université Claude-Bernard Lyon I,
43, boulevard du 11-Novembre-1918, 69621 Villeurbanne Cedex, France

(Reçu le 19 mars 1979, accepté le 14 mai 1979)

Résumé. — Des précipités de lithium sont obtenus par recuits thermiques de monocristaux d'oxyde de magnésium implantés avec ce métal. Ceux de taille inférieure à 200 Å ont une structure inhabituelle cubique à faces centrées ($a = 4,4$ Å) et sont en orientation simple avec la matrice. Lorsque leur taille est supérieure à 400 Å, leur structure est cubique centrée ($a = 3,51$ Å) et leur orientation par rapport à la matrice est :

$$(011) \text{ Li} // (111) \text{ MgO et } [11\bar{1}] \text{ Li} // [0\bar{1}1] \text{ MgO.}$$

Abstract. — Lithium precipitates are obtained by thermal annealing of magnesium oxide single crystals implanted with this metal. Those under 200 Å size have an unusual face-centred cubic structure ($a = 4.4$ Å) and are in simple orientation with the matrix. For a size above 400 Å, the structure is body-centred cubic ($a = 3.51$ Å) and the orientation with respect to the matrix is :

$$(011) \text{ Li} // (111) \text{ MgO and } [11\bar{1}] \text{ Li} // [0\bar{1}1] \text{ MgO.}$$

1. Introduction. — Lithium precipitates in a dielectric matrix have been identified by X-ray diffraction : M. Lambert *et al.* [1, 2] (LiF irradiated with thermal neutrons) and Gordon S. Smith [3] (LiH irradiated with γ rays). However, these precipitates could not be observed directly by transmission electron microscopy, because, in these materials, the electron beam very quickly creates point defects which make the observation impossible. Consequently it is interesting to observe directly such precipitates in a MgO matrix without defects created by electronic irradiation and with a lattice parameter (4.213 Å) very close to those of LiF (4.02 Å) or LiH (4.08 Å).

In a previous letter [4], we concluded that lithium precipitates could have two different structures : face-centred cubic and body-centred cubic. In this letter, we shall determine the lithium parameter in its face-centred cubic structure from the measurement of the spacing of the moiré fringes. Then, we shall study more particularly the orientation of the body-centred cubic lithium precipitates with respect to the MgO matrix, and we will compare our results with those obtained in LiF [1, 2] and in LiH [3].

2. Study of lithium precipitates by transmission electron microscopy. — Lithium precipitates are obtained after thermal annealing of Li^+ ions implanted in magnesium oxide single crystals [4]. The samples are implanted in the $\langle 100 \rangle$ direction with 250 keV or 60 keV ions of up to about 10^{17} ions. cm^{-2} flux. The mean projected range R_p is, in these conditions, 6 500 Å and 2 900 Å with standard deviations in projected range of 800 Å and 540 Å respectively for the two energies considered. The thin foil preparation technique has been described in two previous articles [4, 5].

For a 973 K thermal annealing, the precipitates are under 150 Å in size and they all have the unusual face-centred cubic structure. They are in simple epitaxy with the matrix :

$$(001) \text{ Li} // (001) \text{ MgO and } [100] \text{ Li} // [100] \text{ MgO.} \quad (1)$$

For a 1 073 K thermal annealing, their size is under 350 Å, and most of them have the face-centred cubic structure. Nevertheless the larger ones already have the body-centred cubic structure (A — Fig. 1a). For 1 173 K thermal annealing, the size is under 1 000 Å and most of them have the body-centred cubic structure.

(*) La version française a été acceptée aux C.R.A.S.

(*) Associé au C.N.R.S.

Fig. 1. — MgO implanted with 60 keV Li^+ ions (10^{17} ions. cm^{-2}) and annealed at 1 073 K : moiré fringes (dark field) in Li precipitates : a) $\mathbf{g} = (1\bar{1}1)$; b) $\mathbf{g} = (\bar{1}11)$; c) $\mathbf{g} = (111)$; d) $\mathbf{g} = (1\bar{1}\bar{1})$.

3. **Determination of the lattice parameter of face-centred cubic precipitates.** — On the dark field micrographs of figure 1, obtained under Bragg conditions, on several (111) matrix reflections, we can see moiré fringes (perpendicular to $\mathbf{g}$: parallel moiré) inside precipitates. These equally spaced fringes exist whatever the vector $\mathbf{g}$ may be. However, for some precipitates (A — Fig. 1), we only observe fringes for one type of vector $\mathbf{g}$, and with a larger spacing. These precipitates are larger than the previous ones and they then have the usual body-centred cubic structure.

The measured moiré spacing of first type precipitates (f.c.c.) is : $D = 53 \text{ \AA}$.

Now, in the case of parallel moirés, the spacing is connected to the matrix d_0 and precipitate d_1 interplanar distances by the relation :

$$D = \frac{d_0 d_1}{|d_0 - d_1|} \simeq \frac{d_0^2}{|d_0 - d_1|}$$

if $d_1 \simeq d_0$, which is generally the case when moiré fringes are obtained.

The interplane distance misfit between matrix and precipitate is given by :

$$\delta = \frac{d_0 - d_1}{\frac{d_0 + d_1}{2}} \simeq \frac{d_0 - d_1}{d_0}$$

therefore $D \simeq \pm \frac{d_0}{\delta}$, whether d_0 is above or under d_1 .

From the spacing value ($D = 53 \text{ \AA}$), knowing the (111) MgO interplanar distance ($d_{(111)} = 2.431 \text{ \AA}$), we can calculate δ :

$$\delta = \pm \frac{d_0}{D} = \pm 4.6 \%$$

The precipitate being in simple epitaxy with the matrix (orientation 1), the interplanar distance misfit

The interplanar distance misfit between parallel planes is : $\delta = -2.1\%$, and for (111) matrix reflection the moiré spacing must be : $D = 116 \text{ \AA}$.

The measured spacing for the body-centred precipitates (Figs. 1a and 2d) is in good agreement with this calculated value.

5. Discussion. — For face-centred cubic lithium, the calculated lattice parameter can be 4.0 or 4.4 Å. The distance deduced between nearest neighbouring atoms can be 2.8 Å or 3.1 Å. Now, the distance between nearest neighbours of body-centred lithium is 3.04 Å, and A. Julg *et al.* [6] have pointed out that, for the Li face-centred cubic structure, it must be larger; the face-centred cubic structure will exist only for a 3.12 to 3.16 Å distance between nearest neighbours. Therefore the 4.0 Å parameter value seems to be excluded, and in our study the admissible parameter value for face-centred cubic lithium precipitates is 4.4 Å.

By plastically deforming lithium at 77 K, C. S. Barrett [7] obtained a f.c.c. phase. In these conditions, the measured lattice parameter (4.41 Å) is very close to the value we have just determined.

In the case of body-centred cubic lithium, we find that the close-packed atomic planes of the two materials coincide. For MgO, only the {111} planes contain one kind of atom (Mg or O). Moreover, we notice that the interplanar distances of (110) lithium and (111) MgO planes are very close. It is probably these three conditions together which entail the parallelism of (011) lithium and (111) magnesium oxide planes.

Also, for lithium, the orientation relationship between the usual b.c.c. phase and the f.c.c. one (observed when the precipitate was smaller, orientation 1) is as follows :

$$(011) \text{Li}_{\text{b.c.c.}} // (111) \text{Li}_{\text{f.c.c.}}$$

and

$$[1\bar{1}\bar{1}] \text{Li}_{\text{b.c.c.}} // [0\bar{1}\bar{1}] \text{Li}_{\text{f.c.c.}}$$

This orientation relationship between the two structures is exactly that obtained by C. S. Barrett [8] for the martensitic transformation of lithium.

Nevertheless, the orientation (2) is different from that observed by M. Lambert *et al.* [2] :

$$(110) \text{Li} // (111) \text{LiF} \text{ and } \langle 110 \rangle \text{Li} // \langle 211 \rangle \text{LiF}$$

and by Gordon S. Smith [3] :

$$\{110\} \text{Li} // \{111\} \text{LiH} \text{ and } \langle 100 \rangle \text{Li} // \langle 110 \rangle \text{LiH}$$

which furthermore are equivalent expressions of the same orientation.

The coinciding planes are the same, but in these planes the common directions are different. We nevertheless note that these two orientations can be derived from that observed in our study by a 5.3° rotation.

To attempt an explanation of the difference, in table I we have recorded the interatomic distances in the $\langle 110 \rangle$ and $\langle 211 \rangle$ directions for MgO, LiF and f.c.c. Li, and in table II, the interatomic distances in the $\langle 110 \rangle$ and $\langle 111 \rangle$ directions for b.c.c. lithium.

Table I

	MgO	LiF	LiH	f.c.c. Li
$\langle 110 \rangle$	2.98 *	2.84	2.89	3.12 *
$\langle 211 \rangle$	5.16	<u>4.92</u>	<u>5.01</u>	5.40

Table II

	$\langle 110 \rangle$	$\langle 111 \rangle$
b.c.c. Li	<u>4.96</u>	3.04 *

(Interatomic distances in the indicated directions for MgO, LiF, LiH, f.c.c. and b.c.c. Li.)

We find out, that for the atoms located in the b.c.c. (110) Li and (111) MgO, LiF, LiH or f.c.c. Li planes, the best agreement for interatomic distances is observed in different rows :

$\langle 211 \rangle$ LiF or LiH parallel to $\langle 110 \rangle$ (b.c.c.) Li (underlined values), and $\langle 110 \rangle$ MgO (Fig. 4) or f.c.c. Li parallel to $\langle 111 \rangle$ b.c.c. Li (values marked with an asterisk).

In our study, the coincidence between rows giving the best agreement for interatomic distances entails the relative orientation between (110) b.c.c. Li planes and (111) matrix (MgO) planes.

References

- [1] LAMBERT, M. and GUINIER, A., *C.R. Hebd. Séan. Acad. Sci.*, Paris **246** (1958) 1678.
- [2] LAMBERT, M., MAZIERES, Ch. and GUINIER, A., *J. Phys. Chem. Solids* **18** (1961) 129.
- [3] SMITH, Gordon S., *J. Phys. Chem. Solids* **36** (1975) 797.
- [4] TREILLEUX, M. and CHASSAGNE, G., *J. Physique Lett.* **40** (1979), to be published.
- [5] TREILLEUX, M., THEVENARD, P., CHASSAGNE, G., HOBBS, L. W., *Phys. Status Solidi* **48** (1978) 425.
- [6] JULG, A., BENARD, M., BOURG, M. GILLET, M. and GILLET, E., *Phys. Rev. B* **9** (1974) 3248.
- [7] BARRETT, C. S., *Phys. Rev.* **72** (1947) 245.
- [8] BARRETT, C. S., *Phase transformations in solids* (Wiley and Sons, New-York) 1951, p. 351.