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Crystal Structure of γ_2' Martensite in Au-47.5 at%Cd Alloy

By Takuya Ohba*, Yutaka Emura**, Shuichi Miyazaki* and Kazuhiro Otsuka*

Crystal structure of the γ_2' martensite in a Au-47.5 at%Cd alloy has been analyzed by the single crystal X-ray diffraction method. The lattice constants were $a=0.4859(11)$, $b=0.3151(1)$ and $c=0.4766(1)$ nm. The space group was Pcmm, with 4 atoms in the unit cell as Ölander reported. The structure was refined by the full-matrix least squares method to a final R factor of 4.7%, noticeably improved from that of Ölander. Moreover, the amount of shift of each atom from the ideal stacking positions in the hcp structure was discussed by using a hard sphere model of atoms; *e.g.* atoms in each layer are not arranged centro-symmetric.

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I. Introduction

The Au-47.5 at%Cd alloy has attracted much attention of researchers for many years for the shape memory effect[1] and early application of the phenomenological crystallographic theory[2] and a unique property called rubber-like behavior[3]-[4]. The phenomenological theory was successfully applied to this alloy to predict the crystallographic parameters such as the habit plane, the shape strain in the martensitic transformation[2]. The rubber-like behavior occurs by a reversible twin boundary movement after stabilization (aging) in the γ_2' martensitic state for about 50.4 ks(14 h) or so at room temperature[4]. The origin for the phenomenon still remains unsolved, but it is clearly related to the stabilization effect. Lieberman *et al.*[5] proposed a mechanism, in which a twinning process is separated into twinning shear and shuffles, and that twinning shear occurs instantaneously but shuffling occurs gradually during aging. The stabilization effect increases the A_s temperature (reverse transformation start temperature) in general. The effect was observed in other β-phase alloys, such as Cu-Zn-Al and Cu-Al-Ni, and it is a serious problem in the practical applications of shape memory alloys[6]-[8]. The stabilization effect in this respect was also found in an Au-Cd alloy[9]. The origin for the stabilization is not understood yet, and the re-ordering of martensite is proposed to be responsible for the phenomenon[7].

The first step to understand the above behavior is to know the crystal structure of the martensite. Besides, if there is a structural change on aging or stabilization, it is very important to know the accurate structure in the martensitic phase. Furthermore, an exact equiatomic alloy Au-50 at%Cd shows a different mechanical behavior[10] and has a different crystal structure[11]. In order to clarify the difference between Au-50 at%Cd and Au-47.5 at%Cd, it is also important to determine the crystal structure accurately.

Table 1 The lattice constants of γ_2' martensite in Au-47.5at%Cd alloy.

at%Cd	a (nm)	b (nm)	c (nm)	Reference
47.5	0.4861	0.3150	0.4765	Ölander[12]
47.6	0.4861	0.3150	0.4765	Byström and Almin[21]
47.5	0.48644	0.31540	0.47645	Chang[22]
47.5	0.4859(11)	0.3151(1)	0.4766(1)	Present study

The structure of the γ_2' martensite was first analyzed by Ölander[12] in 1932 by using the X-ray powder diffraction method. The space group they reported was Pcmm, and their lattice constants are shown in Table 1, along with those measured by others. The positional parameters they determined will be described later. In 1977, Tadaki and Shimizu[13] re-examined the crystal structure by using a hard sphere model and gave atomic positions derived from the model, which were different from those reported by Ölander. They calculated structure factors for both structures and compared them with observed electron diffraction patterns. Although they concluded their positional parameters were more reliable than Ölander's, the comparison was not quantitative. No quantitative analysis has been made for this martensite since Ölander's work. One of possible reasons for this lies in the difficulty of obtaining a single crystal of the martensite.

In this paper, structure determination of a Au-47.5 at%Cd alloy is carried out by using a single crystal obtained under a tensile stress.

II. Experimental

An alloy ingot with nominal composition of Au-47.5 at%Cd was prepared by melting 99.99%Au and

* Institute of Materials Science, University of Tsukuba, Tsukuba, Ibaraki 305, Japan.
** Graduate Student, Doctoral Program in Engineering, University of Tsukuba, Tsukuba, Ibaraki 305, Japan.