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# Structural Study of R-Phase in Ti-50.23 at.%Ni and Ti-47.75 at.%Ni-1.50 at.%Fe Alloys

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The crystal structure of the R-phase was determined by combined use of the electron diffraction and the powder X-ray diffraction method. The Rietveld method was applied for the analysis of the powder diffraction data. The structure of the R-phase belongs to the space group $P3$ and is similar to that of $\zeta_2'$ Au-Cd martensite. The deviations of the atomic coordinates from the mirror plane of the $P\bar{3}1m$ are smaller than that of $\zeta_2'$ Au-Cd. The convergent beam electron diffraction patterns were also observed and discussed with the results.

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## I. Introduction

The R-phase transformation in Ti-Ni(-X) alloys is now widely used in the industrial application of the shape memory effect or superelasticity. The study of the R-phase began with the discovery by Dautovich *et al.*[1] Since then many studies have been done on its characteristic properties and many interesting and useful properties were found[2].

Concerning the crystal structure of the R-phase, there are a few reports. Several researchers explained that the R-phase belonged to the rhombohedral crystal system with the interpretation of shuffling on every three $(1\bar{1}0)_{B2}$ plane and distortion along the $[111]_{B2}$ direction of the parent phase[3]-[5]. Vatanayon and Hehemann[6] reported the crystal structure of the $\zeta_2'$ Au-Cd martensite and suggested the structure of the R-phase is similar to the $\zeta_2'$ Au-Cd martensite. Goo and Sinclair[7] studied the space group of the R-phase using the convergent beam electron diffraction (CBED). They reported that the space group of the R-phase is $P\bar{3}1m$. However, the crystal structure of the R-phase was not solved.

The mechanism of the martensitic transformation is an important issue. The Ti-Ni alloy has been studied for this purpose. Vatanayon and Hehemann[6] pointed out that the transformation mechanism of the Ti-Ni R-phase is similar to that of the $\zeta_2'$ Au-Cd alloy. They explained the transformation with longitudinal waves. Hwang *et al.*[8] reported that an incommensurate phase appears prior to the R-phase transformation. Several researchers[9][10] measured phonon dispersion relation in the parent phase and found a phonon anomaly around $1/3[110]^*$. Shapiro *et al.*[11] studied the diffuse scattering and reported that it appears at 1/3 of the $[110]^*$ direction as a precursor phenomenon. For the study of the transformation mechanism, it is necessary to determine the crystal structure of the R-phase. The situation is similar in the Au-Cd alloy. Although, the structure of the $\zeta_2'$ Au-Cd martensite was not determined for a long time, it was recently solved with the space group $P3$[12]. Based on the result, a transformation mechanism was proposed and phonon softening was found to support it[13].

The purpose of the present paper is to determine the crystal structure of the R-phase by means of X-ray and electron diffraction techniques.

## II. Experimental Procedure

Binary Ti-Ni and ternary Ti-Ni-Fe alloys were used for the X-ray and electron diffraction experiments, respectively. Compositions of the specimens and the conditions of the heat treatments were chosen to obtain the stable R-phase at room temperature. Details of the specimen preparation are described below.

### 1. Electron microscopy experiments

The composition of a 50.75 at.%Ti-47.75 at.%Ni-1.50 at.%Fe ternary alloy was chosen. A part of the specimens were made from a rod shaped sample with a diameter of 10 mm provided by the Tokin corporation. The rest of the specimens were made from the button shaped ingots made by Ar arc melting. The solution treatment condition was made at 1273 or 1223 K following ice water quench. After the heat treatment, differential scanning calorimetry (DSC) measurements were done to check the transformation temperatures. The transformation temperatures of the specimens heat-treated at 1273 K were as follows: $M_s'$=310 K, $M_f'$=299 K, $M_s$=284 K

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