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Phonon Softening in Au–49.5 at%Cd Alloy

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Phonon softening was observed in the parent phase of a AuCd alloy which transforms from the β_2(B2) parent to ζ_2'(trigonal) martensite at M_s=304 K. Since Cd strongly absorbs neutrons, the isotope ^{114}Cd was used in preparing the single crystal for the measurements. The $[\zeta\zeta 0]TA_2$(u//$[1\bar{1}0]$) phonon branch was measured and found to be anomalously low. A minimum is present at ζ=0.35 which softens as M_s approaches from above. The results are consistent with the model proposed by Ohba *et al.* [Materials Trans. JIM **33** (1992) 29] based upon a crystallographic study of the ζ_2' phase.

KEYWORDS: Au–Cd alloy, β phase alloy, neutron diffraction, phonon softening, phonon dispersion curve, isotope ^{114}Cd, martensitic transformation

1. Introduction

The Au–Cd alloy is one of the most interesting and extensively studied materials which exhibit martensitic transformations. Near the equiatomic composition, the high temperature phase, called the β-phase, possesses the CsCl type structure, while in the low temperature phase, there are two martensitic phases called γ_2' and ζ_2'. The structure of γ_2' martensite was determined by Ölander[1] in 1932 by X-ray powder diffraction, and then reexamined by Tadaki and Shimizu using electron diffraction and a hard sphere model.[2] The more accurate structure determination of γ_2' phase was made by Ohba *et al.*[3] using single crystals of the martensite. The ζ_2' phase was first found by Köster and Schneider in 1940.[4] After their report, various crystal structure of the ζ_2' phase were proposed. Ledbetter and Wayman[5] critically reviewed these studies. Vatanayon and Hehemann[6] reported the structure to have the space group P$\bar{3}$1m with 18 atoms in a unit cell. However, they did not show any detail of the structure analysis nor the reliability, R factor for the structure determination. The precise structure of ζ_2' martensite phase remained unsolved for a long time and the transformation mechanism had not been clarified. Recently, however, the structure of the ζ_2' martensite was determined using X-ray diffraction on a stress-induced martensite single crystal and a transformation mechanism was proposed by Ohba *et al.*[7] They found the space group to be P3 rather than P$\bar{3}$1m. Furthermore, they described the transformation mechanism by the superposition of three $\langle 110\rangle\langle 1\bar{1}0\rangle$ transverse displacement waves along with their higher harmonics. Since $\langle 110\rangle\langle 1\bar{1}0\rangle$ shear occurs every three (110) plane, the softening of $[\zeta\zeta 0]TA_2$ phonon mode is expected at $\zeta=1/3$.

Inelastic neutron scattering technique is the only method to observe the phonon softening at finite wave vectors. However, Au, and especially Cd, have a large neutron absorption coefficient which makes an experiment nearly impossible. By use of the isotope ^{114}Cd, the absorption coefficient is reduced by a factor of 1/2000 and the difficulty of absorption has been overcome.

2. Experimental

The single crystal was grown from 99.99%Au and 99. 5%Cd by the Bridgman method. The isotope ^{114}Cd was provided by Advanced Materials Tech. The composition was $Au_{50.5}Cd_{49.5}$ and the size of the sample was approximately 5 mm in diameter and 50 mm long with the [001] direction along the long axis. The lattice parameter at T=400 K is a=0.331 nm and the sample mosaic is uniform and less than 10′. The martensite start and finish temperature (M_s, M_f) was 304 K and reverse transformation start (A_s) and finish (A_f) temperatures were 308 and 316 K, respectively. These temperatures were determined by measuring the intensity of the 110 reflection of the parent phase. The sample was placed in an aluminum can filled with He gas and attached to be cold finger of a closed-cycle refrigerator. The neutron experiments were performed at H4M spectrometer at the High Flux Beam Reactor located at Brookhaven National Laboratory. Pyrolytic graphite crystals were used for the monochromater and analyzer and a filter in the scattered beam. The fixed final energy of the neutrons was 14.7 meV. Collimators used for most of the experiments were 40′ through the spectrometer.

The (001) scattering plane allowed us to measure the $[\zeta\zeta 0]TA_2$ phonon branch in the parent phase about the [110] reciprocal lattice plane. This phonon branch corresponds to a sliding of the closed packed {110} planes along $\langle 110\rangle$. In the limit of $\zeta\rightarrow 0$ the slope corresponds to the elastic constant $C'=(C_{11}-C_{12})/2$.

3. Results and Discussion

Figure 1 shows the spectra of scattered neutrons measured at ζ=0.35 for four different temperatures. Least squares fitting of the peaks with polynomial was done and shown in the figure simultaneously. The peak position which is 1.4 meV at 425 K and shifts toward lower energy with decreasing temperature. At 306 K, just above M_s, the peak has shifted to 0.8 meV.

The phonon dispersion curves of the other $[\zeta\zeta 0]$ LA and TA branches are shown in Fig. 2. The low lying TA_2 branch at various temperatures is shown as well as