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Phonon dispersion curves in disordered $Cu_{0.715}Pd_{0.285}$ alloy

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Abstract. Both the atomic short-range order diffuse intensities and the phonon frequencies along the high-symmetry directions for disordered $Cu_{0.715}Pd_{0.285}$ alloy were measured using neutron experiments, to investigate the relationship between the diffuse maxima due to the atomic short-range order and the Kohn anomalies. The observed phonon dispersion curves were compared with the curves calculated from the second-nearest-neighbour Born–von Karman model. There were no anomalies in the phonon dispersion curves themselves or their derivatives under our experimental conditions. An improvement in energy resolution would be required to search further for the Kohn anomalies in this alloy system.

1. Introduction

Krivoglaz (1969) has pointed out that the form of the Fermi surface of a disordered alloy is reflected in the distribution of atomic short-range order (ASRO) diffuse scattering of x-rays, neutrons and electrons through anomalies which are similar to those predicted by Kohn for phonon scattering and due to the pairwise interaction potential caused by conduction electrons in the alloy. By extending this idea of Krivoglaz, Moss (1969) has noted that the shape of the Fermi surface in disordered Cu–Au alloys was indeed imaged in the diffuse scattering via the singularity in $\chi(q = k_F)$, where k_F is the Fermi wavevector. Ohshima and Watanabe (1973) have already measured the composition-dependent diffuse scattering intensity distributions from disordered Cu–Pd alloys by electron diffraction. The inset in figure 1 shows the schematic illustration of diffuse scattering from disordered Cu–Pd alloys for reference. Twofold and fourfold splittings of diffuse scattering are observed at 100, 110 and their equivalent positions in reciprocal space and the separation m of split diffuse maxima increases with increasing Pd content. This result can be interpreted well using the Krivoglaz–Moss idea. Gyorffy and Stocks (1983) have calculated the Fermi surfaces for the disordered Cu–Pd alloys on the basis of a self-consistent-field KKR CPA calculation. They argued that the observed composition-dependent diffuse maxima in the electron diffraction intensities are due to parallel sheets of flat Fermi surfaces. It is, therefore, confirmed that the positions of diffuse maxima are directly related to the Fermi vector. Rao *et al* (1984) have also calculated the electronic structure of copper-rich Cu–Pd alloys with KKR CPA computation. Recently, Chou *et al* (1990) have measured the phonon frequencies along high-symmetry directions of disordered $Cu_{0.84}Al_{0.16}$ alloy at room temperature to investigate the relationship between the diffuse maxima due to ASRO and the Kohn anomalies in the phonon dispersion curve. No strong anomaly was observed in the phonon dispersion itself or

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in its derivative near the expected wavevector $q = 2k_F$. They have pointed out in their paper that it is interesting to study the Kohn anomalies in the Cu–Pd alloy system due to the detailed calculation of Fermi surfaces in the system.

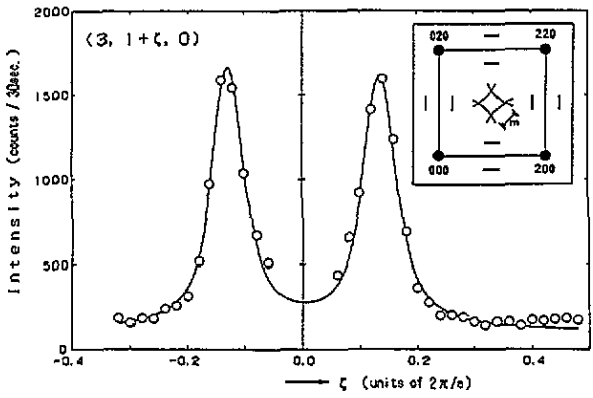

Figure 1. One-dimensional intensity distribution along the [010] direction from (3, 0.68, 0) to (3, 1.48, 0) where the $\lambda/2$ component was eliminated. The inset in the figure shows a schematic illustration of diffuse scattering from disordered Cu–Pd alloys.

We have, therefore, measured the phonon dispersion curves of disordered $Cu_{0.715}Pd_{0.285}$ alloy at room temperature by neutron inelastic scattering. The neutron diffuse scattering intensities were also obtained to compare the split diffuse maxima and Kohn anomalies.

2. Experimental details

An alloy was prepared in a high-purity alumina crucible by melting 99.99% pure Cu and Pd. A single crystal was grown by the Bridgman technique. A sample, 12 mm in diameter and 40 mm in length, was cut from the ingot. It was annealed at 1000 °C for 2 d and quenched into ice–water. The lattice parameter of the specimen was measured with an x-ray Debye–Scherrer camera using Cu Kα radiation. The specimen composition was determined by comparison with the lattice parameter versus composition relation (Pearson 1958). The composition was $Cu_{0.715}Pd_{0.285}$.

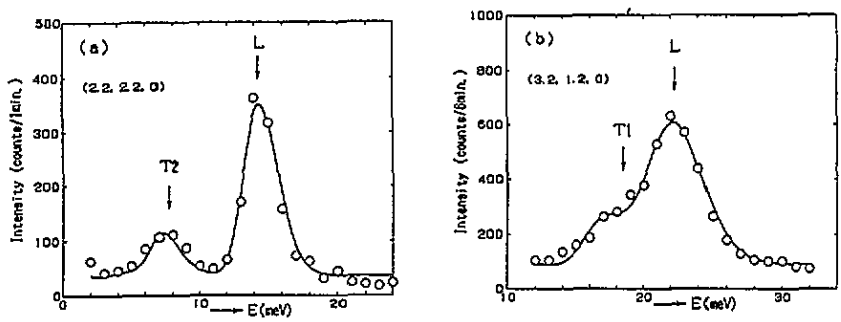

Figure 2. Example of the phonon peaks at (*a*) (2.2, 2.2, 0) and (*b*) (3.2, 1.2, 0) points: ——, least-squares fit with the instrumental resolution function.

The phonon frequencies were measured at room temperature for convenience on the triple-crystal spectrometer TOPAN at the JRR-3M reactor of the Japan Atomic Energy

Research Institute. Pyrolytic graphite was used as both a monochromator and an analyser. A pyrolytic graphite filter was used before the analyser to eliminate the higher-order contamination in the beam. Constant-Q scans were made with fixed final energy E_f = 30.5 meV. The collimations before the monochromator, before and after the sample and after the analyser were 40′, 30′, 30′ and 30′, respectively.

3. Results and discussion

The elastic diffuse scattering intensities were measured on the ($hk0$) reciprocal lattice plane. Fourfold split diffuse maxima due to ASRO were clearly observed around the 310 reciprocal lattice point with a good S/N ratio. Figure 1 shows an example of one-dimensional intensity distribution along the [010] direction from (3, 0.68, 0) to (3, 1.48, 0), together with fits using a Lorentzian distribution convoluted with the instrumental resolution function. In the figure the $\lambda/2$ component was eliminated by estimating the line shape of (620) Bragg reflection. The distance m between the diffuse maxima was found to be 0.095±0.01 in terms of the distance between the 000 and 200 Bragg points. This is in good agreement with that obtained by x-ray diffraction within the experimental error (m = 0.107±0.005 (Saha *et al* 1992)) and a little smaller than that estimated from the band-structure calculation by Gyorffy and Stocks (1983).

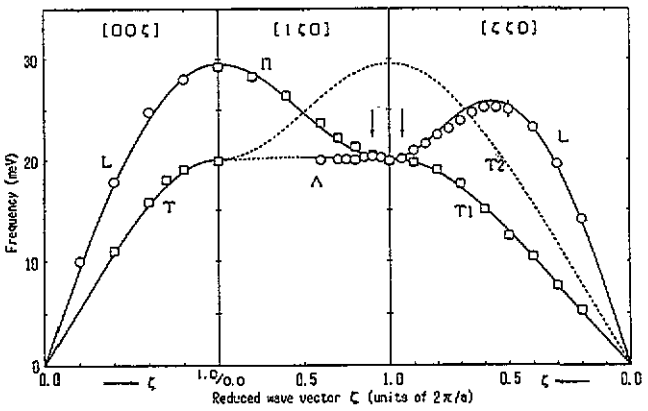

Figure 3. The phonon dispersion curves of $Cu_{0.715}Pd_{0.285}$ alloy for the [ζ00], [ζζ0] and [1ζ0] directions: ——, results for the second-neighbour Born–von Karman model. The point where the intensity maximum of ASRO diffuse scattering appears is indicated by an arrow.

Table 1. Interatomic force constants for disordered $Cu_{0.715}Pd_{0.285}$ alloy.

	Interatomic force constant (dyn cm^{-1})
$1xx$	15 790 ± 190
$1zz$	− 1 220 ± 240
$1xy$	17 360 ± 330
$2xx$	740 ± 430
$2xy$	− 1 810 ± 330

The phonon frequencies were measured along the high-symmetry directions [ζ00], [1ζ0] and [ζζ0]. Figures 2(a) and 2(b) show examples of observed phonon peaks at the (2.2, 2.2, 0) and (3.2, 1.2, 0) points, respectively, together with a least-squares fit with the instrumental resolution function. The peak position can be determined with a

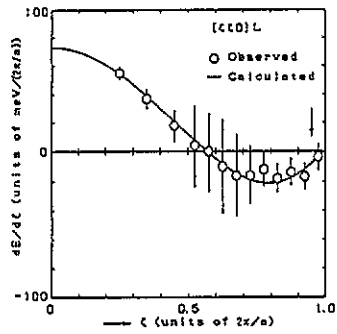

Figure 4. $dE/d\zeta$ for the (110)-L branch of $Cu_{0.715}Pd_{0.285}$ alloy. The point where the intensity maximum of ASRO diffuse scattering appears is indicated by an arrow.

standard deviation of 0.20 meV. Figure 3 shows the phonon dispersion curves for the three directions. The full curves in the figure represent the results for the fit to the Born-von Karman model. The interatomic force constants up to the second-nearest-neighbour distance, given in table 1, were used in this study because of the limited number of phonon dispersion curves. The point where the intensity maximum of ASRO diffuse scattering appears is indicated by an arrow. No apparent anomaly in the phonon dispersion curves was observed near the expected point by comparison with the full curve. We have, therefore, tried to search for an anomaly in the derivative of the phonon dispersion curves as Chou *et al* (1990) did for disordered $Cu_{0.84}Al_{0.16}$ alloy. Figure 4 shows the derivative of the phonon dispersion curves for the (110)-L branch. The full curve is the derivative calculated with the Born–von Karman fit. There is no systematic deviation between the observed and calculated curves around $\zeta = 0.95$ in the figure, where the Kohn anomaly is expected. It is thought that the reason why the anomaly was not found originated from the weak electron–phonon interaction as suggested by Chou *et al* (1990) for the phonon dispersion curves in $Cu_{0.84}Al_{0.16}$ alloy. We have also found that the linewidth of phonons is finite for the transverse branch and nearly zero for the longitudinal branch. We expect that some anomaly on the phonon dispersion curves may appear if the energy resolution is improved.

Acknowledgments

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