Lattice Modulation in the Long Period Ordered Alloys Studied by X-Ray Diffraction. II : CuAuII

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Lattice Modulation in the Long Period Ordered Alloys Studied by X-Ray Diffraction. II. CuAuII*

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Abstract

The crystal structure of the long period ordered alloy CuAuII has been investigated by X-ray diffraction using an alloy single crystal with the composition of Cu-50 at.%Au. Half of the long period of the alloy has been measured to be 5.0 in units of the fundamental Ll_0-type cell, differing from the result of Jehanno and Perio on a polycrystalline alloy. The Fourier synthesis has been made using H, K, 0 type reflections recorded on Weissenberg photographs. Taking into account the information obtained from the synthesis, the structure parameters including atomic coordinates, temperature factor and occupancy ratio of each atomic site have been refined by a modified least squares method. It has been confirmed that atoms are periodically displaced from the normal lattice points of the fundamental cell. Copper atoms shift by distances ranging from 0.079Å to 0.028Å toward the anti-phase boundary and gold atoms by distances ranging from 0.048Å to 0.004Å in the opposite direction. The atomic disordering occurs considerably in the neighborhood of the anti-phase boundary, while it is not much in the center of the antiphase domain.

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