On the Anti-Phase Domain Structure of the Ordered Phase CuAu₃*

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Abstract

A model for the anti-phase domain structure of CuAu₃ is proposed which can account well for the particular feature of the superlattice reflections observed by Hirabayashi in his single crystal X-ray diffraction pattern. In this model, the imperfectly ordered lattice consists of anti-phase domains with the shape of dodecahedron. Domain boundaries are {110} planes, across which direct contact between like atoms takes place more frequently than inside domains. The shape and size of domains may considerably be irregular in the actual lattice.