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Thermal expansion of α-AuCu, AuCu(II) and AuCu(I) at low temperatures

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Abstract

The thermal expansion of α-AuCu, AuCu(II) and AuCu(I) at low temperatures has been studied by X-ray powder experiment. Volume expansion coefficients remain positive down to 15 K for all phases. The negative expansion parallel to the tetragonal unique axis is observed in AuCu(I). No anomalous anisotropy is observed in AuCu(II).

1. Introduction

It is well known that AuCu alloy, depending on annealing temperature, can be obtained in different phases: cubic phase with statistical disorder (α-AuCu), orthorhombic phase with long-period superstructure (AuCu(II)) and tetragonal, ordered phase (AuCu(I)). The structure and structural phase transitions have been investigated in AuCu by X-ray powder and single-crystal diffraction methods [1–8]. It was concluded in ref. 8 that generally there is an increasing tendency towards the separation of constituent atoms with decreasing temperature. Therefore, we stated that it would be interesting to measure and compare the thermal expansion of AuCu phases at low temperatures.

2. Experimental details

AuCu alloy was prepared from appropriate amounts of gold (99.9% purity) and copper (99.99% purity) melted together in evacuated and sealed quartz tube and then quenched in water. Next the ingot was converted into fillings. Fillings were divided into three parts and appropriately annealed to obtain α-AuCu, AuCu(II) and AuCu(I) phases.

Powder samples of all three phases were measured on Siemens D 5000 X-ray diffractometer using Cu Kα radiation in the temperature range between 15 K and 300 K. The temperature dependences of lattice parameters are shown on Figs. 1–3. For AuCu(II) phase, parameters of the basic lattice are plotted (see Fig. 2). The long-period structure consists of 10 lattice periods along the *c* axis.

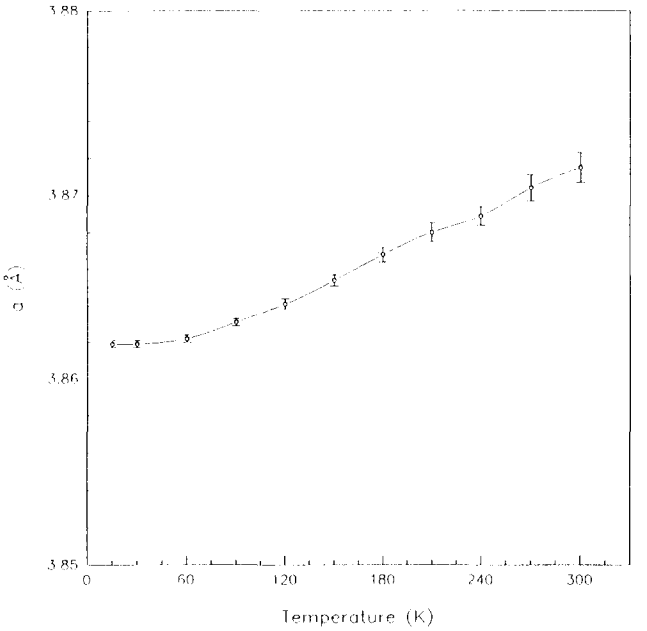

Fig. 1. Temperature dependence of a lattice parameter in α-AuCu.

3. Discussion

The temperature dependences of unit cell volumes for all AuCu phases show qualitatively similar behaviour (see Fig. 4). An interesting anisotropy is observed for lattice parameters in AuCu(I). It shows a positive thermal expansion perpendicular to the unique axis

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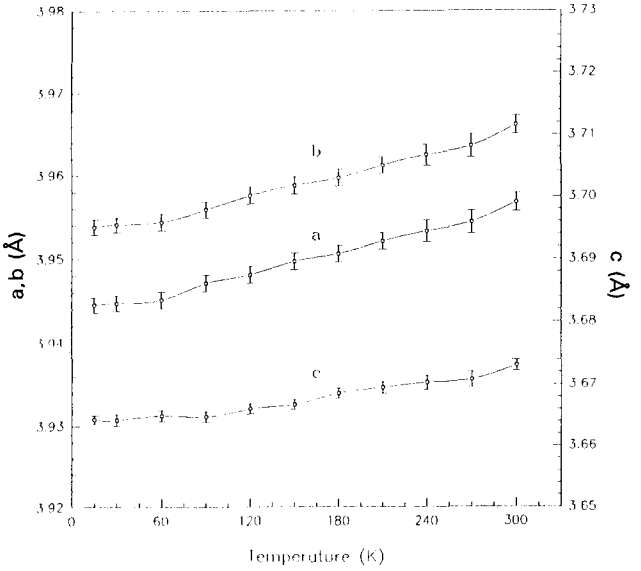

Fig. 2. Temperature dependence of lattice parameters in AuCu(II).

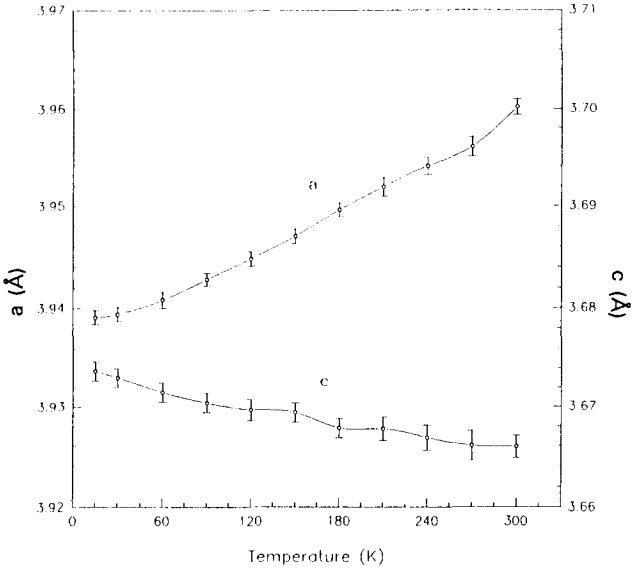

Fig. 3. Temperature dependence of lattice parameters in AuCu(I).

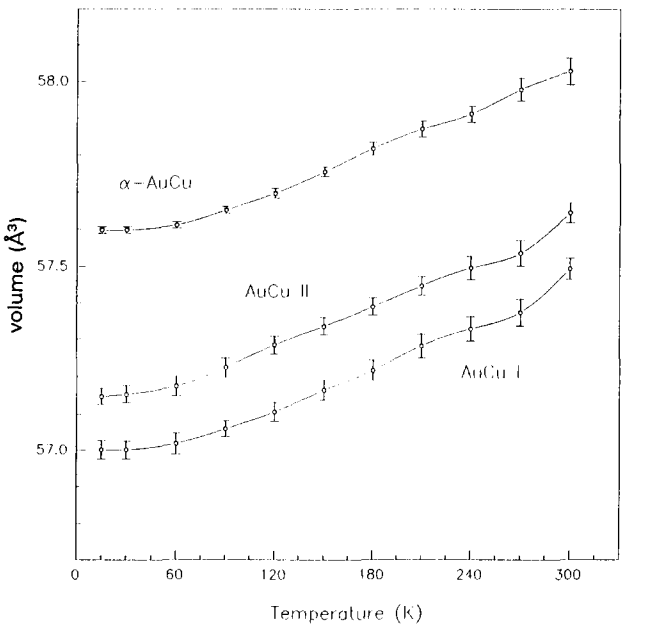

Fig. 4. Temperature dependence of unit cell volumes in α-AuCu, AuCu(II) and AuCu(I).

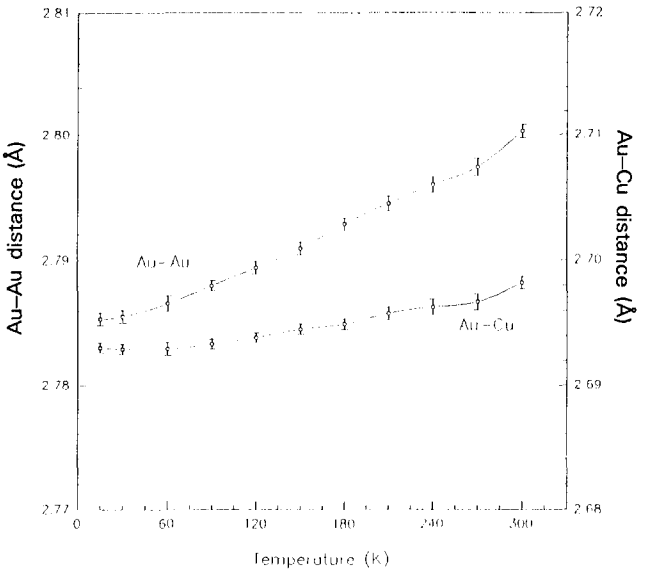

Fig. 5. Temperature dependence of interatomic distances in AuCu(I).

and a negative expansion parallel to the unique axis c. The expansion coefficients are practically constant in the temperature range between 60 K and 270 K. Their values are calculated to be $\alpha_a = 1.88 \pm 0.03\ 10^{-5}$ [K^{-1}] and $\alpha_c = -0.69 \pm 0.04\ 10^{-5}$ [K^{-1}]. The expansion coefficient vanishes on a cone for which half the apex angle ($\simeq 31°$) is equal to the angle between the c^* axis and the [112] direction in reciprocal space.

With decreasing temperature, the Au–Au and Cu–Cu interatomic distances decrease faster than the Au–Cu distance (see Fig. 5). The anisotropy for AuCu(I) gives an indication that, in AuCu alloy, atoms of the same kind attract each other more than atoms of different kinds. This is confirmation for the separating tendency concluded in ref. 8.

No anomalous anisotropy in thermal expansion is observed in AuCu(II) (see Fig. 2). We think that the anomalous anisotropy is suppressed by the anti-phase domain structure of AuCu(II).

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