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Al-C-Co (Aluminum-Carbon-Cobalt)

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Since the early work of [1960Hut], new experimental investigations were carried out on this system by [1995Kim, 2006Kim]. [2004Oht] presented a thermodynamic analysis that includes ab initio calculations.

Binary Systems

In the Al-C system [1991Har], the stoichiometric compound Al_4C_3 ($D7_1$-type rhombohedral) is known. The calculated Al-Co phase diagram [2004Oht] shows the following intermediate phases: CoAl (48-78.5 at.% Co; $B2$, CsCl-type cubic), Co_2Al_5 ($D8_{11}$-type hexagonal), $CoAl_3$ ($D0_{11}$, Fe_3C-type orthorhombic), Co_4Al_{13} (three modifications found by [1996God]), and Co_2Al_9 ($D8_d$-type monoclinic). A metastable phase Co_3Al with the $L1_2$-type of structure was suggested by [1995Kim], which is stabilized by C into the $E2_1$-type compound Co_3AlC_x (κ). The C-Co system is of the simple eutectic type, with the eutectic reaction at 1320 °C.

Ternary Phase Equilibria

[1995Kim] remelted in an arc furnace 17 pre-prepared alloys made with high purity elements. The alloys were annealed at 1100 °C for 30 h or at 1000 °C for 7 d and cooled in air. The phase equilibria were studied with optical and electron metallography, energy dispersive x-ray spectroscopy and x-ray powder diffraction. Differential thermal analysis was carried out at a heating/cooling rate of 10 °C per min. On the basis of their results, [1995Kim] constructed a liquidus projection and an isothermal section at 1100 °C, both for Co-rich alloys. The liquidus projection is shown in Fig. 1. The primary crystallization fields are (Co), κ, CoAl, and graphite (gr). Three vertical sections were constructed at 3 and 10 at.% C and 30 at.% Al respectively, as shown in Fig. 2-4. Also, a pseudobinary section along the CoAl-C line was deduced from the thermal arrests.

[2006Kim] arc-melted under Ar atm four Co-rich alloys and annealed them at 1100 or 1000 °C for 144 h. The phase equilibria were studied by means of electron metallography, x-ray diffraction and electron probe microanalysis. An updated version of the isothermal section at 1100 °C was constructed, which is redrawn in Fig. 5.

Combining ab initio energetic calculations with the CALPHAD approach, [2004Oht] calculated the phase equilibria in this system. The regular solution approximation was used to describe the liquid phase. The face-centered cubic (fcc) solid solution was modeled with two sublattices, one for the metal atoms and the other for C and V_a (vacancy). The body-centered cubic (bcc) phase was

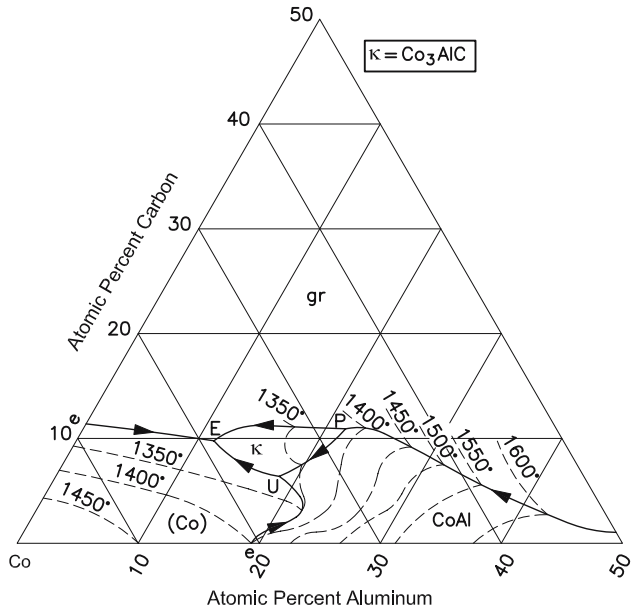

Fig. 1 Al-C-Co liquidus projection [1995Kim]

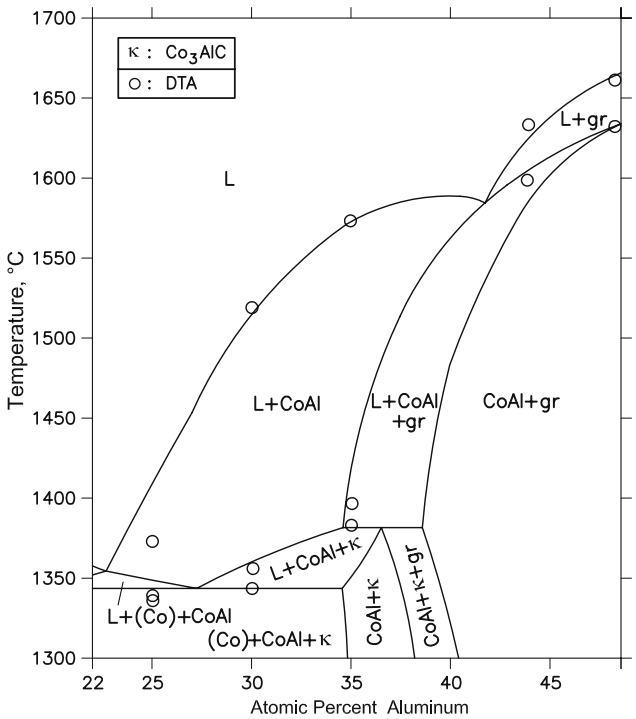

Fig. 2 Al-C-Co vertical section at a constant 3 at.% C [1995Kim]

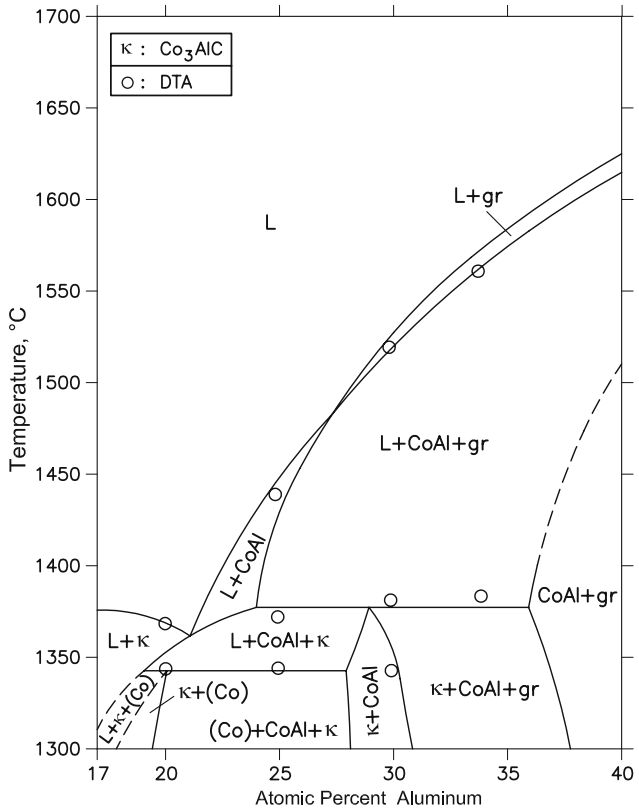

Fig. 3 Al-C-Co vertical section at a constant 10 at.% C [1995Kim]

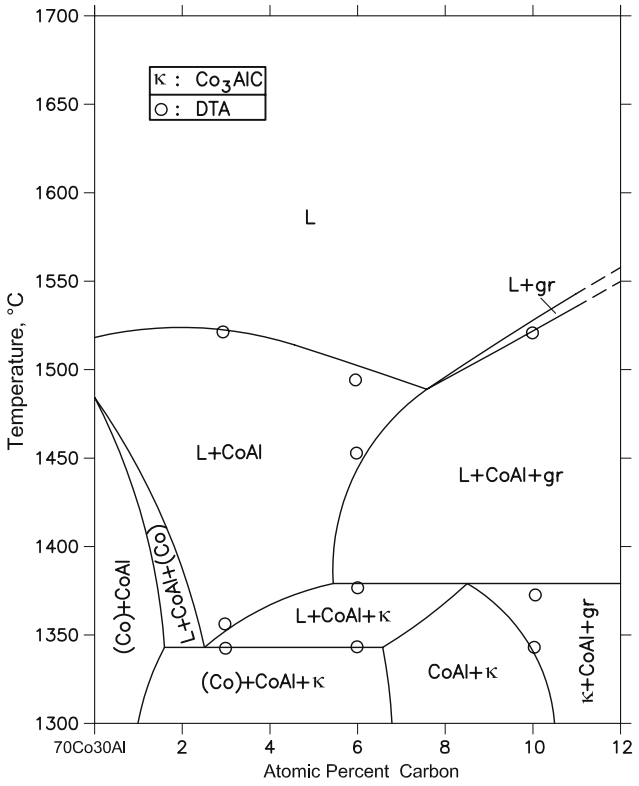

Fig. 4 Al-C-Co vertical section at a constant 30 at.% Al [1995Kim]

modeled with three sublattices. Two metal sublattices provide for *B*2 ordering and the third sublattice is for C and V_a. In the modeling of the $E2_1$-type Co_3AlC structure, Co and Al occupy the $L1_2$ superlattice, in which the C atom is in the body-centered, interstitial site.

New interaction parameters optimized by [2004Oht] for the Al-Co, Al-C, and C-Co binary systems were listed along with the parameters adopted from the literature. The interaction parameters for the Al-C-Co system were optimized using the experimental results of [1995Kim]. The formation energy of Co_3AlC was estimated from the energetic calculations, using the Full-Potential Linearized Augmented Plane Wave (FLAPW) method. A liquidus projection and three isothermal sections at 1300, 1000 and 900 °C were computed. The section at 1100 °C was compared with the experimental results of [1995Kim], showing satisfactory agreement. Two vertical sections at 10 at.% C and 30 at.% Al respectively were computed by [2004Oht]. The comparison with the experimental data of [1995Kim] shows some differences in the nature and the temperature of occurrence of the invariant reactions.

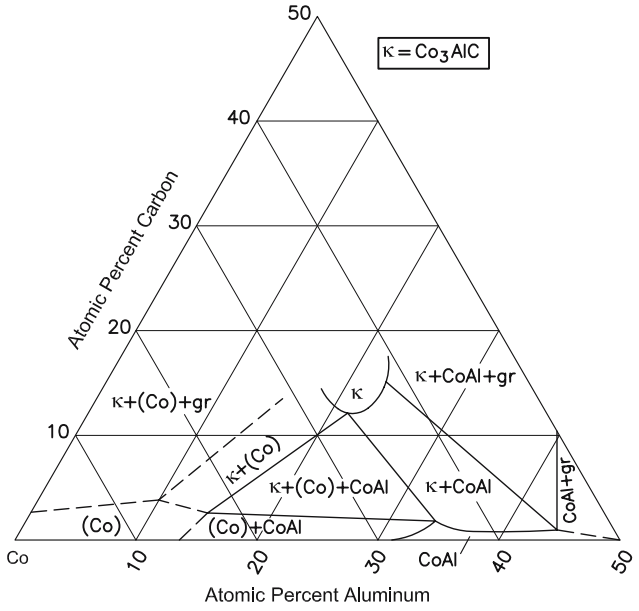

Fig. 5 Al-C-Co partial isothermal section at 1100 °C [2006Kim]

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