

## Aluminium – Chromium – Iron

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### Literature Data

Although the Al–Cr–Fe system has undergone many investigations, the Al–Cr–Fe equilibrium diagram has not been determined in the whole composition range. After assessment of [1991Gho] in accordance with which there are no ternary phases in the system, many reports with data on ternary phases in the Al-rich part of phase diagram appeared. The major part of the earlier work has been done by Kornilov [1940Kor1, 1940Kor2, 1945Kor, 1946Kor] and Kozheurov [1970Koz1] and [1970Koz2]. Kornilov used Armco grade Fe (0.25 mass% C, 0.05 mass% Si and traces of Mn), Al pigs (0.1 mass% Si, 0.1 mass% Cu), Al powder (0.1 mass% Si, 0.1 mass% Cu), chromium oxide of unspecified purity and analytically pure iron oxide. The Fe and Cr rich alloys were prepared by the aluminothermic process, which was also used by other investigators [1932Tai1, 1932Tai2, 1943Mon, 1951Pra, 1953Cas, 1954Chi, 1955Tag] and [1958Chu]. Thermal analysis was performed to monitor the solidification process in an induction furnace in insulated corundum crucibles and under an inert atmosphere of He–Ar. [1932Tai1] and [1932Tai2] used Armco grade Fe (0.14 mass% Si), Al (0.17 mass% Si, 0.6 mass% Fe), and the liquidus surface was determined by thermal analysis. Atomic ordering and lattice parameters of  $\text{Cr}_{1-x}\text{Fe}_x\text{Al}$  alloys were studied by [1969Kal] using neutron diffraction. [1951Pra] have experimentally determined two isothermal sections at 425 and 600°C, in the Al-rich corner. [1958Chu] determined isothermal sections using high-purity Al (99.994 mass%), iodide Cr (99.988 mass%), and electrolytic Fe (99.994 mass%) having extremely low contents of interstitial elements C, H, O, and N. Alloys were prepared by arc melting, followed by homogenizing treatment at 1000°C for 100 h. Final heat treatments were done under an argon atmosphere in silica capsules with subsequent quenching into water. Phase analysis was carried out by optical metallography, X-ray diffraction, and hardness testing. [1955Tag] and [1958Tag] studied the effect of Al addition to Cr–Fe binary alloys on the formation of the  $\sigma$  phase by means of optical microscopy, X-ray diffraction and hardness measurements. The effect of Cr on the stability of  $\alpha_1\text{Fe}_3\text{Al}$  and  $\alpha_2\text{FeAl}$  and the transition from ( $\alpha\text{Cr}$ ), ( $\alpha\text{Fe}$ ) or  $\alpha_1$  to  $\alpha_2$  has been studied by X-ray diffraction, dilatometry [1968Bul, 1969Bul1] and [1969Bul2] and also by high-temperature X-ray diffraction [1969Sel]. The details of the ordering nature in the ternary  $(\text{Cr,Fe})_3\text{Al}$  alloys have been studied by X-ray and neutron diffraction [1972Kaj, 1974Niz, 1975Lit] and [1977Tys]. [1982Yea] investigated Al-based alloys of four compositions prepared by extrusion at 260°C and annealed at 400°C for 100 h. [1997Pal] reported an isothermal section in the Al-rich corner at 1000°C established by metallography, EMPA and X-ray investigations of quenched samples. [1997Pal] used iron 99.97, aluminium 99.99, and chromium 99.53 mass% with 0.35 mass% iron as a main impurity. Alloys of 18 compositions with more than 50 at.% Al were prepared by levitation melting and annealed at 1000°C for 100 h followed by quenching in ice brine. [1988Ten, 1989Law1, 1989Law2, 1992Don, 1995Sui, 1995Zha, 1997Sui, 1998Lia, 1999Sui, 2000Mo, 2000Dem, 2001Dem, 2002Dem1] and [2002Dem2] reported ternary phases of monoclinic, orthorhombic as well as hexagonal structures found in alloys in the range of compositions 65 to 81 at.% Al and 6 to 15 at.% Cr, which were under investigation. Initial Al used in these studies was of 99.99 or higher purity, Fe 99.5, Cr 99.9 mass%. The alloys were prepared by either arc melting [1995Sui, 1997Sui, 1998Lia, 1999Sui] or induction levitation melting under pure helium atmosphere [2000Dem, 2001Dem, 2002Dem1, 2002Dem2] and investigated in the as-cast or annealed state. [2001Dem, 2002Dem2] annealed the samples at temperatures in the range 900 to 1050°C for 20 h depending on the alloy and cooled at a conventional rate. TEM, HREM, at a SEM-(EDX, WLDX), XRD were used for investigation of alloys. [2000Mo] established the crystal structure of the hexagonal ternary  $\text{Cr}_{11}\text{Fe}_8\text{Al}_{81}$  phase, labelled by him as v, using TEM, HREM and X-ray diffracton methods. The alloy of the nominal composition  $\text{Cr}_2\text{FeAl}_{12}$  was prepared by induction melting a mixture of high-purity Al (99.9999 mass%), Fe (99.5 mass %), and Cr (99.9 mass %) and cooled in a sand bath. The chemical composition of a hexagonal needle-like single crystal of the  $\text{Cr}_{11}\text{Fe}_8\text{Al}_{81}$  phase selected in the cavities of the cast ingots was determined by electron microprobe analysis. The hexagonal phase is supposed to have

the largest cell among intermetallics. The icosahedral ternary *i* phase in coexistence with the Al solid solution was found by [1995Zia] and [1995Sta] in Cr-3.1Fe-94.7Al and Cr-8Fe-86Al (at.%) alloys, respectively. The alloys were prepared by induction melting followed by centrifugal atomization after heating at 1200°C and then degassed at 330°C for 3 h [1995Zia] and by arc melting followed by a spinning process [1995Sta]. As-cast and annealed alloys were investigated by TEM, SEM-EDX, X-ray, convergent beam technique (CBT), DSC [1995Zia] and XRD, DSC, Moessbauer spectroscopy and magnetic susceptibility [1995Sta].

### Binary Systems

The Al–Cr and Al–Fe systems are accepted from [2003Cor] and [2003Pis], respectively. Data concerning the Cr–Fe system are from [Mas2, 1982Kub].

### Solid Phases

Crystallographic data on the known unary and binary phases as well as recently reported ternary ones are listed in Table 1. Seven ternary phases with crystal structures different from those of the binary intermetallics are reported in the ternary Al rich alloys solidified and consequently (directly or after homogenization) cooled at conventional rate. One of them,  $\nu$  Cr<sub>11</sub>Fe<sub>8</sub>Al<sub>81</sub>, can be believed to be a stable ternary compound at high temperature. This hexagonal phase investigated by [2000Mo] was found in the CrFe<sub>2</sub>Al<sub>12</sub> alloy by [1999Sui] as the main phase together with orthorhombic “O–CrFeAl” and monoclinic “M–CrFeAl”. Body centered orthorhombic phase, labelled as “O–CrFeAl” was observed in Al rich as-cast alloys (prepared by arc melting) by [1995Sui, 1996Ros, 1997Sui, 1998Lia] and also [2000Dem]. Found together with O phase, C-centered monoclinic ternary phase “M–CrFeAl” has a structure which is considered a superstructure of “O–CrFeAl”. The lattice correspondence between the lattice parameters of the M- and O-phases are as follows:

$$\begin{aligned} a_m &= c_o - b_o \quad (a_m = c_o / \sin\beta), \\ b_m &= a_o \\ c_m &= 2b_o \end{aligned}$$

Three orthorhombic phases “O–CrFeAl”, “O<sub>1</sub>–CrFeAl” and “C<sub>3,1</sub>–CrFeAl” additionally to Al-solid solution were found by [2000Dem] in as-cast alloy of Cr<sub>11</sub>Fe<sub>8</sub>Al<sub>81</sub> nominal composition, prepared by levitation melting. Phases with the same crystal structure as the two latter ones, O<sub>1</sub>- and the O<sub>3,1</sub>-, earlier were observed in Al–Cr–Cu–Fe by [1992Don], as well as in Al–Mn–Ni and Al–Pd–Ru by [1988Ten] and [1995Zha], respectively. A new “O<sub>2</sub>–CrFeAl” phase together with orthorhombic phases “O–CrFeAl”, “O<sub>1</sub>–CrFeAl” as well as Al<sub>8</sub>Cr<sub>5</sub>, which is isostructural with  $\gamma$ -brass, were obtained by [2001Dem] in alloys of the compositions (at.%): Cr-6.0Fe-77.5Al (O+O<sub>1</sub>+hexagonal phase  $\gamma$  type), Cr-8.0Fe-72.5Al (O+O<sub>2</sub>+hexagonal  $\gamma$  type), Cr-6.0Fe-72.5Al (O<sub>1</sub>+O), as well as Cr-9.1Fe-67.6Al (hexagonal  $\gamma$  type). The alloys after induction melting were annealed in the range 900 to 1050°C for 20 h. The O<sub>2</sub>-phase is for the first time observed in this system, but a phase with the same structure was identified before in Al–Cr–Cu–Fe by [1992Don, 1995Li]. The orthorhombic O<sub>1</sub> and O<sub>2</sub> phases were observed by [2002Dem1, 2002Dem2] in the alloy of Cr-6.0Fe-77.5Al (at.%) composition, prepared by induction melting, subsequently crushed and pressed in a graphite mold and then sintered at 980 and 1060°C. In the alloy of the same composition which was annealed at 900 to 1050°C for 20 h directly after melting the O<sub>1</sub>- and O-phases coexist. Both [2002Dem1] and [2002Dem2] found a  $\gamma$ -brass-like phase in the Cr-7Fe-65Al (at.%) alloy as single phase with somewhat shorter lattice parameters. The last fact, which is in agreement with data of [1997Pal] for 1000°C, demonstrates the high solubility of Fe in the Cr<sub>8</sub>Al<sub>5</sub>(r) phase, and supports the results concerning orthorhombic phases. As one can see, most of the investigated alloys were not in an equilibrium state. Quenching experiments were not made. Except for the  $\nu$  Cr<sub>11</sub>Fe<sub>8</sub>Al<sub>81</sub>, the composition of the reported ternary phases are unknown. The latter may be either ternary compounds or stable or unstable polymorphous modifications of the binary intermetallics because of their close structural relationship to each other.

There is a body centred cubic continuous solid solution  $\alpha$ (Fe,Cr,Al) in the system and a wide field of ordered phases  $\alpha_2$  (FeAl) and  $\alpha_1$  (Fe<sub>3</sub>Al) based on the b.c.c. lattice. FeAl dissolves more than 30 at.% Cr at

600°C at the equiatomic Al/Fe ratio according to [1991Tre, 1997Pal].  $\text{Fe}_3\text{Al}$  can dissolve a considerable amount of Cr (more than 26%) [1968Bul, 1969Bul1] and [1969Bul2], which leads to some increase in both  $\text{Fe}_3\text{Al} \rightleftharpoons \text{FeAl}$  and  $\text{FeAl} \rightleftharpoons (\alpha\text{Fe})$  transition temperatures [1969Bul2] and [1969Sel]. [1972Kaj] suggested that at certain compositions Fe occupies one sublattice while Cr and Al occupy the other. [1993Kni] found that the alloys on the basis of  $\text{Fe}_3\text{Al}$  with 2 and 5 mass% Cr (about 1.3 and 3.3 at.% Cr, respectively) have an equilibrium structure of the  $\text{BiF}_3$  type ( $cF16$ ) at low temperatures which transforms to the CsCl type structure ( $cP2$ ) above 500°C. The crystal structures of alloys in a similar range of compositions were investigated also by [1999Wit]. [1976Vla] studied the decomposition behavior of a Cr-68.3Fe-10.4Al (at.%) alloy after quenching from 750°C and subsequent annealing at 490°C for up to 200 h by means of Mössbauer spectroscopy, low-angle X-ray scattering and TEM. Though no ternary phase was detected upon annealing, the authors observed phase separation into two isomorphous solid solutions which were depleted or enriched with Cr. Coordinates of the  $((\gamma\text{Fe})+(\alpha\text{Fe})) / (\alpha\text{Fe})$  surface of the  $(\gamma\text{Fe})$ -loop in the Al–Cr–Fe system are given in Table 2 based on the microstructural, hardness, electrical resistivity, and dilatometry results on eight ternary alloys heat treated between 800 and 1300°C [1946Kor].

All binary intermetallics of the ternary system dissolve the third component.  $\text{Cr}_2\text{Al}$  is reported by [1969Kal] to dissolve Fe up to  $x = 0.25$  replacing Cr atoms in the lattice. Data on the lattice parameters of  $(\text{Cr}_{1-x}\text{Fe}_x)_2\text{Al}$  as a function of  $x$  are listed in Table 1. [1951Pra] reported that the extracted crystals of  $(\text{Cr}_2\text{Al}_{13})$  and  $(\text{Cr}_2\text{Al}_{11})$  (from alloys cooled slowly to room temperature from the liquid phase) dissolved iron. The observed compositions of  $\text{Cr}_2\text{Al}_{13}$  and  $\text{Cr}_2\text{Al}_{11}$  at maximum Fe solubilities were Cr-5.49Fe-75.05Al (mass%) Cr-3.02Fe-85.48Al (at.%) and Cr-13.47Fe-67.96Al (mass%) Cr-7.73Fe-80.81Al (at.%), respectively. [1960Zol1] and [1960Zol2] also analyzed  $\text{Cr}_2\text{Al}_{13}$  crystals from alloys with various Fe contents. The solid solubility data of [1960Zol1] and [1960Zol2] showed a lower Fe solubility in  $\text{Cr}_2\text{Al}_{13}$  of 2.36 mass% (1.3 at.%) Fe, but it was not certain to be a maximum value. The data of [1951Pra] show that the replacement of Cr for Fe deviates from a simple one-to-one atomic substitution scheme, but that in [1960Zol1] and [1960Zol2] is somewhat closer to one-to-one atomic replacement. Solution of Fe in  $\text{Cr}_2\text{Al}_{13}$  is reported to cause a reduction in the lattice parameter of the  $\text{Cr}_2\text{Al}_{13}$  phase [1960Zol1] and [1960Zol2].  $\text{FeAl}_3$  is reported to dissolve some Cr, and the  $\text{FeAl}_3$  composition, according to chemical analysis data, is Cr-39.89Fe-56.17Al (mass%) (Cr-24.87Fe-72.49Al (at.%) [1951Pra]. But the value 2.64 at.% for Cr solubility in  $\text{FeAl}_3$  can not be accepted as maximal, because according to [1997Pal], the solid solubility of Cr in  $\text{FeAl}_3$  at 1000°C is considerably higher - about 6.4 at.%. All Al-rich phases that are in a solid state at 1000°C (based on  $\text{FeAl}_3$ ,  $\text{Fe}_2\text{Al}_5$ ,  $\text{FeAl}_2$ ,  $\text{Cr}_4\text{Al}_9$  and  $\text{Cr}_5\text{Al}_8$ ) extend deep into the ternary system. The maximum solubilities of the third component at 1000°C are observed for the  $\text{Cr}_5\text{Al}_8$  and  $\text{Cr}_4\text{Al}_9$  phases - 32.5 and 9.6 at.% Fe, respectively. The lattice parameters of the,  $\text{Cr}_5\text{Al}_8$  ( $r$ ) ( $\gamma_2$ ) phase versus Fe content are presented in Fig. 1. [1990Ioa] found that the rapidly solidified alloy Cr-1Fe-95Al (mass%) (Cr-0.5Fe-97.37Al at.%) exhibits a mixed microstructure composed of featureless and cellular morphologies. According to X-ray data, the equilibrium  $\text{Cr}_2\text{Al}_{13}$  phase coexists in the alloy with the aluminium matrix and an unknown phase. Taking into account the data of [1995Zia] and [1995Sta], the latter could be a ternary quasicrystalline phase with an icosahedral symmetry, see Table 1. [1995Zia] found the  $i$  phase, named Q by him, in the  $\text{Cr}_3\text{Fe}_z\text{Al}_x$  ( $z = 0, 1$  or  $3$  at.%) alloys, using X-ray diffraction. The accepted composition of the phase  $\text{Cr}_{12\pm1}\text{Fe}_{12\pm1}\text{Al}_{75\pm0.5}$ , was established using chemical microanalysis. During the “low” temperature sequences of the rapidly solidified alloys, the Q phase reacts with the Al matrix giving rise to the non-equilibrium and equilibrium phases:  $(\text{Al}) + \text{Q} \rightarrow \text{FeAl}_6 + \text{Cr}_2\text{Al}_{13} + \text{FeAl}_3$ . At higher temperatures (450 to 550°C), the quasicrystal transforms directly into the stable phases, by-passing the step of the metastable  $\text{FeAl}_6$  phase formation. At the quasicrystal/matrix interface the orthorhombic phase was observed. According to EDX analysis, the ratio  $(\text{Al})/(\text{Cr}+\text{Fe})$  is equal to  $3.1 \pm 0.1$  and the content of Cr  $\ll 1$  at.%. [1995Zia] concludes that this phase is the allotropic variant of  $\text{FeAl}_3$ , which is monoclinic in the binary system. The structure of the  $i$  phase, found in a melt spun alloy of  $\text{Cr}_8\text{Fe}_6\text{Al}_{86}$  (at.%) composition, is reported by [1995Sta] as simple icosahedral type with the value of the six-dimensional hypercubic lattice constant  $a_{6D} = 654.2 \pm 0.02$  pm. In a rapidly solidified alloy, the  $i$  phase coexisted with the Al-solid solution. This mixture transformed to a mixture of stable phases  $\text{Cr}_2\text{Al}_{13} + \text{FeAl}_3$  after 5 min. heating at 580 or 635°C. Earlier a metastable icosahedral ternary phase was also reported by [1987Wou, 1988Man, 1989Man, 1988Sch, 1989Law1, 1989Law2].

### Invariant Equilibria

Figure 2 gives the tentative invariant equilibria for the Al-rich corner. The equilibrium  $L + Cr_2Al_{11} + FeAl_3$  within the ternary is not known, while equilibrium  $L + Cr_2Al_{13} + FeAl_3$  is unquestioned because the existence of the three-phase equilibrium  $Cr_2Al_{13} + FeAl_3 + (Al)$  is established well at temperatures close to the solidus: 500°C [1995Zia] and 635°C [1995Sta]. [1943Mon] suggested that the invariant  $U_1$  reaction takes place at Cr-4.2Fe-93.7Al (mass%), but the temperature was not given. Careful thermal analysis data of [1932Tai1] and [1932Tai2] show the presence of a ternary eutectic E at Cr-2Fe-97Al (mass%). On the other hand, [1943Mon] and [1976Mon] suggested that E takes place at Cr-1.70Fe-97.95Al (mass%), to which there is no experimental evidence. It remains inconclusive whether the ternary eutectic reaction E exists or not. Thermodynamic calculations of the Al-rich corner of the Al–Cr–Fe system by Saunders [1987Sau] suggest that the reaction E is unlikely and instead he predicted a ternary transition  $U_1$  reaction  $L + Cr_2Al_{11} \rightleftharpoons Cr_2Al_{13} + FeAl_3$  at 709°C (0.63 mass% (0.33 at.%) Cr, 3.09 mass% (1.52 at.%) Fe) followed by the ternary transition  $U_2$  reaction  $L + Cr_2Al_{13} \rightleftharpoons (Al) + FeAl_3$  at 654.5°C (0.19 mass% (0.10 at.%) Cr, 2.02 mass% (0.99 at.%) Fe). The latter shows a good agreement with the findings of [1960Zol2] and [1973Wil] showing no ternary eutectic reaction at 640°C, but a transition reaction at 655°C. Because of this uncertainty, alternative paths for E and U are given by broken lines in Fig. 2.

### Liquidus Surface

Figures 3 and 4 show two versions for the liquidus surface of the Al corner. Fig. 3 is presented after experimental data [1932Tai1, 1932Tai2] and [1943Mon]. The melting troughs separate 4 different areas of primary crystallization. Ternary alloys from 100 to about 94 at.% Al have been investigated by different authors [1932Tai1, 1932Tai2, 1951Pra, 1954Chi, 1960Zol1, 1960Zol2], and no ternary compound has been reported by them in this composition range. The presence of the ternary eutectic E is concluded from thermal analysis data of [1932Tai1] and [1932Tai2], even though limited thermal analysis results of [1960Zol1] and [1960Zol2] failed to confirm it. Figure 4 is the calculated liquidus surface of the Al corner after [1987Sau], showing the presence of the transition invariant reaction  $U_2$  instead of ternary eutectic reaction. [1951Pra] failed to observe the  $\rho(Cr_2Al_{11})$  phase in binary and ternary alloys either slowly-cooled or quenched from 730 to 765°C. In accordance with the old version of the Al–Cr binary phase diagram adopted by [1951Pra], in which a reaction  $L + \rho \rightleftharpoons \theta$  takes place at 755°C instead of 790°C in the presently accepted binary phase diagram, the obtained result seems to reject the existence of the stable  $Cr_2Al_{11}$  compound. Nevertheless, these data are in good agreement with the Al–Cr phase diagram accepted in this assessment. But there is no confidence that the equilibrium  $L + \rho + FeAl_3$  exists. It can be prevented by possible formation of high-temperature incongruently melting ternary compounds with aluminium content less than 94 at.%. Therefore the monovariant curves in the vicinity of  $U_1$  are dotted. The liquidus surface in Fig. 5, after [1945Kor], shows a melting trough defining the primary crystallization field of  $(Cr, \alpha Fe)$ . Approximate isotherms at 50 K intervals are also shown. [1935Gru] reported the melting point of a Cr-64.6Fe-5.3Al (mass%) Cr-59.86Fe-10.17Al (at.%) alloy which agrees reasonably well with Fig. 5. [1970Koz1] and [1970Koz2] compared the calculated and experimental results for liquidus points for compositions from the Cr corner to about 70 mass% Fe and 40 mass% Al. The experimental values were always 30 to 40 K lower than calculated ones, which was attributed to undercooling. Nevertheless, the isotherms between 1500 and 1800°C agree well with those of [1945Kor]. The original publications [1940Kor1, 1940Kor2, 1945Kor, 1946Kor] show the liquidus surface of  $(Cr, \alpha Fe)$  as terminated by the uninterrupted monovariant curve  $p_1p_2$ , corresponding to the equilibrium of liquid with the  $(Cr, \alpha Fe)$  phase and assumed continuous solid solution of the binary  $\gamma_1$  and  $\epsilon$  phases. There is reason to believe that the  $\gamma_1$  phase has a cubic structure. If the cubic  $\epsilon$  phase is isomorphous with  $\gamma_1$ , the continuous cubic solid solution in the ternary system is possible at high temperatures. But until now the existence of a  $(\gamma, \epsilon)$  continuous series has not been established.

### Isothermal Sections

Figure 6 shows the isothermal section at 1150°C based on data of [1945Kor, 1946Kor] and [1991Tre, 1997Pal]. In the original paper [1946Kor], the two-phase “ $\alpha_3 + \epsilon_3$ ” field is not very clear. Even though “ $\alpha_3$ ” is the ternary (Cr, $\alpha$ Fe) solid solution and  $\epsilon_3$  is the  $\epsilon$  or  $\gamma$  phase, the authors made very little investigation of the “ $\epsilon_3$ ” phase and they interpreted it as a continuous solid solution between  $\epsilon$  ( $\text{Fe}_2\text{Al}_3$ ) and  $\gamma_1$  ( $\text{Cr}_5\text{Al}_8$ )(h) [1946Kor]. Since the crystal structure of  $\epsilon$  is unknown, better evidence for the existence of a continuous solid solution between  $\epsilon$  ( $\text{Fe}_2\text{Al}_3$ ) and  $\gamma_1$  ( $\text{Cr}_5\text{Al}_8$ )(h) is required. On the other hand, [1997Pal] established a large extension of  $\gamma_2$  into the ternary system - up to 32.5 at.% Fe at about 48 at.% Al at 1000°C. The  $\alpha_2/\alpha$  transition of the second order is shown according to the binary Al–Fe system and data of [1991Tre] on an FeAl–Cr polythermal section. Figures 7, 8, 9, 10, and 11 show isotherms at 900, 750, 700, 650, and 600°C, respectively, after [1958Chu], with correction in the range of the ordering of the  $\alpha$  phase according to the experimental data of [1991Tre]. Phase equilibria between the  $\gamma$ -brass type phases are assumed by taking into account the data of [1997Pal] for 1000°C. Phase equilibria in the Al-corner are presented after data of [1951Pra, 1961Phi, 1995Zia, 1995Sta]. Annealing times for different alloys used by [1958Chu] are listed in Table 3. More than 50 ternary alloys were studied by [1958Chu], most of them near the region of  $\sigma$  phase formation. As one can see in the isothermal sections at 750, 700, 650, and 600°C, the extent of the  $\sigma$  phase field decreases with increasing Al content. This is in agreement with the results of [1945Kor]. Even though the  $\eta$  phase ( $\text{Cr}_2\text{Al}$ ) is stable up to 911°C according to the accepted Al–Cr binary phase diagram, this phase does not appear in the isothermal section at 900°C shown in Fig. 7. Such a difference of 11 K is not unreasonable when comparing data from different sources [1980Riv]. In his original paper, Chubb [1958Chu] presented a wide two-phase  $\alpha_2 + \alpha$  field in all isothermal sections of the ternary system, as well as two three-phase ( $\alpha\text{Fe}$ )+ $\text{FeAl}\alpha_2$ + $\text{Cr}_2\text{Al}(\eta)$  and  $\text{FeAl}\alpha_2$ + $\text{Cr}_2\text{Al}(\eta)$ + $\text{Cr}_4\text{Al}_9(\zeta)$  ones, the latter two being contiguous, which is not likely. The existence of the wide  $\alpha_2 + \alpha$  field, because of very narrow (to 1 or 2 at.% Cr)  $\alpha_2$  region shown by [1958Chu], is rather doubtful when the data of [1991Tre] and [1997Pal] are taken into account. FeAl dissolves at 1000°C about 30 at.% Cr at 45 at.% Al after [1997Pal]. In agreement with the above mentioned data, [1991Tre] showed that the extension of  $\alpha_2$  in the FeAl–Cr section increases with decreasing temperature down to about 28 at.% Cr at 36 at.% Al at 1000°C. The phase transition  $\alpha/\alpha_2$  of the second order in binary Al–Fe at high temperatures becomes first order below 665°C [1993Oka, 2003Pis]. A rise in the  $\alpha/\alpha_1$  temperature with increasing Cr content is reported by [1968Bul, 1969Bul1] and [1969Bul2]. The influence of Cr on the type of the ordering transition  $\alpha/\alpha_2/\alpha_1$  in ternary solid solution has not been studied in detail. In the isothermal sections at 900, 750, 700, 650, and 600°C,  $\alpha$  phase ordering is presented based on binary Al–Fe as well as on the compared data of [1991Tre, 1997Pal]. There is some contradiction between the results of [1958Chu] and those of [1955Tag] and [1958Tag] as far as the formation of the  $\sigma$  phase in the ternary alloys is concerned. Based on the purity of the material, heat treatment regime and number of alloys used, the results of [1955Tag] and [1958Tag] seem to be more reliable than those of [1958Chu]. The results of [1955Tag] and [1958Tag] on  $\sigma$  phase formation in alloys containing up to 32 mass% Al are in accordance with those of [1958Chu], but they disagree with [1958Chu] for ternary alloys containing 35 mass% Cr. It should be emphasized that the formation of the  $\sigma$  phase is reported to be sensitive to non-equilibrium factors arising from impurities in ternary alloys [1955Tag, 1969Mue]. Phase equilibria above 50 at.% Al proposed in Figs. 7 to 11 are based on significant solubility of Fe in  $\gamma$  ( $\zeta$ ) phases at 1000°C found by [1997Pal]. A very strong temperature dependence of the solubility of Fe in  $\gamma$  and  $\zeta$  phases can be assumed taking into account the low thermodynamic stability of the binary  $\epsilon$  phase, which coexists in equilibrium with  $\gamma$  and is stable only within close limits of the equilibrium parameters at high temperature. It is seen in the isothermal sections. The isothermal section at 1000°C for Al content greater than 50 at.% is presented in Fig. 12 according to [1997Pal]. The data presented by [1997Pal] for the ternary alloys fit well to those for Al–Fe [Mas2] and Al–Cr [1992Cos, 1995Aud], respectively, as accepted in the [2003Cor] assessment of Al–Cr. The Al solubility within the ternary Fe based solid solutions is near to that for 1150°C but higher than reported for 900°C by [1958Chu]. While no ternary intermetallic phases have been found at 1000°C in this work, in contradiction to above mentioned observation of the ternary phases, the solubility of the third component in the Al–Cr and Al–Fe binary phases in some cases is very high. Solubility of Fe in the  $\gamma_2$  phase reaches about 30 at.% at 10 at.% Cr and 60 at.% Al. Fe stabilizes the  $\gamma_2$

structure so that at a content higher than about 13 at.% Fe only the  $\gamma_2$  phase (but not  $\gamma_1$ ) is reported to participate in phase equilibria at temperatures under investigation. The solubility of Cr in the Al–Fe binary phases is less than that of Fe in the binary Al–Cr phases as seen in Table 1. When the aluminium content exceeds 80 at.%, the liquid and liquid-solid regions appear. Fig. 13 shows the partial isothermal section for the Al corner at 600°C, according to the data of [1951Pra, 1961Phi]. [1951Pra] reported that undercooling suppresses the reaction  $L + Cr_2Al_{11} \rightleftharpoons Cr_2Al_{13}$  in both binary and ternary alloys. In the composition range shown in Fig. 13, no ternary phase has been reported and the phase fields remain the same at 425°C with a small shift in the phase boundaries [1951Pra]. Saunders [1987Sau] calculated the isothermal sections of the Al-rich corners at 600 and 425°C. The agreement between the calculated (presented by dashed line in Fig. 13) and the experimental (Al) +  $Cr_2Al_{13}$  / (Al) +  $Cr_2Al_{13}$  + FeAl<sub>3</sub> phase boundary accepted by [1951Pra] was reported to be very good, whereas that for the (Al) + FeAl<sub>3</sub> / (Al) +  $Cr_2Al_{13}$  + FeAl<sub>3</sub> boundary was less satisfactory. After [1995Zia, 1995Sta], in ternary alloys at Al contents greater than 94 at.% at 635°C and below, only (Al),  $Cr_2Al_{13}$  and FeAl<sub>3</sub> phases coexist in equilibrium, in agreement with [1951Pra, 1961Phi] and [1987Sau]. The sections through the surface  $((\gamma Fe) + (\alpha Fe)) / (\alpha Fe)$  of the  $\gamma$ -loop in the ternary system are given in Fig. 14. Further work is necessary to clarify the phase equilibria in the Al corner of the system.

### Temperature – Composition Sections

Figure 15 shows the polythermal FeAl–Cr section of the phase diagram according to [1991Tre]. The alloys containing up to 70 at.% Cr were prepared by arc melting from aluminium (99.5 mass% purity), electrolytic chromium and carbonyl iron. The annealings were carried out at 1200°C and 1300°C for 70 h each. As can be seen from Fig. 15, the temperature of the  $\alpha \rightleftharpoons \alpha_2$  transformation decreases with increasing the chromium content. The  $\alpha_2$  field extends to about 28 at.% Cr at 1000°C. Fig. 16 shows the variation in the order-disorder reaction temperature as a function of the Cr content along the Fe<sub>3</sub>Al–CrFe<sub>3</sub> section. In the Fe<sub>3</sub>Al–CrFe<sub>3</sub> isopleth taken from [1969Bull], additional dashed boundaries are given approximately according to the phase transformations in Fe<sub>75</sub>Al<sub>25</sub> (at.%) by [1993Oka]. The partial isopleth along Fe<sub>3</sub>Al–Cr<sub>3</sub>Al [1969Bull] is in poor agreement with the general data set discussed above and is not considered here.

[1946Kor] gave four isopleths at constant mass ratios Cr/Fe. These diagrams partially contradict the isothermal sections shown in Figs. 6, 7, 8, 9, 10, 11, 12 and therefore are not reproduced here.

### Thermodynamics

Information on thermodynamic properties of the Al–Cr–Fe alloys is incomplete. [1975Kau] used a simple thermodynamic model to calculate the phase boundaries between liquid and (Cr,  $\alpha$ Fe) at 1747, 1647, 1547 and 1527°C. In general, there is a substantial disagreement between the calculated [1975Kau] and the experimental phase boundaries [1970Koz2]. Applying a defect model, [1988Hoc] calculated the activity of Cr in FeAl, assuming that FeAl is either a compound or a solid solution. The calculated results do not show a significant discrepancy and both cases suggest complete solid solubility between Cr and FeAl. [1992Hil] studied the vaporization of the alloy Cr-75.4Fe-4.8Al (mass%) (Cr-70.72Fe-9.32Al (at.%)) using Knudsen effusion mass spectrometry in the temperature range 1313–1556 K. This composition virtually agrees with those of the commercial Aluchrom and MA956 alloys. The obtained thermodynamic data are presented in Tables 4 and 5. The heat capacities of the Fe<sub>3</sub>Al-based compound with a Cr content of 5 at.% have been measured in the temperature range from 20 to 700°C by [1997Rud]. The results of the  $C_p(T)$  measurement are shown in Fig. 17. [2000Sub] have reported a thermodynamic assessment of the Al–Cr–Fe system, which was performed applying the standard CALPHAD methodology. There the old version of the Al–Cr phase diagram [Mas2] was accepted, and no ternary phases have been assumed. A four-sublattice model for the  $\gamma$ -brass type phases was developed. [2001Sch] calculated isopotential curves of the thermodynamic forces for ternary diffusion as a function of composition for the Al–Cr–Fe system at 1073 and 1273 K.

### Notes on Materials Properties and Applications

Mechanical properties of the Al–Cr–Fe alloys were investigated by [1982Nao, 1991Pra, 1991Sik1, 1991Sik2, 1993Kni, 1996Jim, 1998Su] and [2000Spi]. In particular, [1982Nao] obtained the ductile supersaturated ferrite solid solution with high hardness and strength by the rapid quenching technique. The range of its formation is limited to less than about 35 at.% Cr and 23 at.% Al. The hardness, yield strength and tensile fracture strength increase with increasing amounts of chromium and aluminium. [1991Pra] studied mechanical properties of ordered alloys in the composition range 50 to 80 at.% Fe, 0 to 20 at.% Cr, that were rapidly solidified by melt spinning. An increasing preponderance of cleavage fracture with increasing ternary substitution for iron was observed. Mechanical properties of Fe<sub>3</sub>Al-based alloys were investigated by [1991Sik1, 1991Sik2] and [1993Kni]. According to [1991Sik1], room-temperature tensile ductility of the samples with 2 to 5 mass% Cr (1.3 and 3.3 at.%, respectively) approach 20%, which should be acceptable for many practical applications, and [1993Kni] established that increasing the Cr content from 2 to 5 mass% has a small effect on the ductility of the alloys based on Fe<sub>3</sub>Al. The tensile properties of the Cr-65Fe-30Al (at.%) alloy in air and in vacuum were investigated by [1998Su]. The yield strength of the Fe<sub>3</sub>Al alloy was reduced by the addition of 5 at.% Cr, indicating a softening with the addition of chromium, but the ultimate tensile strength (UTS) was increased slightly. [1996Jim] studied the creep behavior of several Al–Cr–Fe alloys ranging in aluminium from 21.7 to 48 at.% and established that the ternary alloys exhibit an improvement in strength under high temperature compressive creep. The microstructure of four Al–Cr–Fe alloys containing 9.3 to 18.0 at.% Cr and 7.6 to 25.5 at.% Al was investigated by [2000Spi] using TEM after different heat treatments and different degrees of compressive deformation. The maximum of the work-hardening curves is found to be shifted to higher strains with increasing aluminium concentration. At a deformation temperature of 400°C dynamic strain aging occurs. [1976Vla] investigated three alloys (mass%): Cr-7Fe-92Al, Cr-7.0Fe-92.5Al and Cr-7.0Fe-91.5Al (in at.%: Cr-3.5Fe-95.9Al, Cr-3.5Fe-96.2Al and Cr-3.5Fe-95.7Al) designed to be used at elevated temperatures. Extrusion bars were made from powders. The as-extruded and annealed at 482°C alloys, investigated by optical microscopy, TEM and XRD, had a microstructure consisting of equiaxed grains of aluminium matrix and two types of precipitates, namely (Cr,Fe)Al<sub>3</sub> and a metastable (Cr,Fe)Al<sub>6</sub> phase.

Data on the magnetic behavior of the Al–Cr–Fe alloys were obtained by [1969Kal, 1974Niz, 1975Lit, 1983Bus, 1985Okp, 1995Sta] and [1997Sat]. [1969Kal] studied the antiferromagnetic behavior and Neel temperature of ternary alloys based on the  $\eta$ (Cr<sub>2</sub>Al) phase. [1974Niz] and [1975Lit] reported the magnetic atomic moment, Curie temperature, temperature dependence of magnetic coercivity and susceptibility in the temperature range from 627 to -196°C. [1983Bus] obtained the values of Curie temperature, saturation moment at 4.2 K and Kerr rotation angle for the CrFe<sub>2</sub>Al alloy annealed at 800 K (527°C) for 11 d. [1985Okp] studied the ferromagnetism of ternary alloys based on FeAl, with Cr contents up to 50 at.%, quenched from 830°C. Ferromagnetism was observed in alloys with Cr contents no less than 35 at.%. [1995Sta] investigated magnetic susceptibility of the Cr<sub>8</sub>Fe<sub>6</sub>Al<sub>86</sub> (at.%) alloy solidified by melt spinning, of the phase content  $i+\theta+\text{FeAl}_3+(\text{Al})$ . The icosahedral symmetry was concluded not to produce any magnetic properties in the studied alloy. [1997Sat] determined the magnetic moment of chromium in Fe<sub>3</sub>Al-based alloys with chromium content up to 15 at.% in the temperature range 10 to 300 K. The overall moment was found to be small and that of neighboring iron atoms was reduced by about 0.1  $\mu_B$  per Cr atom. [1982Nao] reported that the room temperature electric resistivity of the alloys with less than about 35 at.% Cr and less than 23 at.% Al increases with increasing chromium and aluminium contents and reaches a maximum value for the Cr<sub>30</sub>Fe<sub>50</sub>Al<sub>20</sub> (at.%) alloy. The temperature coefficient of resistivity in the temperature range between room temperature and 500°C decreases with increasing chromium and aluminium contents and becomes zero in the vicinity of 20 to 30 at.% Cr and 15 at.% Al. The influence of aluminium on the kinetics of  $\sigma$  phase formation in alloys at the equiatomic Cr/Fe ratio with fine- and coarse-grained structures was studied by [2000Bla] using <sup>57</sup>Fe Mössbauer spectroscopy. It was found that the addition of 0.2 at.% Al slightly accelerated the kinetics in the coarse-grained samples, and practically did not affect in the fine-grained samples. On the other hand, doping with 1 at.% Al resulted in a significant retardation of the  $\sigma$  phase formation both in the fine-grained samples as well as in the coarse-grained samples. [2001Dem] presented the results of surface oxidation studying on the alloys containing the

O<sub>1</sub>-(CrFeAl) and O<sub>2</sub>-(CrFeAl) phases. It was found that under mild conditions only aluminium oxidizes, but under extreme conditions (water immersion at room temperature, or oxygen exposure at high temperatures), chromium oxidizes as well. [2001Rod] obtained a nanocomposite with an amorphous matrix containing metallic nanocrystals through the controlled crystallization of an amorphous Cr-5Fe-90Al (at.%) alloy. Milling of this alloy for 60 h resulted in the formation of amorphous and nanocrystalline regions and the crystallization temperatures for the primary and intermetallic phases occurred with an interval of 50°C. The effect of heat treatment and grain size on the damping capacity of the Cr-70Fe-5Al (mass%) (Cr-63.4Fe-12.3Al (at.)) has been investigated by [2002Zho]. It has been shown that annealing temperature and grain size have a significant influence on the damping capacity and strain amplitude dependence of this alloy. It has a rather low damping capacity after being water quenched or cold worked due to a high internal stress in the structure. [2002Dem2] studied the optical conductivity of the ternary phases and interpreted the obtained data on the basis of a tunneling transition. Good agreement between the obtained results and a theoretical approach developed for aperiodic intermetallics assuming an anomalous diffusion of the electron wavepacket was found.

### Miscellaneous

[1970Koz3] reported the solubility of C in liquid Al-Cr-Fe alloys at different temperatures. [1974Vya] used the “simplex lattice method” to construct the liquidus and solidus surfaces and reported a good agreement with data of [1970Koz1].

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**Table 1:** Crystallographic Data of Solid Phases

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
(Al) ≤ 660.452  $\text{Cr}_x\text{Fe}_y\text{Al}_{1-x-y}$	$cF4$ $Fm\bar{3}m$ Cu	$a = 404.88$	pure Al, $T = 24^\circ\text{C}$ [V-C]  $x = 0$ to 0.00375 [2003Cor] $y = 0$ to 0.004 [2003Pis]
(Cr) ≤ 1863  $\alpha$ , ( $\alpha\text{Fe}$ )(r) ≤ 912 $\alpha$ , $\text{Cr}_x\text{Fe}_{1-x-y}\text{Al}_y$	$cI2$ $Im\bar{3}m$ W	$a = 288.4$  $a = 286.65$ $a = 286.60$  $a = 287.67$ $a = 288.55$ $a = 289.2$ $a = 289.99$  $a = 288.13$ $a = 288.96$ $a = 289.43$ $a = 289.59$  $a = 2912.0$ $a = 2971.4$	pure Cr, $T = 27^\circ\text{C}$ [V-C] $x = 0$ to 0.46 [V-C2]  pure Fe, $T = 27^\circ\text{C}$ [V-C] pure Fe, room temperature [1961Lih, 1993Oka] $x = 0$ , $y = 0$ to 0.46 [1980Sch] $x = 0$ , $y = 0.06$ [1961Lih, 1993Oka] $x = 0$ , $y = 0.105$ [1961Lih, 1993Oka] $x = 0$ , $y = 0.155$ [1961Lih, 1993Oka] $x = 0$ , $y = 0.19$ [1961Lih, 1993Oka] Quenched from $250^\circ\text{C}$ [1958Tay, 1993Oka]: $x = 0$ , $y = 0.0985$ $x = 0$ , $y = 0.141$ $x = 0$ , $y = 0.177$ $x = 0$ , $y = 0.188$ Quenched from $1000^\circ\text{C}$ (100 h) [1997Pal]: $x = 0.028$ , $y = 0.444$ $x = 0.556$ , $y = 0.444$
( $\delta\text{Fe}$ )(h <sub>2</sub> ) 1538 - 1394	$cI2$ $Im\bar{3}m$ W	$a = 293.80$	[1993Oka]
( $\gamma\text{Fe}$ )(h <sub>1</sub> ) 1394 - 912  $\gamma$ , $\text{Fe}_{1-x}\text{Al}_x$ $\gamma$ , $\text{Cr}_y\text{Fe}_{1-y}$ $\gamma$ , $\text{Cr}_x\text{Fe}_{1-x-y}\text{Al}_y$	$cF4$ $Fm\bar{3}m$ Cu	$a = 366.60$ $a = 364.67$	pure Fe, $T = 1167^\circ\text{C}$ [1993Oka] $T = 915^\circ\text{C}$ [Mas2]  $x = 0$ to 0.013 [1993Oka] $y = 0$ to 0.119 [Mas2] $y = \sim 0.04$ at $x = 0.083$ , $T = 1200^\circ\text{C}$ [1946Kor] $y = 0.06$ at $x = 0.083$ , $T = 1100^\circ\text{C}$ [1946Kor] $y = 0.077$ at $x = 0.082$ , $T = 1000^\circ\text{C}$ [1946Kor]

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
$\alpha_2$ , FeAl $\leq 1310$	$cP8$ $Pm\bar{3}m$		$x = 0.22$ at $T = 600^\circ\text{C}$ to $x = 0.545$ at $T = 1102^\circ\text{C}$ [1993Oka]
$\alpha_2$ , $\text{Fe}_{1-x}\text{Al}_x$	CsCl	$a = 289.48$	$x = 0.345$ [1961Lih, 1993Oka]
		$a = 289.60$	$x = 0.389$ [1961Lih, 1993Oka]
		$a = 289.86$	$x = 0.422$ [1961Lih, 1993Oka]
		$a = 290.50$	$x = 0.475$ [1961Lih, 1993Oka]
		$a = 290.9$	$x = 0.5$ [1958Tay, 1993Oka]
		$a = 289.81$	Quenched from $T = 500^\circ\text{C}$ [1997Kog]: $x = 0.397$
		$a = 291.01$	$x = 0.509$
		$a = 289.53$	Quenched from $T = 250^\circ\text{C}$ [1958Tay]: $x = 0.362$
		$a = 289.66$	$x = 0.383$
		$a = 289.77$	$x = 0.409$
		$a = 290.17$	$x = 0.438$
$\alpha_2$ , (Fe,Cr,Al) <sub>1</sub> (Al,Cr,Fe) <sub>1</sub>		$a = 291.9$	30 at.% Cr, 40 at.% Fe [2001Alo]
		$a = 291.7$	35 at.% Cr, 35 at.% Fe [2001Alo]
$\alpha_1$ , $\text{Fe}_3\text{Al}$ $\leq 547$	$cF16$ $Fm\bar{3}m$	$a = 579.23$	$x = 0.225$ to $0.365$ [V-C] $x = 0.25$ [V-C]
$\alpha_1$ , $\text{Fe}_{1-x}\text{Al}_x$	$\text{BiF}_3$	$a = 579.30$	$x = 0.247$ [1961Lih, 1993Oka]
		$a = 579.28$	$x = 0.263$ [1961Lih, 1993Oka]
		$a = 579.30$	$x = 0.28$ [1961Lih, 1993Oka]
		$a = 579.24$	$x = 0.307$ [1961Lih, 1993Oka]
		$a = 578.92$	$x = 0.317$ [1961Lih, 1993Oka]
			Quenched from $T = 250^\circ\text{C}$ [1958Tay, 1993Oka]:
		$a = 579.30$	$x = 0.231$
		$a = 579.28$	$x = 0.237$
		$a = 579.18$	$x = 0.243$
		$a = 579.30$	$x = 0.254$
		$a = 579.32$	$x = 0.261$
		$a = 579.38$	$x = 0.272$
		$a = 579.32$	$x = 0.283$
		$a = 579.06$	$x = 0.295$
		$a = 578.94$	$x = 0.315$
		$a = 578.96$	$x = 0.34$
		$a = 578.86$	$x = 0.35$
$\alpha_1$ , (Fe,Cr,Al) <sub>3</sub> Al,Cr,Fe) <sub>1</sub>		$a = 578.86$	CrFe <sub>2</sub> Al alloy, annealed at $T = 527^\circ\text{C}$ [1983Bus]
$\epsilon$ , $\text{Fe}_2\text{Al}_3$ 1232 -1102	$cI16$ (?) -		$x \approx 0.58$ to $0.65$ [1993Oka]
$\epsilon$ , $\text{Fe}_{1-x}\text{Al}_x$		$a = 598.0$	$x = 0.61$ [1934Osa]



Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
FeAl <sub>2</sub> ≤ 1156 Fe <sub>1-x</sub> Al <sub>x</sub>	<i>aPI8</i> <i>PI</i> FeAl <sub>2</sub>	$a = 488$ $b = 646$ $c = 880$ $\alpha = 91.70^\circ$ $\beta = 73.3^\circ$ $\gamma = 96.90^\circ$	$x = 0.655$ to $0.670$ [V-C] $T = 900^\circ\text{C}$ [V-C]
		$a = 487.8$ $b = 646.1$ $c = 880.0$ $\alpha = 91.75^\circ$ $\beta = 73.27^\circ$ $\gamma = 96.89^\circ$	$x = 0.669$ ; $\rho = 4200 \text{ kg}\cdot\text{m}^{-3}$ [1973Cor]
	A-base-centred pseudomonoclinic	$a = 759.4$ $b = 1688.6$ $c = 486.2$ $\alpha = 89.55^\circ$ $\beta = 122.62^\circ$ $\gamma = 90.43^\circ$	[1978Bas]
	Triclinic <i>PI</i>	$a = 487.8$ $b = 646.1$ $c = 880.0$ $\alpha = 91.75$ $\beta = 73.27$ $\gamma = 96.89$	$x = 0.666$ , quenched from $T = 1000^\circ\text{C}$ (100 h) [1997Pal]
(Cr <sub>y</sub> Fe <sub>1-y</sub> )Al <sub>2</sub>	Triclinic <i>PI</i>	$a = 486.3$ $b = 645.4$ $c = 880.1$ $\alpha = 91.92$ $\beta = 72.95$ $\gamma = 96.87$	$y = 0$ to $0.045$ , $T = 1000^\circ\text{C}$ [1997Pal] $y = 0.045$ , quenched from $T = 1000^\circ\text{C}$ (100 h) [1997Pal]
Fe <sub>2</sub> Al <sub>5</sub> ≤ 1169 Fe <sub>1-x</sub> Al <sub>x</sub>	<i>oC24</i> <i>Cmcm</i>	$a = 767.5$ $b = 640.3$ $c = 420.3$	$x = 0.70$ to $0.73$ [1993Oka] $x = 0.72$ [1953Sch]
		$a = 765.73$ $b = 640.87$ $c = 422.65$	$x = 0.7145$ [1986Gri]
		$a = 765.59$ $b = 641.54$ $c = 421.84$	$x = 0.715$ [1994Bur]
		$a = 767.5$ $b = 640.3$ $c = 420.3$	$x = 0.7145$ , quenched from $T = 1000^\circ\text{C}$ (100 h) [1997Pal]
(Cr <sub>y</sub> Fe <sub>1-y</sub> ) <sub>2</sub> Al <sub>5</sub>		$a = 769.4$ $b = 644.3$ $c = 422.7$	$y = 0$ to $0.062$ , $T = 1000^\circ\text{C}$ [1997Pal] $y = 0.062$ , quenched from $T = 1000^\circ\text{C}$ (100 h) [1997Pal]

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
FeAl <sub>3</sub> ≤ 1160 Fe <sub>1-x</sub> Al <sub>x</sub>	<i>mC102</i> <i>C2/m</i>		$x = 0.745$ to $0.766$ [1993Oka] Sometimes called Fe <sub>4</sub> Al <sub>13</sub> in the literature $x = 0.767$ [1986Gri]
		$a = 1548.7$ $b = 808.4$ $c = 1248.8$ $\beta = 107.99^\circ$	
		$a = 1548.3$ $b = 807.9$ $c = 1250.9$ $\beta = 108.11^\circ$	$x = 0.7665$ [1986Gri]
		$a = 1548.9$ $b = 808.31$ $c = 1247.6$ $\beta = 107.72^\circ$	$x = 0.766$ , single crystal [1955Bla1, 1955Bla2]
		$a = 1550.4$ $b = 807.0$ $c = 1247.2$ $\beta = 107.71^\circ$	$x = 0.7602$ [1986Gri]
		$a = 1549.2$ $b = 807.8$ $c = 1247.1$ $\beta = 107.69^\circ$	$x = 0.76$ [1994Gri]
		$a = 1550.9$ $b = 806.3$ $c = 1247.7$ $\beta = 107.74^\circ$	$x = 0.7594$ [1986Gri]
		$a = 1551.3$ $b = 805.1$ $c = 1248.6$ $\beta = 107.80^\circ$	$x = 0.7463$ [1986Gri]
		$a = 1552.7$ $b = 803.5$ $c = 1244.9$ $\beta = 107.70^\circ$	$x = 0.7416$ [1986Gri]
		$a = 1548.9$ $b = 808.3$ $c = 1247.6$ $\beta = 107.72^\circ$	$x = 0.75$ , quenched from $T = 1000^\circ\text{C}$ (100 h) [1997Pal]
(Fe,Cr,Al) <sub>1</sub> (Al,Cr,Fe) <sub>3</sub>			From 0 to 3 at.% Cr, at $600^\circ\text{C}$ [1951Pra] From 0 to 6.4 at.% Cr, from 22 to 25 at.% Fe, at $1000^\circ\text{C}$ [1997Pal] 6.4 at.% Cr, 21.1 at.% Fe, quenched from $1000^\circ\text{C}$ (100 h) [1997Pal]
	orthorhombic, <i>A2mm</i> or <i>Amm2</i> or <i>A<sub>2/m</sub>A<sub>2/m</sub>A<sub>2/m</sub></i>	$a = 640$ $b = 840$ $c = 620$	<< 1 at.% Cr at 23.3 at.% Fe; in the alloys (at.%) Cr <sub>3</sub> Al <sub>97</sub> , Cr <sub>3</sub> FeAl <sub>96</sub> and Cr <sub>3</sub> Fe <sub>3</sub> Al <sub>94</sub> prepared by hot extrusion of rapidly solidified powder, followed annealing at $400^\circ\text{C}$ [1995Zia]

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
Fe <sub>2</sub> Al <sub>9</sub>	<i>mP22</i> <i>P2<sub>1</sub>/c</i> Co <sub>2</sub> Al <sub>9</sub>	$a = 869$ $b = 635$ $c = 632$ $\beta = 93.4^\circ$	Metastable 81.8 at.% Al [1977Sim, 1993Oka]
FeAl <sub>6</sub>	<i>oC28</i> <i>Cmc2<sub>1</sub></i> FeAl <sub>6</sub>	$a = 744.0$ $b = 646.3$ $c = 877.0$ $a = 744$ $b = 649$ $c = 879$	Metastable 85.7 at.% Al [1993Oka]  [1998Ali]
FeAl <sub>4+x</sub>	<i>t**</i>	$a = 884$ $c = 2160$	Metastable, $0 < x < 0.4$ [1998Ali]
$\theta$ , Cr <sub>2</sub> Al <sub>13</sub> $\leq 791$	<i>mC104</i> <i>C2/m</i> V <sub>7</sub> Al <sub>45</sub>	$a = 2519.6$ $b = 757.4$ $c = 1094.9$ $\beta = 128.7^\circ$	Room temperature, 13.5 at.% Cr [1975Ohn, 1995Aud, 2003Cor] Sometimes called CrAl <sub>7</sub> in the literature
$\theta$ , (Cr,Fe,Al) <sub>2</sub> (Al,Cr,Fe) <sub>13</sub>			From 0 to 3.2 at.% Fe; 11.5 at.% Cr at 3.2 at.% Fe; cooled slowly from the liquid state [1951Pra]
$\rho$ , Cr <sub>2</sub> Al <sub>11</sub> $\leq 941$	<i>oC584</i> <i>Cmcm</i>		16.9 to 19.2 at.% Cr [1995Aud, 2000Mah, 2003Cor] Sometimes called CrAl <sub>5</sub> in the literature
		$a = 1240$ $b = 3460$ $c = 2020$	Quenched from 920°C, 16.9 to 19.2 at.% Cr [1995Aud, 2000Mah, 2003Cor] “eCrAl <sub>4</sub> ” [1992Wen]
$\rho$ , (Cr,Fe,Al) <sub>2</sub> Al(Cr,Fe) <sub>11</sub>		$a = 1260$ $b = 3460$ $c = 2000$	From 0 to 7.74 at.% Fe; 11.45 at.% Cr at 7.74 at.% Fe; cooled slowly from the liquid state, in equilibrium with FeAl <sub>3</sub> [1951Pra]
$\mu$ , CrAl <sub>4</sub> $\leq 1031$	<i>hP574</i> <i>P6<sub>3</sub>/mmc</i>		$x = 0.78$ to $0.80$ [2003Cor] $y = 0.788$ to $0.794$ , at $800^\circ\text{C}$ [1995Aud]
$\mu$ , Cr <sub>1-x</sub> Al <sub>x</sub>	$\mu\text{MnAl}_4$	$a = 1998$ $c = 2467$	$x = 0.791 \pm 0.003$ [1995Aud, 2000Mah, 2003Cor] $y = 0.777 \pm 0.001$ , quenched from $1000^\circ\text{C}$ [2000Mah, 2003Cor]
		$a = 2010$ $c = 2480$	From 0 to 11.9 at.% Fe, $T = 1000^\circ\text{C}$ [1997Pal]
$\mu$ , (Cr,Fe,Al) <sub>1</sub> Al(Cr,Fe) <sub>4</sub>		$a = 2146.9$ $c = 1634$ $a = 2165.1$ $c = 1644.9$	at 10.9 at.% Fe, 19.1 at.% Cr, quenched from $1000^\circ\text{C}$ (100 h) [1997Pal] The Cr <sub>19.9</sub> Fe <sub>75.0</sub> Al <sub>5.1</sub> sample quenched from $1000^\circ\text{C}$ (100 h) [1997Pal]
$i$ , CrAl <sub>4</sub> (or CrAl <sub>5</sub> )	icosahedral		In melt spun alloys Al–Cr at 8 to 13 at.% Cr; by decomposition of amorphous of 20 at.% Cr, metastable [1998Mur]

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
$\zeta_1$ , Cr <sub>4</sub> Al <sub>9</sub> (h) $\zeta_1$ , Cr <sub>1-x</sub> Al <sub>x</sub>	<i>cI52</i> <i>I43m</i> Cu <sub>4</sub> Al <sub>9</sub>	$a = 912.3$	$x \approx 0.55$ to 0.69 [Mas2] $x = 0.71$ at Al-rich limit, quenched from $T = 920^\circ\text{C}$ [1995Aud]
$\zeta_2$ , Cr <sub>4</sub> Al <sub>9</sub> (r) $\zeta_2$ , Cr <sub>1-x</sub> Al <sub>x</sub>  $\zeta_2$ , (Cr,Fe,Al) <sub>4</sub> (Al,Cr,Fe) <sub>9</sub>	<i>hR52</i> <i>R3m</i> Cr <sub>4</sub> Al <sub>9</sub>	$a = 1291$ $c = 1567.7$  $a = 1284.7$ $c = 1545.9$	$x = 0.650$ to 0.672 [Mas2] In the alloy Cr <sub>15</sub> Fe <sub>15</sub> Al <sub>70</sub> quenched from 1000°C (100 h) [1997Pal] From 29 to 39 at.% Cr, from 0 to 9.6 at.% Fe (or to 12.5 at.% Fe estimated), $T = 1000^\circ\text{C}$ [1997Pal] 29 at.% Cr, 9.6 at.% Fe, quenched from 1000°C (100 h) [1997Pal]
$\gamma_1$ , Cr <sub>5</sub> Al <sub>8</sub> (h) $\geq 1100$ (?)	<i>cI52</i> <i>I43m</i> Cu <sub>5</sub> Zn <sub>8</sub>	$a = 904.7$ to 910.4	30.0 to 42.0 at.% Cr, quenched from liquid [1989Ell]
$\gamma_2$ , Cr <sub>5</sub> Al <sub>8</sub> (r) $\leq 1100$ (?) $\gamma_2$ , Cr <sub>1-x</sub> Al <sub>x</sub>	<i>hR26</i> <i>R3m</i> Cr <sub>5</sub> Al <sub>8</sub>	$a = 1271.9$ $c = 793.6$ $a = 1276.5$ to 1271.5 $c = 795.4$ to 782.8 $a = 1272.8$ $c = 794.2$	[1994ICD], No. 29-15] $x = 0.58$ to 0.65 [1989Ell] [1977Bra]
$\gamma_2$ , (Cr,Fe,Al) <sub>5</sub> (Al,Cr,Fe) <sub>8</sub>		$a = 1267.0$ $c = 790.0$ $a = 1258.4$ $c = 785.0$ $a = 1255.4$ $c = 783.0$ $a = 1254.0$ $c = 782.0$ $a = 1253.0$ $c = 779.0$	37 to 40 Cr, 0 to 32.5 Fe (at.%) $T = 1000^\circ\text{C}$ [1997Pal] 6 at.% Fe, quenched from 1000°C (100h) [1997Pal] 18.5 at.% Fe, quenched from 1000°C (100 h) [1997Pal] 24 at.% Fe, quenched from 1000°C (100h) [1997Pal] 25.5 at.% Fe, quenched from 1000°C (100 h) [1997Pal] 5 at.% Fe, quenched from 1000°C (100h) [1997Pal]
$\eta$ , Cr <sub>2</sub> Al < 910	<i>tI6</i> <i>I4/mmm</i> MoSi <sub>2</sub>	$a = 300.45$ $c = 864.77$ $a = 300.5 \pm 0.1$ $c = 864.9 \pm 0.1$	$\sim 65.5$ to 71.4 at.% Cr [1998Mur] [1937Bra, 1998Mur] [1989Ell]
$\eta$ , (Cr <sub>1-x</sub> Fe <sub>x</sub> ) <sub>2</sub> Al		$a = 300.1$ to 299.0 $c = 864.7$ to 865.9 $a = 299.5$ $c = 865.8$ $a = 298.8$ $c = 867.1$ $a = 298.4$ $c = 867.5$ $a = 298.0$ $c = 867.6$ $a = 297.7$ $c = 868.0$	$0 \leq x \leq 0.25$ , annealed at 700 to 1000°C [1969Kal] $x = 0.025$ $x = 0.045$ $x = 0.075$ $x = 0.085$ $x = 0.120$

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
X ≤ 400	Cr <sub>5</sub> Al <sub>3</sub> or Cr <sub>3</sub> Al superlattice		Possibly metastable [1998Mur]  ~75 to ~80 at.% Cr [1981Bro, 1981Ten]
T			In quenched alloys Cr–Al at 60 to 100 at.% Cr, like metastable ωTi in Ti alloys [2000Sha1, 2000Sha2]
σ, CrFe 830–440	<i>tP</i> 30 <i>P</i> 4 <sub>2</sub> / <i>mnm</i> CrFe	<i>a</i> = 879.95 <i>c</i> = 454.42	44.5 to 50.0 at.% Cr [V–C]
* v	<i>P</i> 6 <sub>3</sub> / <i>m</i>	<i>a</i> = 4068.0±0.07 <i>c</i> = 1254.6±0.01 atoms/cell = 1184.56  <i>a</i> = 4000 <i>c</i> = 1240	Cr <sub>10.71</sub> Fe <sub>8.68</sub> Al <sub>80.61</sub> single crystal, elicited from ingot after inductive melting followed cooling in sand bath [2000Mo]. Sometimes called “H-(CrFeAl)”. Cr <sub>11</sub> Fe <sub>8</sub> Al <sub>81</sub> together with κ-(CrFeAl) in as-cast CrFe <sub>2</sub> Al <sub>12</sub> alloy [1999Sui]
* “κ-(CrFeAl)”	hexagonal, κ-Cr <sub>18</sub> Ni <sub>6</sub> Al <sub>76</sub>		In as-cast CrFe <sub>2</sub> Al <sub>12</sub> alloy together with v [1999Sui]
* “O-(CrFeAl)”	orthorhombic body-centered	<i>a</i> = 1230 <i>b</i> = 1240 <i>c</i> = 3070	In as-cast Cr <sub>11</sub> Fe <sub>8</sub> Al <sub>81</sub> alloy together with O <sub>1</sub> -(CrFeAl) and C <sub>3,1</sub> -(CrFeAl) [2000Dem]. In as-cast Cr <sub>2</sub> FeAl <sub>12</sub> alloy together with H-(CrFeAl) and M-(CrFeAl) [1997Sui, 1999Sui]. In as-cast CrFe <sub>2</sub> Al <sub>12</sub> alloy [1998Lia]
* “O <sub>1</sub> -(CrFeAl)”	orthorhombic base-centered or primitive	<i>a</i> = 3250 <i>b</i> = 1220 <i>c</i> = 2360	In as-cast Cr <sub>11</sub> Fe <sub>8</sub> Al <sub>81</sub> , Cr <sub>16.5</sub> Fe <sub>6</sub> Al <sub>77.5</sub> and Cr <sub>21.5</sub> Fe <sub>6</sub> Al <sub>72.5</sub> alloys together with O-(CrFeAl) and C <sub>3,1</sub> -(CrFeAl) [2000Dem, 2001Dem]
* “O <sub>2</sub> -(CrFeAl)”	orthorhombic	<i>a</i> = 1990 <i>b</i> = 1240 <i>c</i> = 2320	In as-cast Cr <sub>19.5</sub> Fe <sub>8</sub> Al <sub>72.5</sub> alloy together with O-(CrFeAl) [2001Dem]
* C <sub>3,1</sub> -(CrFeAl)”	orthorhombic primitive [1988Ten]	<i>a</i> = 3270 <i>b</i> = 1250 <i>c</i> = 2380	In as-cast Cr <sub>11</sub> Fe <sub>8</sub> Al <sub>81</sub> alloy together with O <sub>1</sub> -(CrFeAl) [2000Dem]
* “M-(CrFeAl)”	monoclinic	<i>a</i> = 3310 <i>b</i> = 1230 <i>c</i> = 2480 β = 112° -	In as-cast CrFeAl <sub>12</sub> alloy [1998Lia]  In as-cast alloy Cr <sub>2</sub> FeAl <sub>12</sub> together with O-(CrFeAl) and H-(CrFeAl) [1997Sui, 1999Sui]
* <i>i</i>	simple icosahedral-type	-  <i>a</i> <sub>6D</sub> = 654.2(2)	Cr <sub>12±1</sub> Fe <sub>12±1</sub> Al <sub>75±0.5</sub> , rapid solidification by centrifugal atomization followed extrusion at 340°C [1995Zia] In Cr <sub>8</sub> Fe <sub>6</sub> Al <sub>86</sub> , rapid solidification by melt spinning [1995Sta]

**Table 2:** Coordinates of the  $((\gamma\text{Fe})+\alpha\text{Fe})/(\alpha\text{Fe})$  Surface of the  $\gamma$ -loop [1946Kor, 1991Gho]

Temperature [°C]	Al		Cr	
	(mass%)	(at.%)	(mass%)	(at.%)
1200	1.7	3.4	4.0	4.2
	2.2	4.4	4.0	4.2
	3.0	6.0	8.0	8.3
	2.9	5.8	4.0	4.2
1100	3.9	7.7	8.0	8.2
1000	1.9	3.8	12.0	12.5
	3.8	7.5	4.0	4.1

**Table 3:** Heat Treatment Schedule for Different Alloys by [1958Chu]

Alloys with > 50 mass% Fe		Alloys with > 10 mass% Al	
Temperature [°C]	Time [h]	Temperature [°C]	Time [h]
750	720	900	100
700	1000	750	200
650	720	700	500
600	720	650	250
500	2000	600	250
480	2200	500	1200

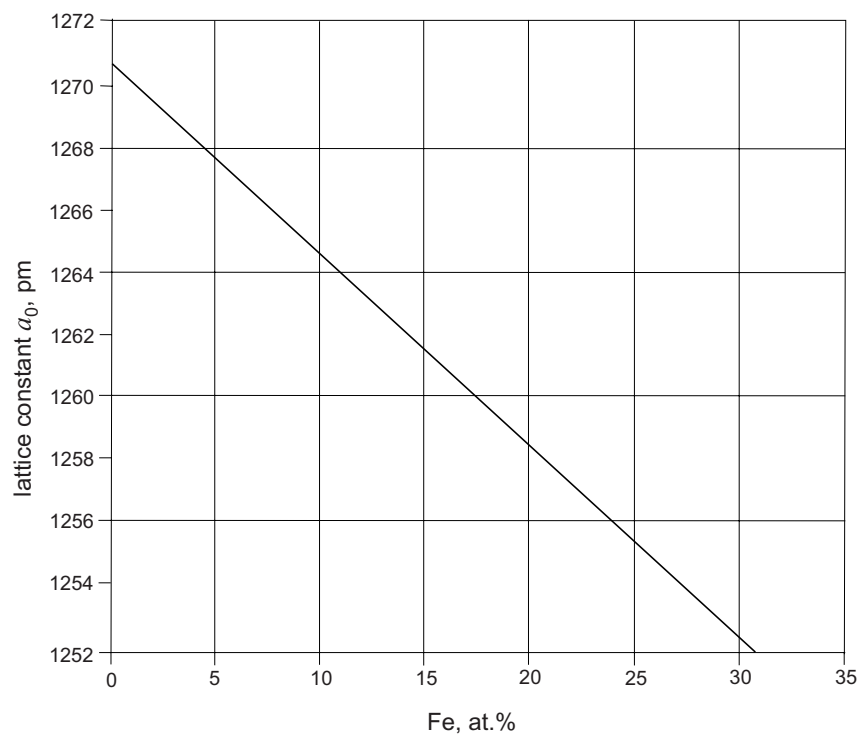
**Table 4:** Partial Pressures of Cr, Fe and Al over the Alloy Cr-75.4Fe-4.8Al (mass%) and Temperature Range of the Measurements  $\Delta T$  [1992Hil]. Errors of A and B values are standard deviations. Errors of  $p_i$  values are probable overall errors

Gaseous species $i$	$p_i$ [Pa] at 1500 K	$\Delta T$ [K]	$\ln p_i = -A \cdot 10^4/T + B$	
			A	B
Cr	$1.6 \cdot 10^{-2} \pm 14 \%$	1313-1556	$4.298 \pm 0.015$	$24.51 \pm 0.05$
Fe	$7.5 \cdot 10^{-3} \pm 15 \%$	1313-1556	$4.622 \pm 0.022$	$25.92 \pm 0.12$
Al	$4.5 \cdot 10^{-3} \pm 43 \%$	1313-1556	$4.501 \pm 0.071$	$24.50 \pm 0.56$

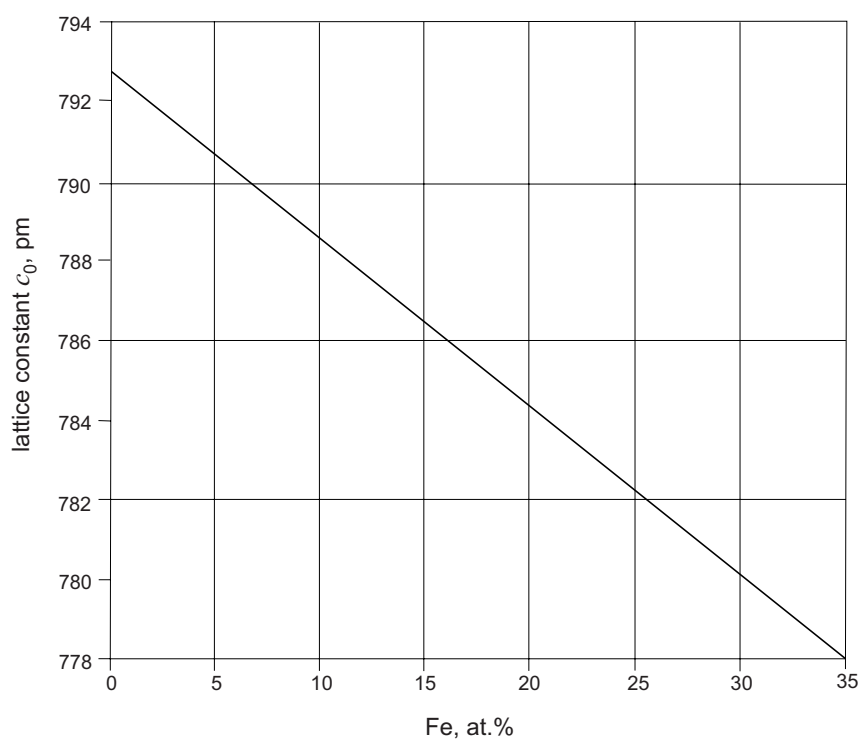
**Table 5:** Chemical Activities  $a_i$ , Excess Chemical Potentials  $\mu_i^E$ , and Partial Excess Enthalpies  $H_i^E$  of the Components in the Alloy Cr-75.4Fe-4.8Al (mass%) for a Temperature of 1500 K [1992Hil]. Errors are probable overall errors

Alloy Component $i$	$a_i$ (at 1500 K)	$\mu_i^E$ (at 1500 K) [kJ·mol <sup>-1</sup> ]	$H_i^E$ (at 1450 K) [kJ·mol <sup>-1</sup> ]
Cr	$0.28 \pm 0.04$	$4.3 \pm 1.9$	$27.6 \pm 8.8$
Fe	$0.50 \pm 0.07$	$-4.4 \pm 2.0$	$13.7 \pm 7.5$
Al	$(3.3 \pm 1.4) \cdot 10^{-3}$	$-42.0 \pm 7.0$	$-66.0 \pm 8.6$

**Fig. 1a: Al-Cr-Fe.**  
Lattice constant  $a_0$  of  
the  $\text{Cr}_5\text{Al}_8(\text{r})$  phase vs  
Fe content. Al content  
is 55 to 58 at.%



**Fig. 1b: Al-Cr-Fe.**  
Lattice constant  $c_0$  of  
the  $\text{Cr}_5\text{Al}_8(\text{r})$  phase vs  
Fe content. Al content  
is 55 to 58 at.%



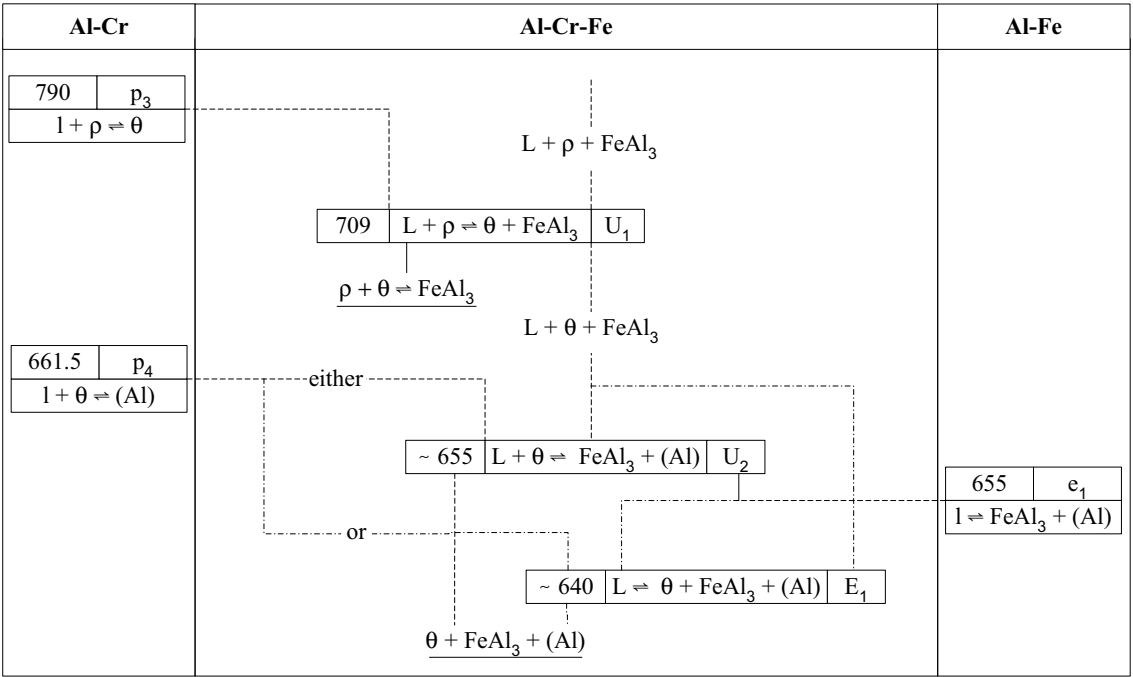
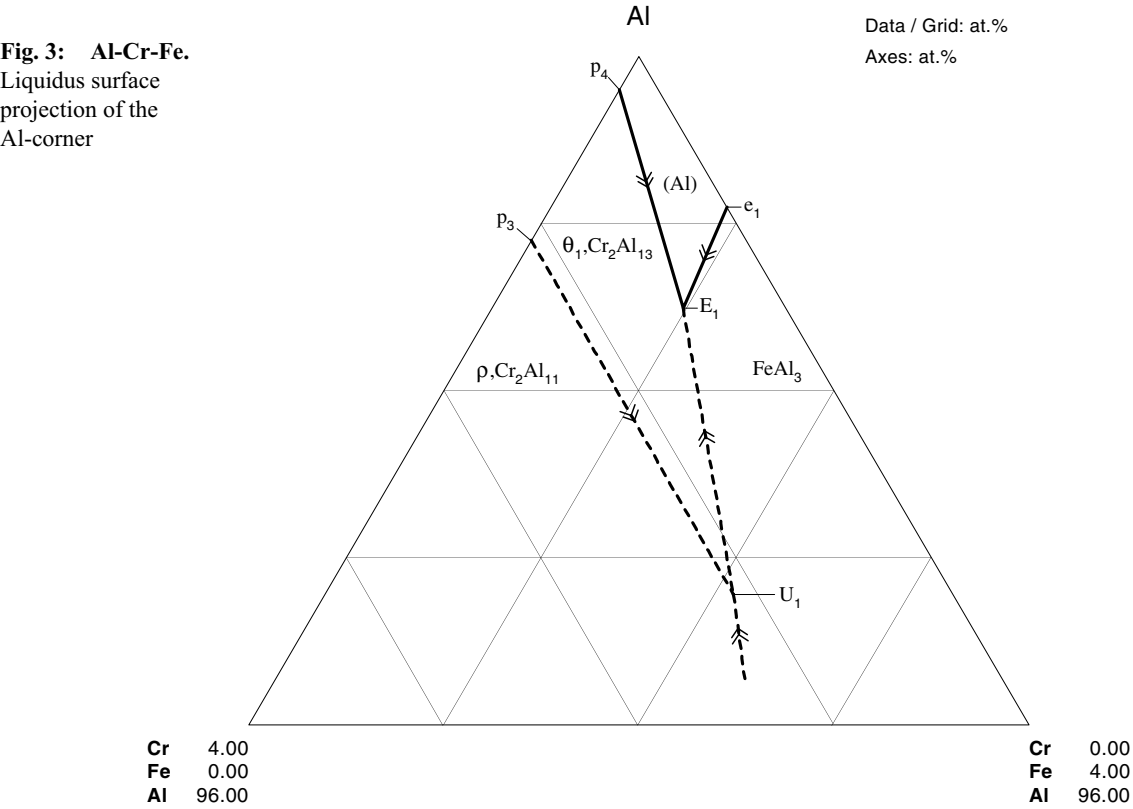
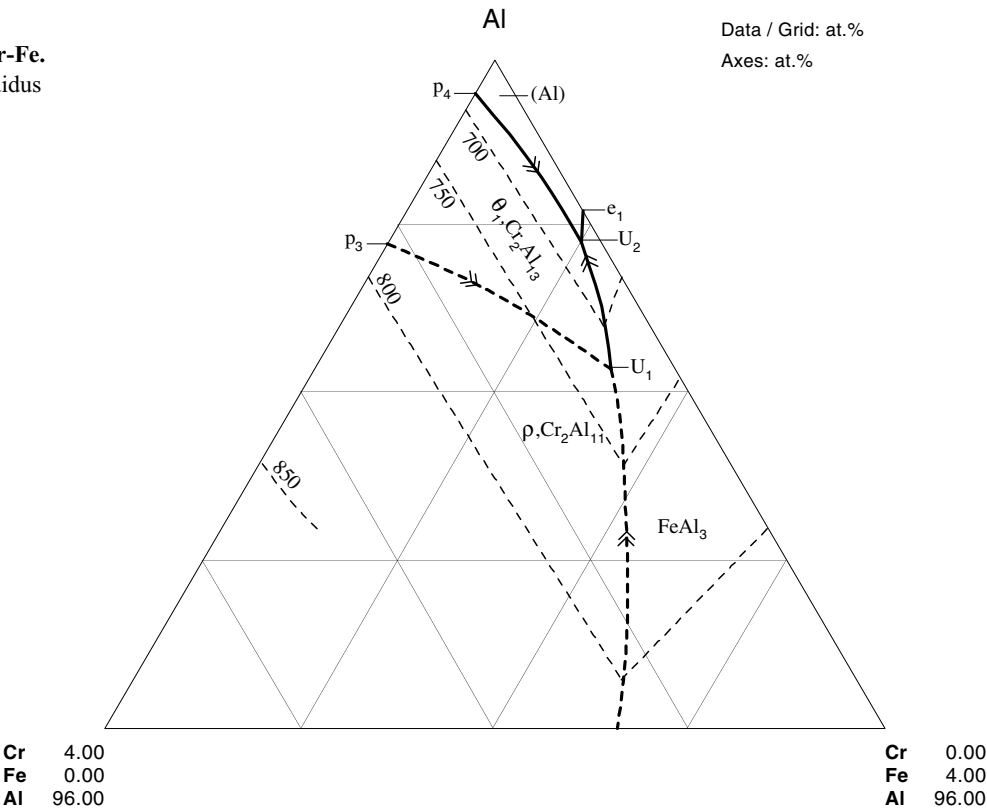


Fig. 2: Al-Cr-Fe. Partial reaction scheme of the Al-rich alloys

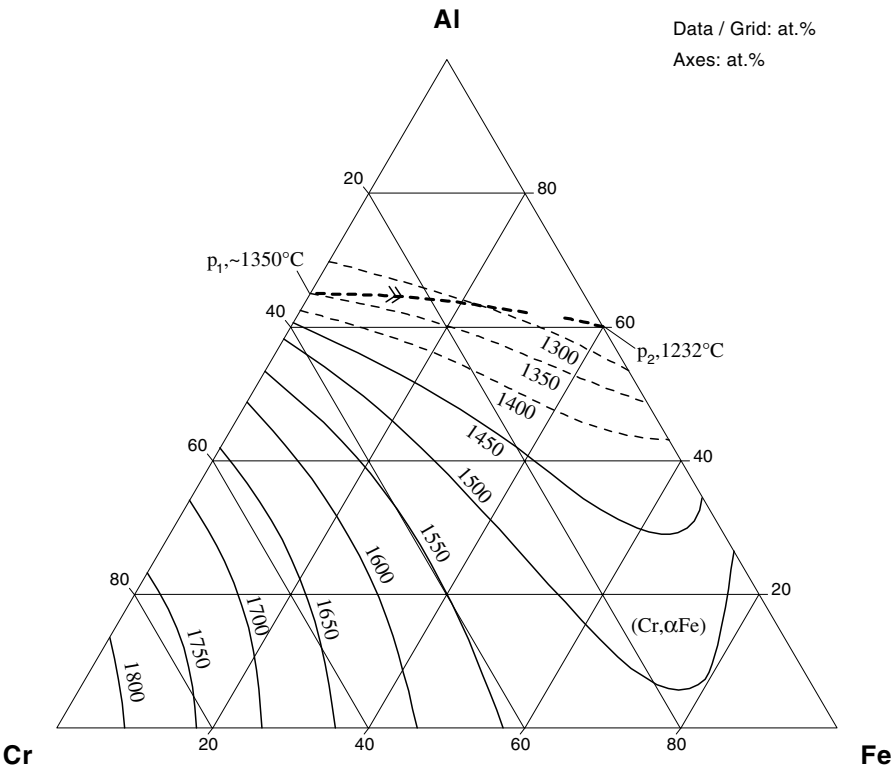




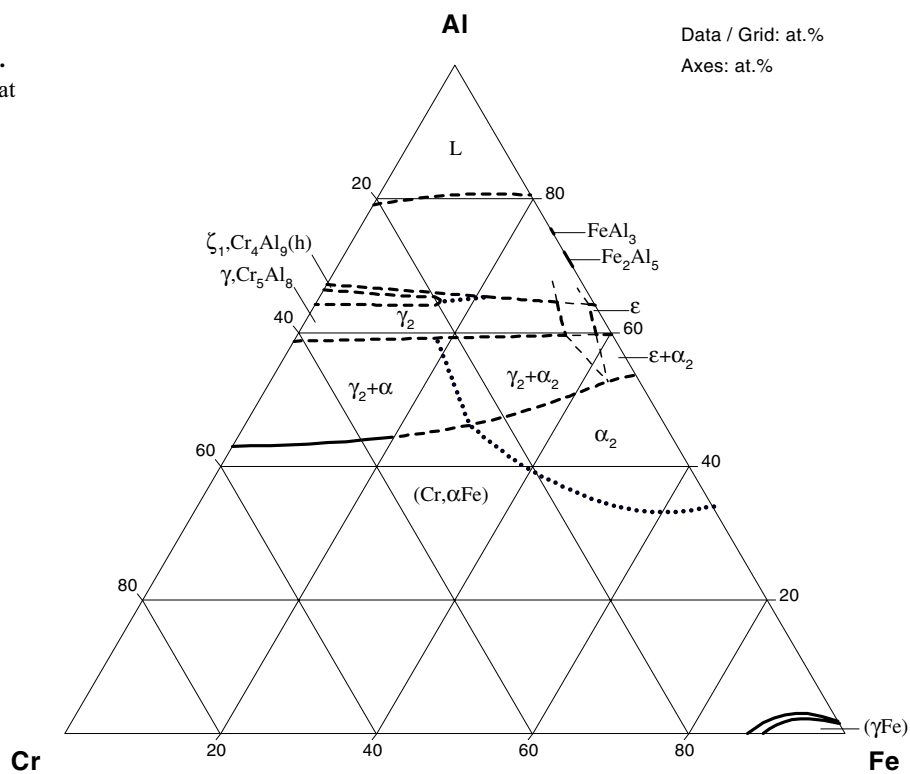
**Fig. 4: Al-Cr-Fe.**  
Calculated liquidus  
surface of the  
Al-corner



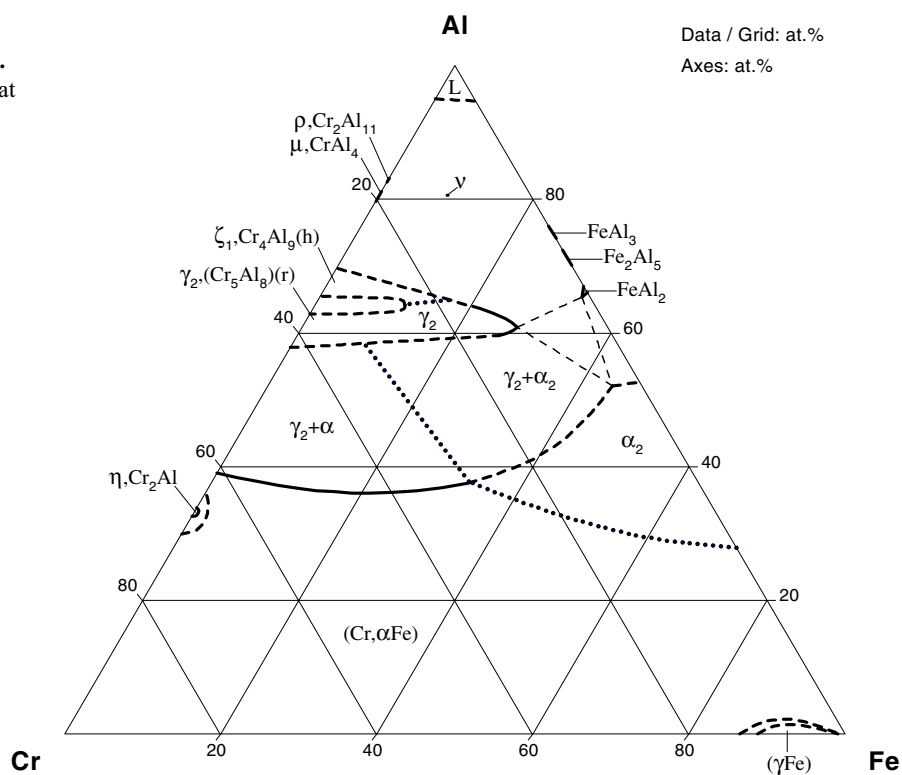
**Fig. 5: Al-Cr-Fe.**  
Partial liquidus  
surface projection



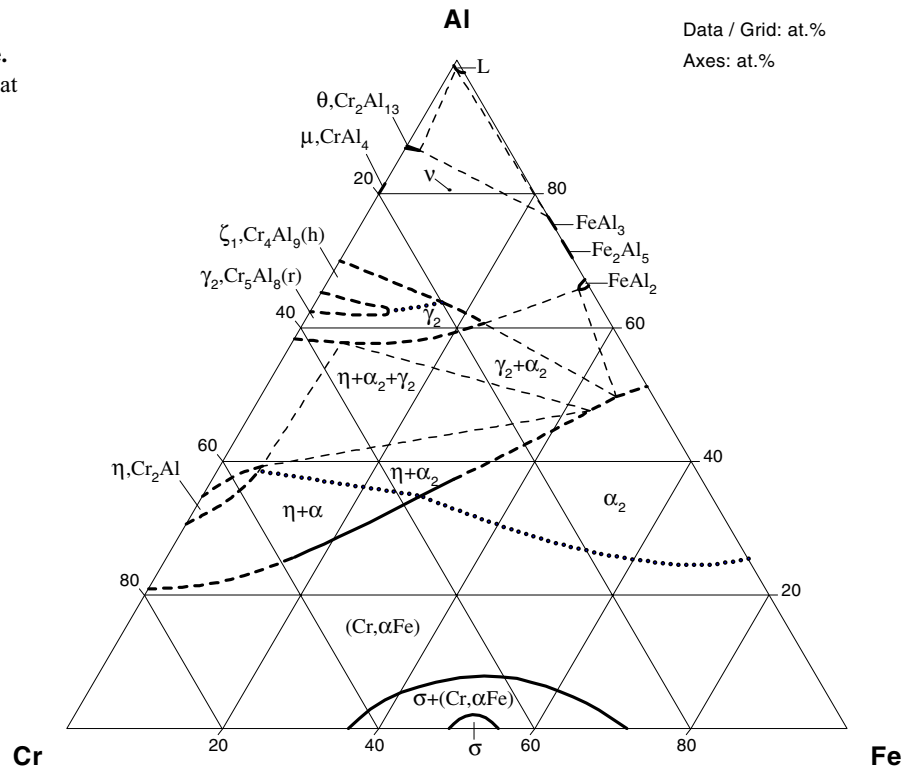
**Fig. 6: Al-Cr-Fe.**  
Isothermal section at  
1150°C



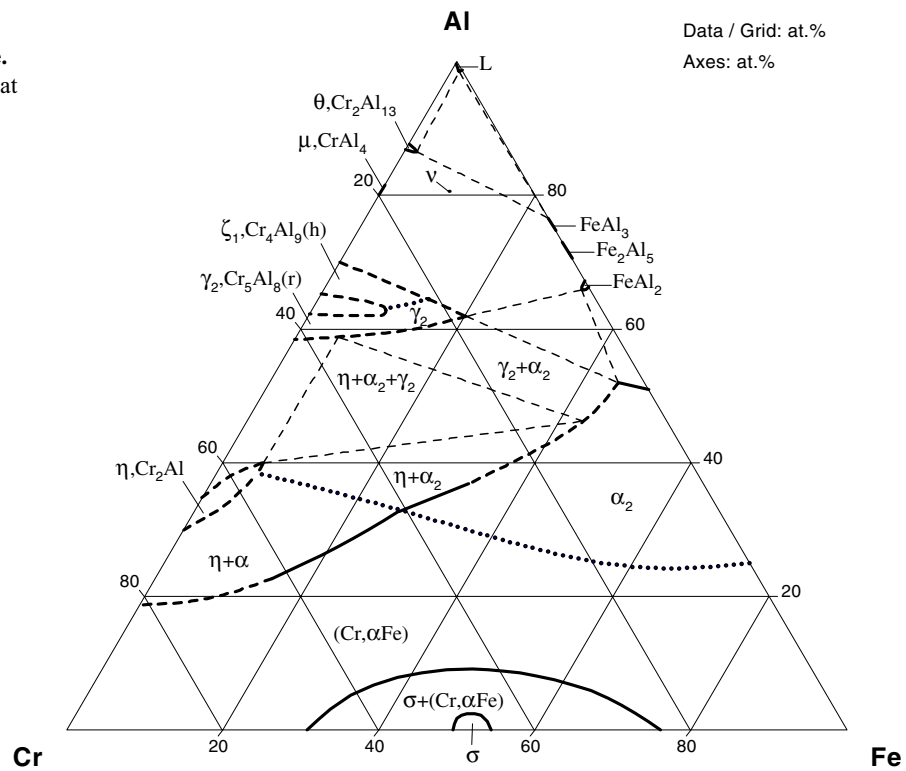
**Fig. 7: Al-Cr-Fe.**  
Isothermal section at  
900°C



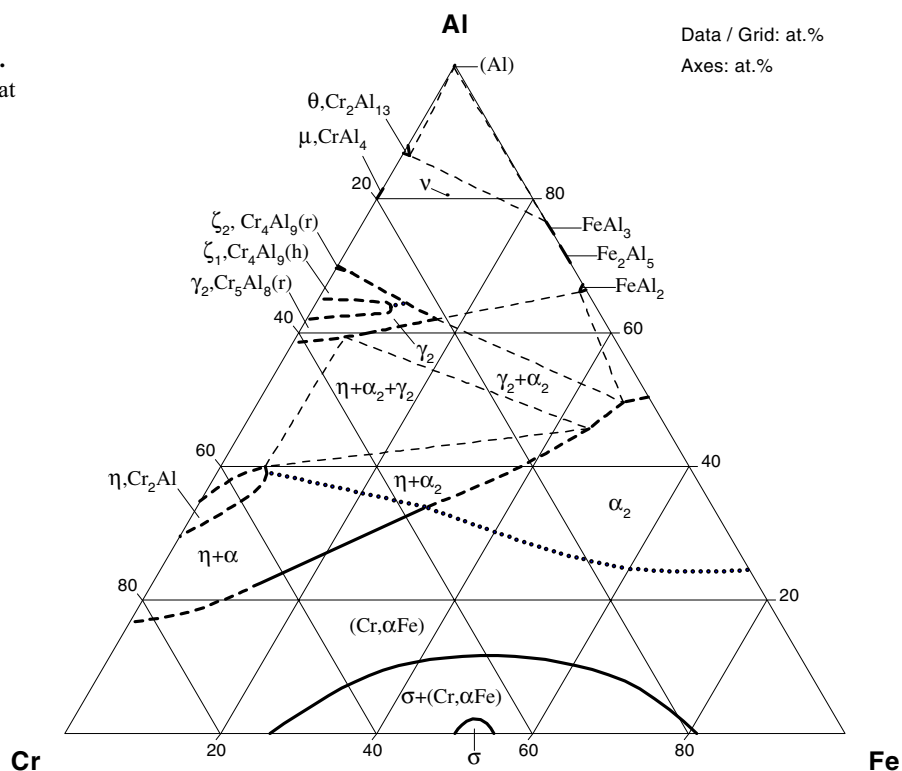
**Fig. 8: Al-Cr-Fe.**  
Isothermal section at  
750°C



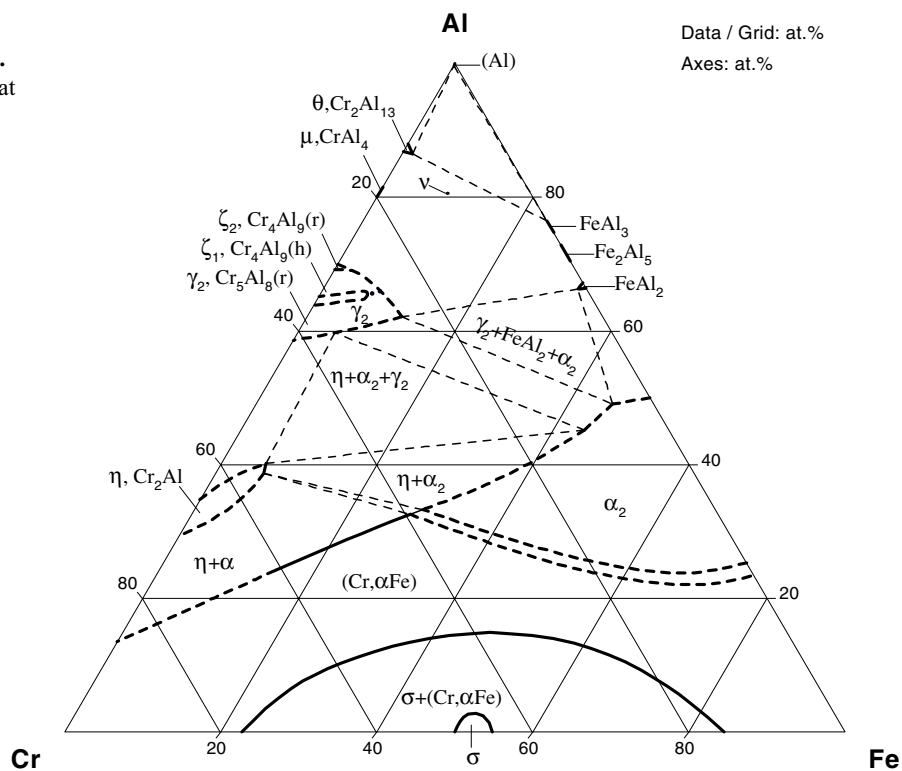
**Fig. 9: Al-Cr-Fe.**  
Isothermal section at  
700°C



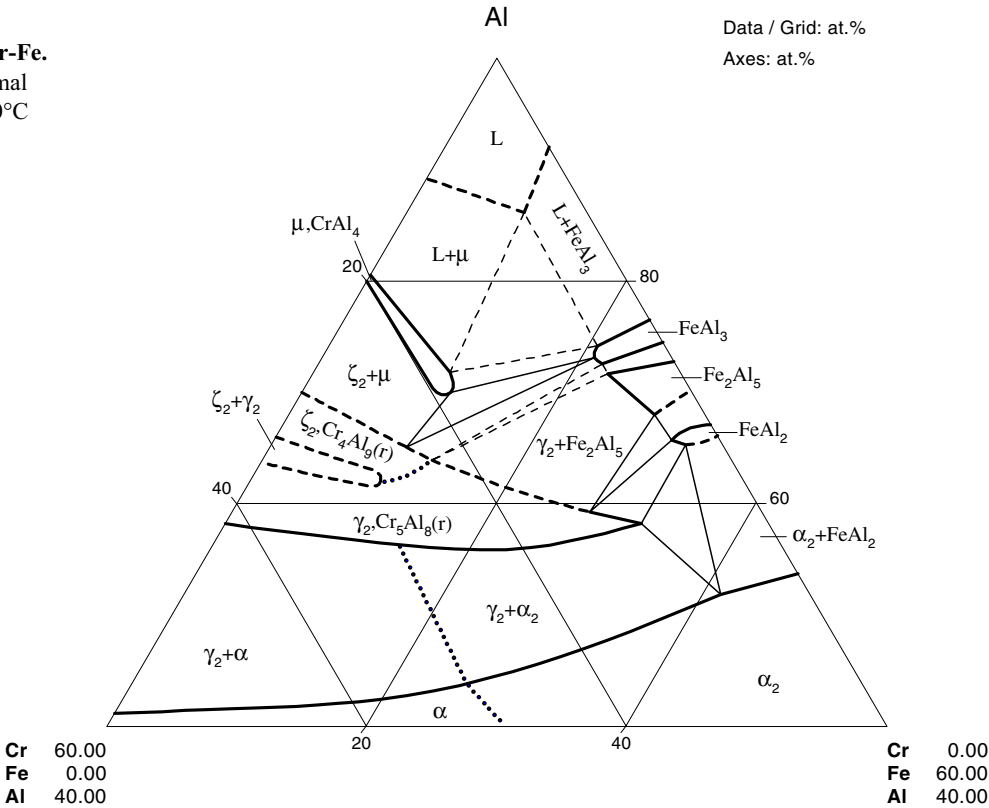
**Fig. 10: Al-Cr-Fe.**  
Isothermal section at  
650°C



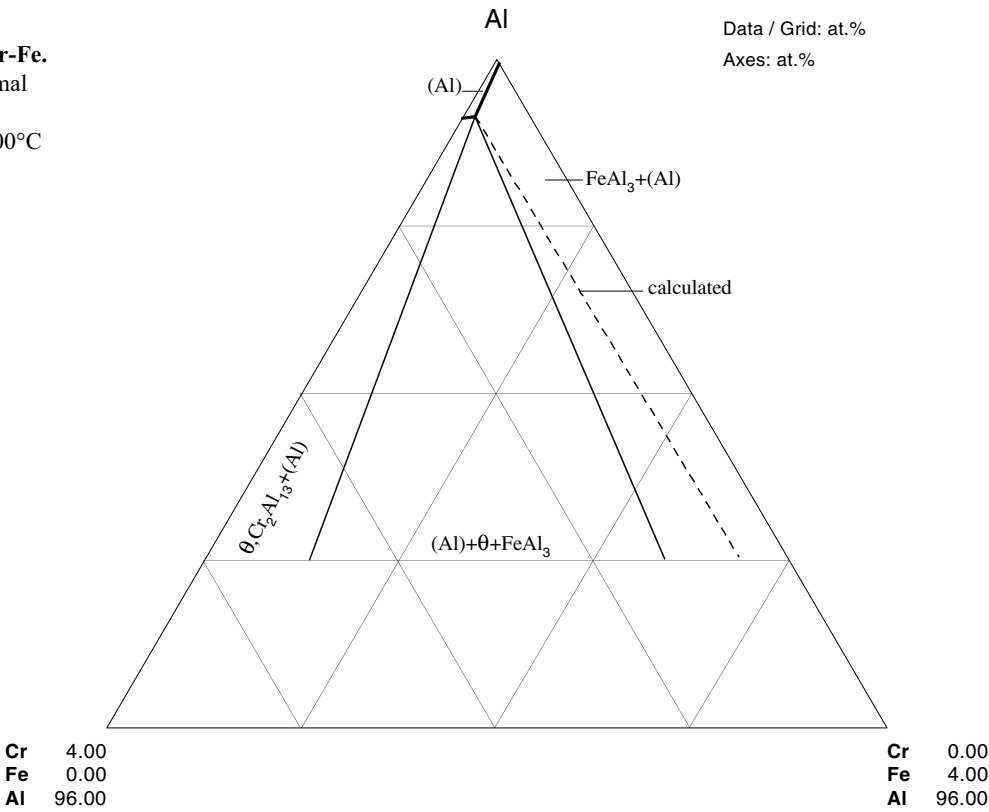
**Fig. 11: Al-Cr-Fe.**  
Isothermal section at  
600°C



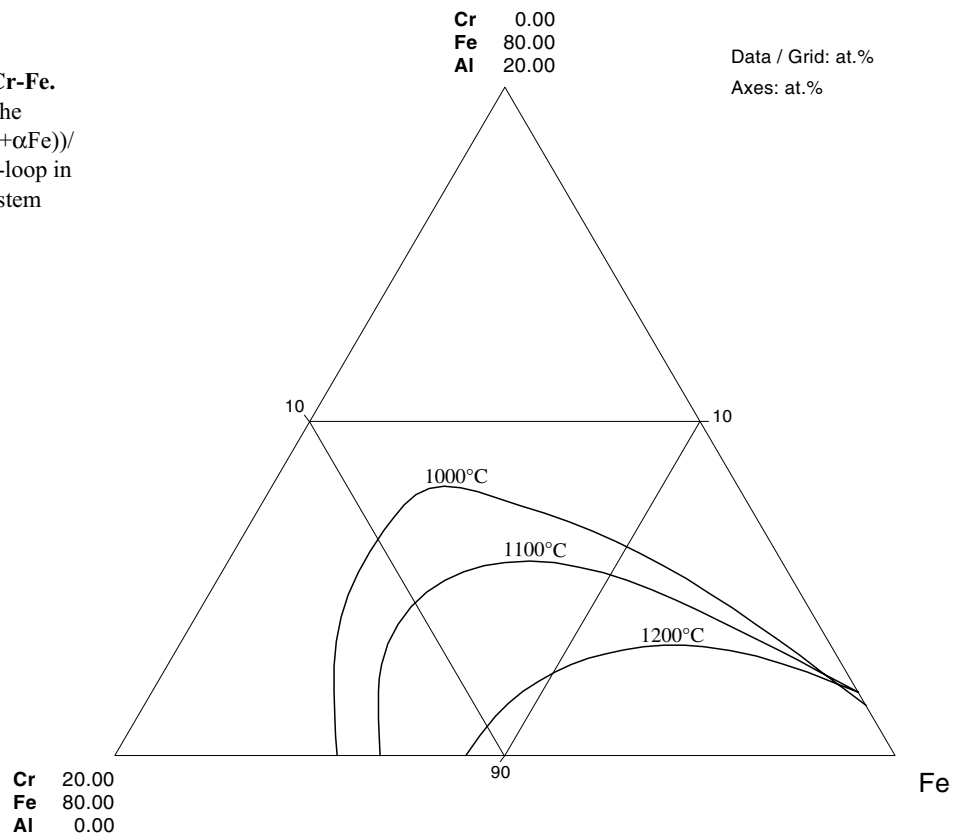
**Fig. 12: Al-Cr-Fe.**  
Partial isothermal  
section at 1000°C



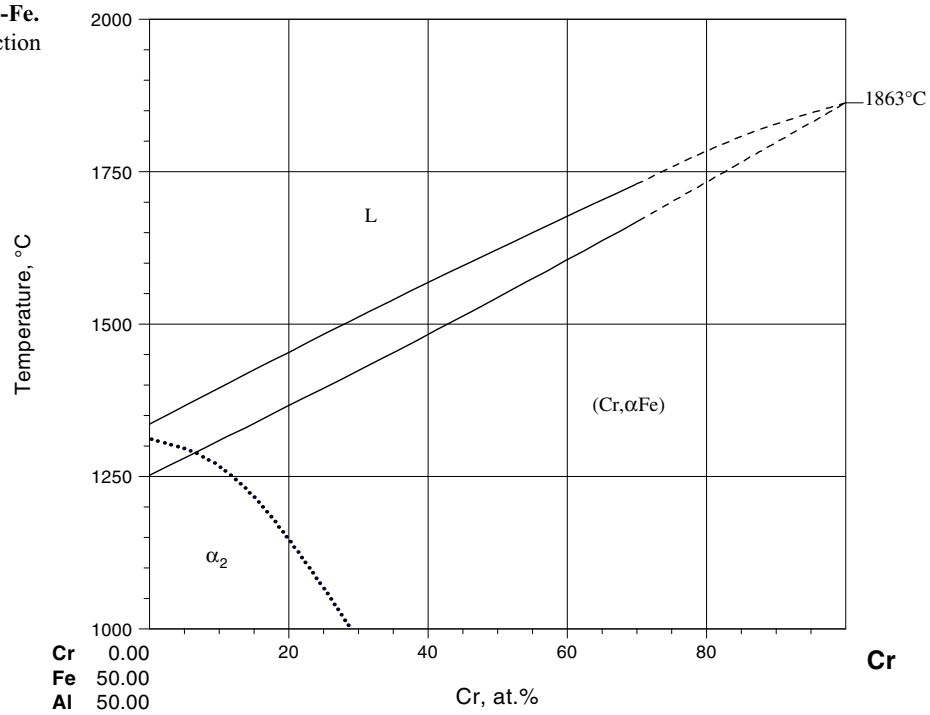
**Fig. 13: Al-Cr-Fe.**  
Partial isothermal  
section of the  
Al-corner at 600°C



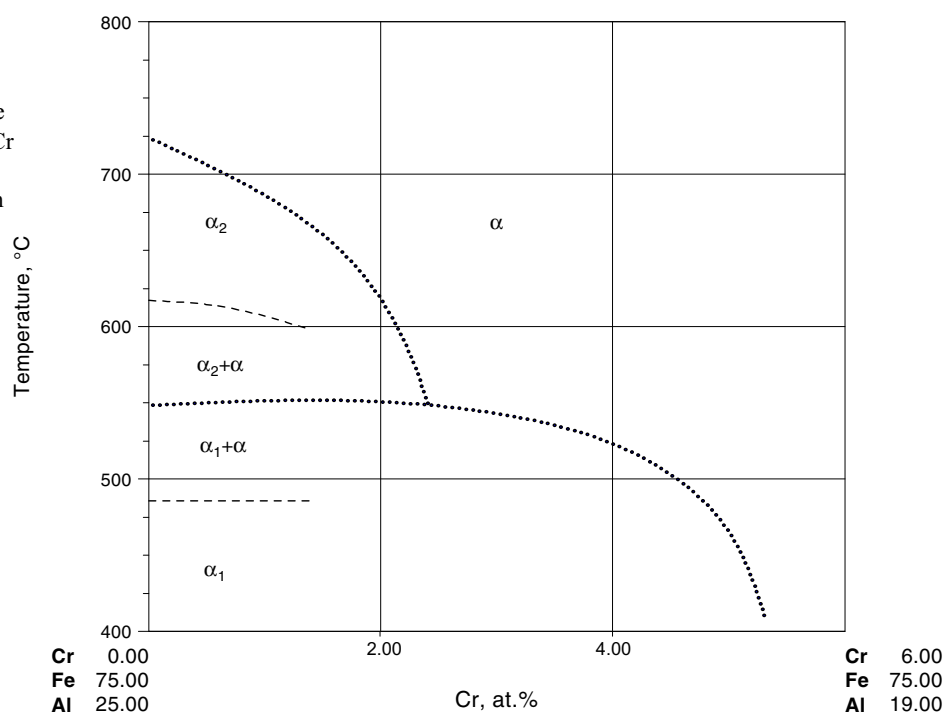
**Fig. 14: Al-Cr-Fe.**  
Isotherms of the  
surface  $((\gamma\text{Fe})+\alpha\text{Fe})/$   
 $(\alpha\text{Fe})$  of the  $\gamma$ -loop in  
the ternary system



**Fig. 15: Al-Cr-Fe.**  
Polythermal section  
FeAl - Cr



**Fig. 16: Al-Cr-Fe.**  
Variation of  
order-disorder  
reaction temperature  
as a function of the Cr  
content along the  
 $\text{Fe}_3\text{Al-CrFe}_3$  section



**Fig. 17: Al-Cr-Fe.**  
Temperature  
dependence of the  
heat capacity  $C_p$  of  
the  $\text{FeAl}_3$ -based  
compound with  
chromium content  
5 at.%

