

Ternary Alloys

Volume 21

Ternary Alloys

A Comprehensive Compendium of
Evaluated Constitutional Data and Phase Diagrams

critically evaluated by MSIT[®]

Volume 21

Selected Al-Fe-X Ternary Systems for Industrial Applications

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Introduction

There is a number of reasons for the scientific interest in the phase relations in the Al–Cr–Fe system, particularly as alloys of this system are employed as lightweight materials for structural applications and as accident-tolerant fuel-rod cladding materials due to very good oxidation and radiation resistance. The existence of quasicrystal approximants is also an interesting peculiarity of the Al–Cr–Fe system.

Reviews of the literature data concerning phase equilibria have been conducted by [1943Mon, 1953Cas, 1961Phi, 1969Wat, 1973Wil, 1976Mon, 1994Rag, 2003Rag, 2005Pal, 2012Rag, 2011Kho1, 2016Li1, 2019Eze, 2019Ran, 2020Ran], concerning crystal structures of the phases - by [2009Bau, 2013Bau]; critical assessments of the available data - by [1970Koz1, 1970Koz2, 1980Riv, 1987Sau, 1991Gho, 2004Gho, 2007Gho]. The most recent MSIT evaluation of [2007Gho] covers the literature data published before 2007. New works of [2011Kho2, 2019Eze, 2019Ran, 2020Ran] presented information about the liquidus surface. Recent data about the melting points of the alloys and the solidus surface projection constitution are given in the papers of [2008Pav3, 2009Pav, 2010Pav, 2011Kho1, 2019Eze, 2019Ran, 2020Ran]. The results of experimental investigations of phase relations at different temperatures along with isothermal sections have been recently presented by [2008Pav2, 2008Pav3, 2014Pav, 2015Zho, 2019Ran, 2020Ran]. No new experimental information besides the data of [1946Kor, 1969Bul1, 1991Tre] has been reported for the temperature-composition sections. There is a large number of papers concerning the data on the crystal structure of the ternary phases in the Al–Cr–Fe system, including the most recent findings of [2009Bau, 2010Bau, 2010Pav, 2011Bau, 2012Ume, 2014Gas]. [2008Jac, 2013Mar] reported new data on the thermodynamic properties of the (Cr, $\alpha\delta$ Fe) phase. The most recent thermodynamic assessments of the system were performed by [2017Wan, 2019Cha, 2020Ran]. The experimental methods used by the investigators, as well as the temperature and composition ranges studied, are presented in Table 1. Despite the fact that the knowledge of the phase equilibria in the system has been significantly expanded, certain issues are still to be clarified.

Binary Systems

The Al–Cr system was evaluated within the MSIT Binary Evaluation Program in 2013 by [2013Khv] involving literature data available at that moment. Later, [2014Ste, 2014Wu, 2015Kur] further studied the phase equilibria in the system. Compared to [2013Khv], these experimental studies provided the following information. [2014Ste] performed the DTA measurements of the Cr-rich part of the diagram and adjusted the liquidus and solidus for the (Cr) phase, as well as phase boundaries involving the γ brasses and Cr_2Al . [2014Wu] confirmed that $\text{Cr}_4\text{Al}_{11}$ is stable in the system and reported the temperature of its decomposition. [2015Kur] performed planar front solidification experiments and found (Al) to form *via* a peritectic reaction. The Al–Cr phase was thermodynamically assessed by [2013Hu, 2015Wit, 2017Cui]. All thermodynamic assessments result in certain discrepancies with respect to the data of [2014Ste] and melting temperatures of $\text{Cr}_2\text{Al}_{11}$ and CrAl_7 as assessed by [2013Khv].

The phase diagram of [2013Khv] was modified here to take the recent data into account. For the Cr-rich part, the phase boundaries were adjusted according to [2014Ste]. The liquidus and homogeneity range of $\beta\text{Cr}_5\text{Al}_8$ were modified according to [2015Wit], whose calculations show better agreement with the experimental data. For (Al), the peritectic reaction is accepted. The coordinates of the reaction are according to [2015Wit]. The temperature of $\text{Cr}_4\text{Al}_{11}$ decomposition is according to [2014Wu]. Below 1100°C, a series of γ -brasses exists in the central part of the Al–Cr diagram. The corresponding phase equilibria were presented by [2013Khv]. Since no experimental information relevant to different γ -brasses modifications is available for the Al–Cr–Fe system, this part of the diagram was simplified by removing the phase boundaries between different modifications of γ -brasses below 1100°C. The resulting homogeneity range corresponds to a rhombohedrally distorted γ -brass structure denoted as $\alpha\text{Cr}_5\text{Al}_8$. The final phase diagram is presented in Fig. 1. The phase equilibria below 450°C are not included because of their uncertainty and lack of experimental data for the ternary phase diagram. [2013Khv] mentioned several possible crystal structures for $\text{Cr}_2\text{Al}_{11}$. According to the observations of [2008Gru, 2009Che, 2008Cao], this compound has a monoclinic $C2/c$ structure. The $Cmcm$ structure corresponds to the metastable $\epsilon\text{-CrAl}_4$ compound.

The accepted Al–Fe binary phase diagram is according to [2022Ste] and presented in the ‘Aluminium – Iron’ chapter. [2010Xio] thoroughly reviewed the phase equilibria in the Cr–Fe system. This system was subsequently assessed by [2011Xio, 2017Cui]. The phase diagram, as compiled by [2010Xio], is accepted in the present evaluation since it provides the best agreement with the available experimental data.

Solid Phases

Crystallographic data on the known unary and binary phases, as well as recently reported ternary ones, are listed in Table 2. Only binary phases that are relevant to the phase transformation in the ternary system have been included.

Solid solutions. According to [2011Kho1, 2019Eze], the addition of Cr slightly increases the solubility of iron in the (Al) phase, while Fe almost does not affect the Cr solubility in this solid solution. Similar to the Al–Cr and Al–Fe systems, the highest solubility of Cr and Fe is observed at solidus temperatures.

Experimental observations of [1946Kor] are the only source of data concerning the (γ Fe) homogeneity range in the ternary system. The extended (γ Fe) solubility range, which reaches up to 7.7 at.% Al and 8.2 at.% Cr at 900 and 1000°C, is most probably due to the low purity of the samples. The as-prepared alloys contained in average 0.04 mass% C and 0.15 mass% Si.

Disordered (Cr, $\alpha\delta$ Fe) solution and its ordered polymorphs. There is a variety of studies on the phase equilibria involving (Cr, $\alpha\delta$ Fe) and its ordered polymorphs – $B2$ (FeAl), $D0_3$ (Fe_3Al) and its ternary $L2_1$ equivalent – Heusler phase CrFe_2Al . These phases have the same cubic lattice with a similar lattice parameter but differ in the ordering of the Fe and Al atoms. Therefore, the ordered polymorphs can easily precipitate coherently in the Al–Fe matrix even during severe quenching of the samples and have a very fine scale. Consequently, the XRD measurements of the quenched structures at room temperature may show the existence of an ordered phase, though a sample had a disordered structure at the annealing temperature. In general, the ordering type can be observed using *in-situ* TEM technique. But the analysis of anti-phase domain (APD) structures in TEM foils at room temperature also allows to retrieve the structure which has been stable at a particular annealing temperature before quenching. The chemical driving forces for ordering in the Al–Cr–Fe are very low, so the formation of an ordered phase in the ternary system may become apparent after long annealing at high Cr concentration. This also affects the establishment of the order-disorder transformation temperatures resulting in a high scatter of the reported data and difficulties in interpretation of the transformations occurring at a particular temperature. Thus, systematic and comprehensive studies of the order-disorder transformations require the production of a series of samples at different annealing temperatures and times, as well a combination of various techniques, such as high-resolution SEM, *in-situ* TEM and TEM APD examination at room temperature, DSC and DTA. For the Al–Cr–Fe system, there are no such experimental investigations that meet all these requirements. But several studies reveal the complex nature of the phase equilibria involving (Cr, $\alpha\delta$ Fe) and its ordered polymorphs.

[1945Kor, 1946Kor, 1958Chu, 1976Vla, 1991Tre, 1997Pal, 2014Pav, 2012Ume, 2019Ran, 2020Ran] reported the compositions of the disordered (Cr, $\alpha\delta$ Fe) solution at different temperatures. For the Cr-rich side of the triangle, [2019Ran, 2020Ran] found that the addition of iron slightly increases Al solubility in the phase at 900°C. Only [2012Ume] used a TEM technique to study the concentration region in which the formation of ordered polymorphs was expected. They analyzed the APD structure of the $\text{Cr}_{25}\text{Fe}_{50}\text{Al}_{25}$ (at.%) sample annealed at 1150°C and subsequently quenched. [2012Ume] found that the sample had a disordered (Cr, $\alpha\delta$ Fe) structure at this temperature. During quenching from 1150°C, FeAl precipitated so that the structure at room temperature was two-phase.

Below 500°C, the (Cr, $\alpha\delta$ Fe) miscibility gap exists in the Cr–Fe system. [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. The authors observed phase separation into two isomorphous solid solutions, which were depleted or enriched in Cr, respectively.

There is a variety of studies on the phase equilibria involving the ordered $B2$ (FeAl), and $D0_3$ (Fe_3Al)/ $L2_1$ (CrFe_2Al) phases. Note that in some papers, [2004Zha, 2012Sah] for example, usage of the term “Heusler phase” is misleading since no $L2_1$ ordering was observed by the authors. The majority of the studies [1968Bul, 1969Bul1, 1969Bul2, 1969Sel, 1994Hyd, 1995Ant, 1995Yos, 1997Nis1, 1997Nis2, 2012Yil, 2019Ran, 2020Ran] is focused on the establishment of the order-disorder transition temperatures though. [1972Kaj, 1974Niz, 1975Lit, 1977Tys, 1995Yos, 1997Nis1, 1997Nis2, 1997Sat, 1998Kim, 1999Wit, 2001Alo, 2007Pad] studied the crystal structure of the samples after slow cooling using different methods (see Table 1). [1981Bus, 1985Okp, 1991Tre, 1997Pal, 1998Sun, 2001Alo, 2008Shr, 2012Lam] produced annealed samples but detailed TEM examinations were not available to the authors.

The studies of annealed samples performed using *in-situ* TEM or TEM APD examination are limited to the works of [1989McK, 1994Mor, 2012Ume]. [2006Gol1, 2006Gol2, 2008Gol, 2009Gol] also examined the APD structures using TEM. Their samples contained from 0.005 to 0.004 at.% C though, and the authors suspected the formation of carbides in their films but did not perform further investigation of this issue. [2012Ume] observed the $B2$ (FeAl) phase at $\text{Cr}_{25}\text{Fe}_{50}\text{Al}_{25}$ (at.%) and 600°C. The $D0_3$ (Fe_3Al) single-phase structure was reported to exist up to 6 at.% Cr at 28 at.% Al and 500°C by [1989McK, 1994Mor], at $\text{Cr}_5\text{Fe}_{69}\text{Al}_{26}$, $\text{Cr}_8\text{Fe}_{67}\text{Al}_{25}$ (at.%) and 477°C by [2006Gol1,

2006Gol2, 2008Gol, 2009Gol]. [1994Mor] performed further *in-situ* TEM observations between 500 and 600°C but did not discuss their finding for the Al–Cr–Fe system in detail.

TEM APD studies performed by [2006Gol1, 2006Gol2, 2008Gol, 2009Gol] and [2012Ume] revealed formation of very fine $D0_3$ (Fe_3Al)/ $L2_1$ (CrFe_2Al) domains in the $\text{Cr}_{25}\text{Fe}_{50}\text{Al}_{25}$ (at.%) thin films annealed at 477°C and 400°C. Even 20 days of annealing by [2012Ume] did not produce coarsened well-developed $L2_1$ (CrFe_2Al) structure. This shows that the stoichiometric $L2_1$ Heusler phase is not stable at either 477 or 400°C. The energy of formation of the stoichiometric CrFe_2Al compound was calculated by [2003Kel, 2016Dah] using full potential linearized augmented plane waves method and by [2021Liu] using the Perdew–Burke–Ernzerhof functional in the generalized gradient approximation. The calculated energies of formation are negative suggesting that the stoichiometric $L2_1$ (CrFe_2Al) Heusler phase is not thermodynamically unstable in the Al–Cr–Fe system. But whether it is metastable or forms at a lower temperature after extremely long annealing is open to debate.

There are several studies on the occupation of Cr on the lattice sites of ordered phases. Using the mean-field approximation, [2002Ban] has found that Cr has a stronger preference for occupying the Fe sublattice in the $B2$ (FeAl) phase. Based on their neutron studies, [1997Sat, 1998Sun] also reported that preferential occupancy of the Fe_1 sites by Cr.

σ phase. [1955Tag] and [1958Chu] studied the phase equilibria involving the σ phase, which originates from the Cr–Fe system. The alloy used by [1955Tag] contained up to 0.09 mass% C and therefore had lower purity than samples used by [1958Chu]. Furthermore, [1958Chu] employed a thorough heat-treatment regime and a larger number of samples. Nevertheless, the $\sigma + (\text{Cr}, \alpha\delta\text{Fe})$ two-phase boundaries established for the Cr–Fe edge in both studies conflict with the binary Cr–Fe phase diagram accepted in the present evaluation. On the other hand, the σ homogeneity region constructed by [1958Chu] is in satisfactory agreement with the binary data. According to [1958Chu], the σ phase dissolves between 1 at.% Al at 750°C and 3 at.% Al at 600°C. To the best of our knowledge, no experimental data on the Al influence on the σ formation temperatures were published in the literature.

Al–Cr-based compounds. [2019Eze] found that the monoclinic CrAl_7 compound dissolves up to 2.5 at.% Fe at solidus temperatures. [2011Kho1, 2011Kho2] reported approximately the same value in their study of the solidus surface. [2019Eze] also measured the lattice parameters of the phase in a three-phase sample annealed at 650°C for 500 h and subsequently quenched.

[1997Pal] performed the very first detailed study of the phase equilibria involving CrAl_4 . It has been reported that this compound dissolves up to 12 at.% Fe. Unfortunately, a TEM technique was not available for [1997Pal] at that time. By using an XRD technique only, the authors could not distinguish between different ternary quasicrystal approximants, which exist in this part of the diagram as confirmed by later TEM, neutron or electron diffraction measurements, see for example [2008Pav2, 2009Pav, 2010Pav, 2010Bau, 2011Bau]. According to [2010Bau, 2011Bau, 2011Kho1, 2014Pav], the Fe solubility in CrAl_4 does not exceed 2 at.%.

The experimental data about $\text{Cr}_2\text{Al}_{11}$ are contradictory. Based on the powder XRD and TEM examinations, [2010Pav, 2014Pav] suggested that the homogeneity range of $\text{Cr}_2\text{Al}_{11}$ extends up to 4 at.% Fe at around 78 at.% Al. Based on neutron diffraction and TEM measurements, [1995Sui, 1997Sui, 2010Bau, 2011Bau, 2013Bau] found that Czochralski-grown single crystals containing 2–6 at.% Fe and around 78 at.% Al present a ternary orthorhombic phase ($\text{o}-(\text{Cr},\text{Fe})\text{Al}_4$) which has a highly modulated structure as was later reported by [2013Bau, 2014Gas]. The argumentation of [2010Pav, 2014Pav] is essentially based on a comparison of the XRD patterns calculated using [1991Ben]’s structural model for monoclinic $\text{Cr}_2\text{Al}_{11}$ and [2004Den]’s structural model for orthorhombic $\text{o}-(\text{Cr},\text{Fe})\text{Al}_4$ with their own experimental powder patterns for Fe-rich compositions. [2010Pav, 2014Pav] stated that the powder XRD calculated using both structural models showed remarkable similarity and were in good agreement with the experimental powder patterns. However, powder diffraction data used by [2010Pav, 2014Pav] are not enough to determine any modulation in the structure and are less reliable in comparison to the single crystal XRD as performed by [1995Sui, 1997Sui, 2004Den, 2010Bau, 2011Bau, 2013Bau]. Finally, the $\text{o}-(\text{Cr},\text{Fe})\text{Al}_4$ structural model reported by [2004Den], as well as by [2013Bau, 2014Gas], present “average” models of the real modulated structure with the model of [2013Bau] giving the best fitting of the experimental data so far. Thus, a comparison of the powder XRD patterns made by [2010Pav, 2014Pav] is questionable.

The majority of the data on the phase equilibria involving $\text{Cr}_2\text{Al}_{11}$, including liquidus and solidus temperatures, were reported by [2010Pav, 2014Pav] and by [2011Kho1, 2011Kho2], who used the results of the former for the interpretation of the experimental results. Liquidus and solidus temperatures of $\text{Cr}_2\text{Al}_{11}$ reported by [2010Pav] and [2019Eze] are questionable as the temperatures for the $\text{L}+\text{CrAl}_4 \rightleftharpoons \text{Cr}_2\text{Al}_{11}$ and $\text{L}+\text{Cr}_2\text{Al}_{11} \rightleftharpoons \text{CrAl}_7$ reactions in the Al–Cr measured in these studies suggest. [2013Khv] discussed various factors affecting this transformation in the binary system earlier. Hence, phase equilibria with $\text{Cr}_2\text{Al}_{11}$ are still open to debate. In the present evaluation, it has

been assumed that the ternary o-(Cr,Fe)Al₄ exists at 3–6 at.% Fe and ~78 at.% Al, and Cr₂Al₁₁ extends up to 3 at.% Fe at *ca.* 80 at.% Al.

No experimental data regarding the phase equilibria involving Cr₄Al₁₁ can be found in the literature.

[1940Kor1, 1946Kor] suggested that isostructural Fe₅Al₈ and βCr₅Al₈ compounds of the cubic γ-brass-type form continuous solid solution (Cr,Fe)₅Al₈. This was later confirmed by [2011Kho1, 2014Pav, 2019Ran, 2020Ran] by considering the SEM and EPMA data. By cooling, (Cr,Fe)₅Al₈ either transforms to room temperature αCr₅Al₈ in Cr-rich samples or decomposes to the mixture of the neighboring phases in Fe-rich samples. [2011Kho1] also measured the lattice parameters of this compound in several multicomponent alloys. The heat treatment of these samples is not described in detail. Therefore, these data are not included in the present evaluation.

The low-temperature αCr₅Al₈ phase has an extended homogeneity range [1997Pal, 2014Pav]. According to [2014Pav], αCr₅Al₈ can dissolve up to 35 at.% Fe. Lattice parameters of the phase in dependence of Fe content were measured by [1997Pal] (Fig. 2). According to [2011Kho1, 2011Kho2, 2014Pav], the addition of Fe also increases the αCr₅Al₈ melting temperatures. It forms *via* a three-phase peritectic reaction at 1185°C according to [2011Kho1].

Based on their XRD and metallographic observations, [1958Chu] suggested that Cr₂Al (MoSi₂-type) might dissolve a significant amount of Fe. This was experimentally confirmed later by [1969Kal, 2015Sus, 2019Ran, 2020Ran]. According to the EPMA/WDX results of [2019Ran, 2020Ran], the Fe solubility in this compound extends to up to 22 at.% at 700°C. [1969Kal, 2015Sus] measured the lattice parameters for a series of the Cr_{2-x}Fe_xAl alloys. The authors did not describe the heat treatment procedure of the samples in detail. Therefore, it is not clear to which temperature the measured values can be attributed. The results of [1969Kal, 2015Sus] are in good agreement though and show that the *a* parameter diminishes, and the *c* parameter slightly increases with increasing Fe content: *a* = 300.4–295.4 pm and *c* = 864–874 pm for 0–13.3 at.% Fe. The effect of iron on the formation temperature of Cr₂Al is not studied. The Cr₂Al compound exhibits antiferromagnetic behavior. As shown by [1969Kal, 2015Sus], the doping with Fe results in rapid suppression of the antiferromagnetic order and a decrease of the Néel temperature. Reported temperatures differ significantly, especially for higher Fe concentrations.

Al-Fe-based compounds. FeAl₂, Fe₂Al₅, and Fe₄Al₁₃ dissolve up to 4.5, 6.2, and 7 at.% Cr according to [1997Pal, 2014Pav, 2019Ran, 2020Ran]. Cr has no effect on the formation temperatures of these compounds.

Ternary phases. Four quasicrystal approximants and a decagonal phase are usually denoted using either Greek or Latin letters, for which no ideal stoichiometries were reported. This type of denomination with certain amendments was accepted in this evaluation.

The icosahedral ε-(Cr,Fe)Al₄ approximant has an orthorhombic structure. [2011Kho1] found that it belongs the *Pbnm* space group, while [2014Pav] proposed the *Immm* space group. Detailed XRD study of the Czochralski-grown single crystal by [2010Bau, 2011Bau] showed that this phase has a *Cmcm* structure. It originates from the Al–Cr system being however metastable in the binary system. Small additions of the third component stabilize this compound, so it becomes a real ternary phase. ε-(Cr,Fe)Al₄ forms *via* a three-phase peritectic reaction at 1055°C according to [2011Kho1]. It is stable in a narrow composition range at around 2–3 at.% Fe and 78–77 at.% Al [2010Bau, 2011Bau, 2011Kho1].

The decagonal approximant o-(Cr,Fe)Al₄ was for the first observed by [1995Sui] and by [1997Sui] (reported as O-AlFeCr), [1998Lia] and later confirmed by [2004Den, 2009Bau, 2010Bau, 2011Bau, 2013Bau, 2014Gas]. As it was already discussed above, o-(Cr,Fe)Al₄ has a highly modulated structure according to [2013Bau, 2014Gas] and is structurally very similar to the binary Cr₂Al₁₁ compound. The o-(Cr,Fe)Al₄ crystal structure is still not fully solved. The structural models reported by [2004Den, 2010Bau, 2011Bau, 2013Bau, 2014Gas] present an “average” model. The model of [2013Bau] was accepted in the present evaluation since it yields the best fitting of the experimental data. The available experimental data on the phase equilibria with o-(Cr,Fe)Al₄ are scarce. As suggesting the data of [2010Bau, 2011Bau, 2014Pav], this compound most probably forms between 1000°C and 1042°C and has small homogeneity range (see Table 2).

The decagonal approximant O₁ was observed in a slowly cooled multiphase sample by [2000Dem] (denoted as C_{3,1}) and later confirmed by [2008Pav2, 2010Pav, 2014Pav] in their studies of equilibrated samples. Its structure is still not solved, and the lattice parameters were reported without specifying the composition of the phase. While [2000Dem] reported orthorhombic primitive cell with *a* = 3270 pm, *b* = 1250 pm, *c* = 2380 pm, [2008Pav2] suggested a *B*-centered orthorhombic cell with *a* ≈ 3270 pm, *b* ≈ 1240 pm, *c* ≈ 2340 pm. Neither [2010Pav] nor [2014Pav] made attempts to further clarify the O₁ crystal structure. The results of [2010Pav, 2011Kho1, 2011Kho2, 2014Pav] suggest that the homogeneity range extends between approximately Cr_{15.0}Fe_{11.0}Al_{74.0} to Cr_{19.7}Fe_{4.3}Al_{76.0} and Cr_{15.0}Fe_{6.9}Al_{78.1} to Cr_{18.3}Fe_{8.9}Al_{72.8} (at.%). According to [2011Kho1], O₁ forms *via* a three-phase peritectic reaction at 1087°C.

[1999Sui, 2000Mo, 2003Zou, 2008Pav3, 2010Bau, 2011Bau] reported on the formation of a ternary hexagonal icosahedral approximant – H phase. Based on their high-resolution electron microscopy measurements, [1999Sui, 2000Mo] concluded that this compound with a $\text{Cr}_{11}\text{Fe}_8\text{Al}_{81}$ (at.%) composition belongs to the $P6_3/m$ space group. [2008Pav3] and later [2010Pav] claimed that this type of structure was not found in their samples containing the H phase. Detailed study of the $\text{Cr}_{12.26}\text{Fe}_{7.45}\text{Al}_{80.29}$ and $\text{Cr}_{13.35}\text{Fe}_{6.63}\text{Al}_{80.02}$ (at.%) single crystals grown by the Czochralski-method using the XRD method by [2010Bau, 2011Bau] revealed that the H compound has a rhombohedral $R\bar{3}$ structure with a large elementary cell containing 1512 atoms. This structure was accepted in the present evaluation. The H homogeneity range extends between approximately $\text{Cr}_{12.0}\text{Fe}_{8.0}\text{Al}_{80.0}$ to $\text{Cr}_{19.7}\text{Fe}_{4.3}\text{Al}_{76.0}$ and $\text{Cr}_{11.0}\text{Fe}_{6.3}\text{Al}_{82.7}$ to $\text{Cr}_{13.5}\text{Fe}_{7.0}\text{Al}_{79.4}$ (at.%) [2019Eze, 2011Kho1]. According to [2011Kho1], this phase forms *via* a four-phase peritectic reaction at 998°C.

A decagonal phase, D, was for the first time reported by [2008Pav2] as a result of their TEM examination. [2009Pav] and later [2020Ma] reported that this phase has periodicity along the 10-fold symmetry axis, and its structure is similar to the D_3 decagonal phase in the Al–Mn–Pd system [1994Ste, 1999Gru]. According to [2009Pav, 2014Pav], D is structurally related to the O_1 compound so that these phases can be reliably resolved using the TEM technique only. The D homogeneity range extends from 70 to 72 at.% Al and from 14 to 18 at.% Cr. It forms *via* a three-phase peritectic reaction at 1096°C according to [2011Kho1].

Metastable phases. In the Cr–Fe system, the metastable miscibility gap of (Cr, $\alpha\delta\text{Fe}$) is observed between 500 and 600°C - in the temperature range of the σ phase existence, if the formation of the latter is suppressed. In spite of numerous investigations, the determined location of the metastable miscibility gap seems still ambiguous even in the binary system, especially for the critical temperature of the miscibility gap. In the ternary system, [1971Yam] studied the influence of Al on the metastable miscibility gap of (Cr, $\alpha\delta\text{Fe}$). The authors studied several Cr-rich samples that were annealed for 5 hours at around 1200°C and subsequently aged at 480°C. According to [1971Yam], the critical temperatures of the miscibility gap slightly increase due to the addition of aluminium. The region itself extends up to 5 at.% Al inside the ternary system.

[1993Sta, 1995Sta, 1995Zia, 2006Kar] observed an icosahedral six-dimensional structure (denoted as *i* in the present evaluation) in the $\text{Cr}_8\text{Fe}_6\text{Al}_{86}$, $\text{Cr}_{3.4}\text{Fe}_8\text{Al}_{88.6}$, $\text{Cr}_3\text{Fe}_3\text{Al}_{94}$, $\text{Cr}_2\text{Fe}_4\text{Al}_{94}$, $\text{Cr}_3\text{Fe}_1\text{Al}_{94}$ (at.%) alloys. Earlier a metastable icosahedral ternary phase was also reported by [1987Wou, 1988Man, 1989Man, 1988Sch, 1989Law1, 1989Law2, 1989Man]. According to [1993Sta, 1995Sta], the value of the six-dimensional hypercubic lattice constant is $a_{6D} = 654$ pm. [1995Zia] performed the EDX measurements using a scanning transmission electron microscopy and suggested the composition of the phase to be $\text{Cr}_{12\pm1}\text{Fe}_{12\pm1}\text{Al}_{75\pm0.5}$ (at.%). The *i* phase is metastable and emerges during the rapid solidification of the samples. The as-prepared structure usually consists of the icosahedral phase distributed in the (Al) matrix. Upon heating, the *i* phase decomposes into a mixture of stable and metastable phases depending on the heat treatment conditions [1993Sta, 1995Sta, 1995Zia, 2006Kar]. Equilibrium $\text{Fe}_3\text{Al}_{14}$, CrAl_7 , and metastable FeAl_6 phase are often reported among the products of the icosahedral phase decomposition. [1995Zia] also detected an unknown metastable phase with an orthorhombic structure. The authors argued that this structure could be an allotrope of $\text{Fe}_3\text{Al}_{14}$. The crystal structure however remained unsolved.

[1999Sui, 2000Dem, 2001Dem, 2006Dem] reported several other structures to exist in multiphase samples: hexagonal κ -(Al–Cr–Fe) [1999Sui], orthorhombic decagonal O_1 -AlCrFe approximant [2000Dem, 2001Dem], and two decagonal approximants denoted as O_A -(Al–Cr–Fe) and O_B -(Al–Cr–Fe) by [2006Dem]. The orthorhombic O_1 -AlCrFe approximant was also observed in thin films produced by a flash evaporation technique by [2004Dem]. [2004Dem] also reported cubic β -AlCrFe phase, orthorhombic decagonal O_F -AlCrFe and O_E -AlCrFe approximants, and monoclinic X-AlCrFe phase. None of these structures were observed in the subsequent studies on the phase equilibria published since 2008. [2000Dem, 2001Dem, 2006Dem] provided neither compositions nor stoichiometries of the observed phases. The compositions measured by the EDS technique [2004Dem] are doubtful, as suggested by the values measured for the $\text{Fe}_4\text{Al}_{13}$ compound. Hence, the structures reported by [2000Dem, 2001Dem, 2004Dem, 2006Dem] were not included in Table 2.

Invariant Equilibria

The data on the invariant equilibria were reported by [1932Tai1, 1932Tai2, 1943Mon, 1960Zol2, 1973Wil, 1976Mon, 1987Sau, 1995Zia, 1995Sta] (discussed in the previous evaluation by [2007Gho]) and recently by [2011Kho2, 2019Eze]. The reaction scheme shown in Fig. 3 is based on that drawn by [2011Kho2], which is the most detailed one. But further modifications were introduced to preserve consistency with the Al–Fe and Al–Cr phase diagrams accepted in the present evaluation and to take the recent results of [2010Bau, 2011Bau, 2013Bau, 2014Gas] on o-(Cr,Fe)Al₄ and [2019Eze] for liquidus and solidus projections into account. In particular, reactions with

o-(Cr,Fe)Al_4 were introduced in the reaction scheme. They are shown with dashed lines because of the contradictions in the data reported for this compound and closely related $\text{Cr}_2\text{Al}_{11}$ (see the discussion in the ‘Solid Phases’ section). [2010Bau, 2011Bau] observed o-(Cr,Fe)Al_4 instead of $\text{Cr}_2\text{Al}_{11}$ being in equilibrium with the liquid phase at around 1000°C . Based on the experimental data of [2010Bau, 2010Pav, 2011Bau, 2011Kho1, 2011Kho2, 2014Pav], it has been therefore assumed in the present evaluation that o-(Cr,Fe)Al_4 forms at around 1026°C . The peritectic $\text{L} + \varepsilon\text{-(Cr,Fe)Al}_4 + \text{O}_1 \rightleftharpoons \text{Cr}_2\text{Al}_{11}$ reaction as reported by [2011Kho2] was replaced by $\text{L} + \varepsilon\text{-(Cr,Fe)Al}_4 + \text{O}_1 \rightleftharpoons \text{o-(Cr,Fe)Al}_4$ (denoted as P_1 in Fig. 3). In the subsequent U_5 and U_6 reactions, the participation of o-(Cr,Fe)Al_4 instead of $\text{Cr}_2\text{Al}_{11}$ was assumed.

Despite the scatter in the reported liquidus and solidus temperatures measured by [2010Pav, 2011Kho1, 2011Kho2, 2014Pav], the reported values reveal that Fe increases the $\text{Cr}_2\text{Al}_{11}$ melting temperature. Therefore, it has been suggested in the present evaluation that $\text{Cr}_2\text{Al}_{11}$ forms between 913 and 985°C in the ternary system *via* the P_3 peritectic reaction. The additional U_7 reaction at $900 < T < 980^\circ\text{C}$ was introduced in the reaction scheme to preserve agreement with the data reported by [2011Kho1, 2011Kho2, 2014Pav, 2019Eze] for lower temperature.

The $\text{L} + \text{H} \rightleftharpoons \text{CrAl}_7 + (\text{Al})$ and $\text{L} + \text{H} \rightleftharpoons \text{Fe}_4\text{Al}_{13} + (\text{Al})$ reactions reported by [2011Kho1, 2011Kho2] for 660 and 657°C were replaced by $\text{L} + \text{H} \rightleftharpoons \text{CrAl}_7 + \text{Fe}_4\text{Al}_{13}$ (U_9) and $\text{L} + \text{CrAl}_7 \rightleftharpoons \text{Fe}_4\text{Al}_{13} + (\text{Al})$ (U_{10}) found by [2019Eze]. [2019Eze] used longer annealing at sub-solidus temperatures for their samples than [2011Kho1, 2011Kho2], which allowed achieving a greater equilibrium state in the samples at low temperatures. The temperatures of U_9 and U_{10} , as well as of the U_8 reaction, are accepted after [2011Kho2]. The values determined by [2019Eze] for U_8 and U_9 are most probably too high due to the overheating effect as the temperature measured for the $\text{L} + \text{Cr}_2\text{Al}_{11} \rightleftharpoons \text{CrAl}_7$ reaction in the Al–Cr system suggests. The compositions of solid phases participating in the P_2 and U_8 reactions are also accepted according to [2011Kho1], as these values are in better agreement with the data reported by [2010Bau, 2011Bau, 1997Pal, 2014Pav] than those measured by [2019Eze].

The resulting reaction scheme is shown in Fig. 3, and the coordinates of the invariant reactions are given in Table 3.

Liquidus and Solidus Surfaces

[2007Gho] evaluated the experimental data [1932Tai1, 1932Tai2, 1935Gru, 1945Kor, 1951Pra, 1954Chi, 1960Zol1, 1960Zol2, 1970Koz1, 1970Koz2, 1987Sau, 1991Tre] and calculation results [1970Koz1, 1970Koz2, 1974Vya, 1987Sau] published for the Al–Cr–Fe liquidus and solidus surfaces until 2007. At that time, the corresponding information was limited to the partial liquidus surface in the Al corner and tentative isotherms of liquid phase drawn in the composition range between 0–60 at.% Al. The studies of [2011Kho1, 2011Kho2, 2019Eze] significantly contributed to the establishment of liquidus and solidus surface projections at 50–100 at.% Al. For lower Al content, new experimental data are limited to the works of [2019Ran, 2020Ran], who measured liquidus and solidus temperatures for four alloys containing 5–35 at.% Fe at 52.5 at.% Al and three alloys containing 13–28 at.% Fe at 66 at.% Al. [2020Ran] thermodynamically assessed the Al–Cr–Fe system and calculated a liquidus surface projection in the whole composition range. Not all invariant reactions reported by [2011Kho1, 2011Kho2, 2019Eze] could be reproduced in the calculations by [2020Ran], which is probably due to the fact that homogeneity ranges of ternary compounds were not modeled, and O_1 reported by [2004Den, 2008Pav2] and o-(Cr,Fe)Al_4 found by [2010Bau, 2011Bau, 2013Bau, 2014Gas] were considered as the same ternary phase. This assessment is still of high importance as it presents a good attempt to model quite complex phase equilibria in the whole composition range.

The liquidus surface projection in the whole composition range is shown in Fig. 4a. It is a combination of the liquidus surface projection reported by [2011Kho2] for 55–100 at.% with amendments described in the ‘Invariant Equilibria’ section and liquidus surface projection calculated by [2020Ran] for 0–50 at.% Al with modifications described below.

No invariant reactions were reported in the composition range between 0 and 50 at.% Al. The isotherms of the liquid phase calculated by [2020Ran] were adjusted to preserve consistency with the Al–Cr and Cr–Fe phase diagrams. In the Cr-rich part, the deviation between the liquidus lines of the Al–Cr and Cr–Fe phase diagrams accepted in the present evaluation and those used by [2020Ran] is significant. Therefore, the isotherms at 1550 – 1800°C were drawn based on the data for the binary phase diagrams and ternary system reported by [1945Kor, 1991Tre]. The relevant experimental information is scarce and uncertain. Hence, the isotherms are shown with dashed lines. The isotherms at 1350 – 1500°C calculated by [2020Ran] were slightly adjusted.

The type and coordinates of the invariant reaction between liquid, (Cr, $\alpha\delta\text{Fe}$), ordered FeAl , and $(\text{Cr,Fe})_5\text{Al}_8$ were neither established experimentally nor calculated by [2020Ran]. The extension of the corresponding monovariant lines into the ternary system is schematical. The reactions and monovariant lines involving o-(Cr,Fe)Al_4 and $\text{Cr}_2\text{Al}_{11}$ are also tentative since the relevant experimental data are contradictory (Fig. 4b).

Figure 5 shows solidus surface projection in the range of compositions 60–100 at.% Al. It is based on the solidus presented by [2011Kho1] with further amendments required to preserve the consistency with the binary Al–Cr and Al–Fe diagram, as well with the reaction scheme and liquidus surface constructed in the present evaluation. The tie-lines corresponding to the maxima in the monovariant lines were added to the solidus surface projection in the present evaluation. The position of the tie-lines is tentative and drawn with dashed lines based on the experimental data [1997Pal, 2011Kho1, 2011Kho2, 2014Pav]. The solubility of iron in $\text{Fe}_4\text{Al}_{13}$ below 998°C (the P_2 reaction) was adjusted, taking the data reported for the isothermal sections by [1997Pal, 2014Pav] into account.

Isothermal Sections

Partial isothermal sections were constructed by [1945Kor, 1946Kor] at 1150°C, by [1958Chu] at 600–900°C, by [1997Pal] and [2008Pav2] at 1000°C, by [2009Pav] at 1075°C, by [2014Pav] at 700–1160°C, by [2015Zho] at 700°C, and by [2019Ran] at 700, 900°C. [2017Wan] calculated phase equilibria at 50–100 at.% Al and 700–1160°C. Full isothermal sections were calculated by [2019Cha] at 320–925°C and [2020Ran] 700–1160°C. The calculated sections present a simplification of the phase equilibria in the ternary system, since the homogeneity ranges of ternary phases and CrAl_2 were not modeled. None of the assessments includes $\text{o}-(\text{Cr,Fe})\text{Al}_4$ found by [2010Bau, 2011Bau, 2013Bau, 2014Gas]. The sections by [2020Ran] were however used in the present evaluation to construct the phase equilibria in the Cr- and Fe-rich part of the system in view of the lack of reliable experimental data for this composition region. The order-disorder transition as modeled by [2020Ran] is not included in the sections because of the controversial nature of the data used for the modeling (see ‘Solid Phases’ section). The extension of the corresponding phase boundary into the ternary system is tentative in all the sections.

Figure 6 shows an isothermal section at 1160°C. [2014Pav] reported only six tie-lines for this section. The corresponding segments of the $(\text{Cr, Fe})_5\text{Al}_8$ homogeneity range and the $(\text{Cr, Fe})_5\text{Al}_8 + \text{FeAl}$ phase boundary are shown with solid lines. The rest of the phase boundaries are tentative. The $\alpha\text{Cr}_5\text{Al}_8$ homogeneity range, $\text{L} + \alpha\text{Cr}_5\text{Al}_8 + (\text{Cr, } \alpha\delta\text{Fe})$ tie-triangles, and phase boundary involving the liquid phase are constructed based on the liquidus and solidus data by [2011Kho1, 2011Kho2]. The (γFe) homogeneity range is according to [2020Ran]. This section shows a continuous solid solution existing between βCrAl_3 and Fe_5Al_8 . Figure 7 shows the isothermal section at 1100°C. The phase equilibria, which were experimentally confirmed by [2014Pav], are shown with solid lines. The phase equilibria involving the liquid phase were slightly amended in accordance with the liquidus and solidus data by [2011Kho1, 2011Kho2]. The phase boundaries involving $(\text{Cr, } \alpha\delta\text{Fe})$ and (γFe) are reproduced according to the modeling of [2020Ran]. All phase boundaries were adjusted to preserve compatibility with the Al–Cr and Al–Fe diagrams.

The isothermal section at 1075°C in Fig. 8 is based on the data reported by [2014Pav] with the $(\text{Cr, } \alpha\delta\text{Fe})$ and (γFe) phase boundaries accepted after [2020Ran]. Small adjustments to preserve compatibility with the Al–Cr and Al–Fe diagrams were introduced. The main change introduced in this section concerns the O_1 phase. Contrary to [2011Kho1, 2011Kho2], [2009Pav, 2014Pav] stated that O_1 does not exist at 1075°C but forms at 1048°C according to the DTA measurements performed by [2014Pav]. First and foremost, the proposed temperature of the O_1 formation is only 6°C higher than the isothermal section at 1042°C (Fig. 9) also constructed by [2014Pav]. In this section, O_1 already has a large homogeneity range suggesting that the ternary phase forms at temperatures higher than 1048°C. Since [2011Kho1, 2011Kho2] and [2014Pav] used comparable annealing times at approximately the same temperatures, the data of [2011Kho1, 2011Kho2] were preferred to those of [2009Pav, 2014Pav]. The O_1 homogeneity range and the corresponding phase equilibria were added in the section. Figure 8 also shows the U_2 plane as reported by [2011Kho1, 2011Kho2]. Figure 9 shows phase equilibria at 1042°C. The partial isothermal section reported by [2014Pav] was complemented by the $(\text{Cr, } \alpha\delta\text{Fe})$ and (γFe) phase boundaries reported by [2020Ran]. At this temperature, $\varepsilon-(\text{Cr,Fe})\text{Al}_4$ is already stable in the ternary system.

The isothermal section at 1000°C (Figs. 10a and 10b) is based on the data of [1997Pal, 2011Kho1, 2011Kho2, 2014Pav, 2020Ran]. The phase equilibria confirmed experimentally are shown with solid lines. The $\text{o}-(\text{Cr,Fe})\text{Al}_4$ homogeneity range and relevant phase equilibria are constructed taking the data of [2010Bau, 2011Bau, 2013Bau, 2014Gas] into account. The phase transformations involving $\text{o}-(\text{Cr,Fe})\text{Al}_4$, $\varepsilon-(\text{Cr,Fe})\text{Al}_4$, and CrAl_4 (Fig. 10b) are tentative and require further experimental confirmation.

The isothermal sections at 900°C (Figs. 11a and 11b) and 700°C (Figs. 12a and 12b) constructed by [2019Ran] were adopted in the present evaluation. They were further modified to take the homogeneity ranges of D , O_1 , $\text{o}-(\text{Cr,Fe})\text{Al}_4$, $\varepsilon-(\text{Cr,Fe})\text{Al}_4$ and H into account. This was done using the data of [2011Kho1, 2011Kho2, 2014Pav, 2019Eze]. The tie-line and tie-triangles measured by [2015Zho] in the Al-corner at 700°C were ignored in the present evaluation. They contradict other experimental datasets in the ternary system and the Al–Fe and Al–Cr phase diagrams. The phase boundary involving Cr_2Al at 900°C was added in the present evaluation to preserve agreement with the accepted

binary phase diagram. The (γ Fe) and σ phase boundaries are according to [2020Ran]. The σ homogeneity range at 700°C is in good agreement with the experimental data of [1958Chu], while the (Cr, $\alpha\delta$ Fe)+ σ region is much wider than that constructed by [1958Chu].

650°C is the lowest temperature at which the isothermal section was constructed in the present work. The experimental data at this temperature are limited to the data of [2019Eze] in the Al-rich corner and [1958Chu] for the σ phase. The isothermal section at 650°C shown in Fig. 13 is very similar to that at 700°C. The main difference is the $\text{CrAl}_7+(\text{Al})+\text{Fe}_4\text{Al}_{13}$ and $\text{CrAl}_7+\text{H}+\text{Fe}_4\text{Al}_{13}$ tie-triangles that replace $\text{L}+\text{H}+\text{Fe}_4\text{Al}_{13}$ and $\text{L}+\text{H}+\text{CrAl}_7$ as a result of the U_{10} reaction according to [2019Eze]. The σ homogeneity range is reproduced according to [1958Chu]. The (Cr, $\alpha\delta$ Fe)+ σ boundary is drawn in the present evaluation and is tentative.

The partial isothermal sections at 1150°C by [1945Kor, 1946Kor], at 600, 750°C by [1958Chu], and at 800°C by [2014Pav] do not provide any new information on the phase equilibria. The available experimental data are too scarce to construct full sections, and no calculations were performed at these temperatures. Hence, these sections are not reproduced in the present evaluation.

Temperature – Composition Sections

Attempts to construct the vertical sections were made by [1969Bul1, 1946Kor, 1991Tre, 2019Ran, 2020Ran]. [1946Kor] gave four isopleths at constant mass ratios of Cr/Fe. These diagrams contradict the isothermal sections shown in Figs. 6 to 13. Partial isopleths at 25 at.% Al and 75 at.% Fe constructed by [1969Bul1] include the order-disorder transformations only. As discussed in the ‘Solid Phases’ section, the relevant experimental data are contradictory, and the formation of the stoichiometric Heusler phase reported by [1969Bul1] is doubtful. [2019Ran, 2020Ran] constructed a partial isopleth at 52.5 at.% Al. This isopleth contradicts both the Al–Cr and Al–Fe phase diagrams. The available information is not enough to correct it. Therefore, the vertical sections reported by [1969Bul1, 1946Kor, 1991Tre, 2019Ran, 2020Ran] are not reproduced here.

Figure 14 shows the temperature-composition section Cr–FeAl of the phase diagram according to [1991Tre] with slight corrections according to the accepted boundary binary Al–Fe system constitution. The order-disorder transformation reported by [1991Tre] was not included in the diagram.

Thermodynamics

The experimental studies on the thermodynamic properties of the Al–Cr–Fe phases were performed by [1961Gul, 1977Ost, 1992Hil, 1997Rud, 2008Jac, 2013Mar]. [1977Ost] studied the heats of dissolution of aluminium in a melt of $\text{Cr}_{30}\text{Fe}_{70}$ (at.%) at temperatures between 1550 and 1600°C. The experimental results, which have been available in the literature at that time, are in good agreement with calculations based on the application of the subregular model. The heat capacities of the Fe_3Al -based alloy with a Cr content of 5 at.% have been measured in the temperature range from 20 to 700°C by [1997Rud] (also cited in the review of [2004Sim]).

[1961Gul, 1992Hil, 2008Jac, 2013Mar] measured activities of Al, Cr, Fe in the (Cr, $\alpha\delta$ Fe) phase using different methods. [2008Jac] analyzed the experimental data reported by other research groups and came to the conclusion that the results of [1961Gul] are not consistent with those of [1992Hil, 2008Jac]. [1992Hil] studied the vaporization of the $\text{Cr}_{19.8}\text{Fe}_{75.4}\text{Al}_{4.8}$ (mass%) ($\text{Cr}_{19.96}\text{Fe}_{70.72}\text{Al}_{9.32}$ in at.%) alloy using Knudsen effusion mass spectrometry (KEMS) in the temperature range 1040–1283°C. This composition virtually agrees with those of the commercial Aluchrom and MA956 alloys. [2008Jac] studied two samples – $\text{Cr}_{15.1}\text{Fe}_{45.1}\text{Al}_{39.8}$ and $\text{Cr}_{30.2}\text{Fe}_{49.9}\text{Al}_{19.9}$ (at.%) – in the temperature range between 877 and 1277°C using KEMS. [2013Mar] investigated the vaporization of seven ternary alloys in the temperature range 961–1335°C by KEMS. This later study reveals the deviation from Raoult’s law is slightly positive for a_{Cr} , negative for a_{Fe} , and sign-changing for a_{Al} . The obtained thermodynamic data are summarized in Table 4.

Thermodynamic properties of ordered phases were calculated by [1988Hoc, 2003Kel, 2016Dah, 2019Wan, 2021Liu]. 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. The energy of formation of the ordered CrFe_2Al ($L2_1$) compound was calculated by [2003Kel, 2016Dah, 2021Liu]. The calculated energies of formation are negative suggesting that the stoichiometric $L2_1$ Heusler phase can form in the Al–Cr–Fe system. By combining first-principle and cluster variation method calculations, [2019Wan] calculated energies of formation of the phases with different ordering types and isothermal sections between 327 and 2727°C. The authors predicted the formation of a $B32$ ternary ordered phase in the system. The modeling of [2003Kel, 2016Dah, 2019Wan, 2021Liu] does not include other phases which are stable in the ternary system. Hence, they did not give an answer whether the $L2_1$ and $B32$ phases are equilibrium or metastable in

the Al–Cr–Fe system. For the same reason, the isothermal sections of [2019Wan], which include only (Cr, $\alpha\delta$ Fe), and its ordered polymorphs do not reflect the real phase equilibria in the system.

[1975Kau, 1970Koz2, 1987Sau] performed the very first thermodynamic modeling of the phase equilibria in the system. [2000Sub, 2017Wan, 2019Cha, 2020Ran] performed thermodynamic assessments of the Al–Cr–Fe system in the frameworks of the standard CALPHAD method. [2020Ran] presented the most comprehensive assessment of the system by calculating the isothermal sections between 700 and 1160°C, as well as the liquidus surface. However, these works present a simplification of the phase equilibria in the ternary system, since the homogeneity ranges of many phases, in particular ternary ones, were not modeled.

Notes on Materials Properties and Applications

Al–Cr–Fe alloys are of interest as lightweight alloys for structural applications, in particular, for the production of protective coatings formed by alumina scales from alloys of compositions that lie in the Al-rich corner of the system. Al–Cr–Fe quasicrystal approximants are also potential candidates for new applications because of their specific properties. Alternatively, the addition of chromium to Fe₃Al- and FeAl-based alloys produces excellent candidates for moderate and high-temperature applications. The Al–Cr–Fe alloys serve as a basis of high-chromium-containing single-phase ferritic alloys surfaces that are commonly used in high-temperature radiant heating applications. Data on some investigations regarding materials properties are listed in Table 4.

[2005Pal] showed that strengthening of Al–Fe-based alloys at high temperatures could be achieved through solid-solution hardening, precipitation of incoherent or coherent particles and by ordering. However, in the Al–Cr–Fe ternary system, within a large composition region (up to 50 at.% Al) strengthening of the alloys can be achieved only through solid solution hardening. At higher Al contents, the possibility of precipitating a second phase, *e.g.* (Cr,Fe)₅Al₈ phase, exists.

Mechanical properties of Fe₃Al-based alloys were investigated by [1991Sik1, 1993Kni, 1998Sun, 2004Hua]. According to [1991Sik1], room-temperature tensile ductility of the samples with 2 to 5 mass% Cr (1.3 and 3.3 at.%, respectively), prepared using the melting process described in [1991Sik2], 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 Fe₃Al. [1998Sun] established that chromium significantly affected the room temperature tensile properties in a vacuum. In comparison with binary Fe₃Al, in the Cr_{5.38}Fe_{70.42}Al_{24.20} (at.%) alloy (arc melted, then forged at 1000°C, rolled into plates with thickness of 1.0–1.2 mm within the temperature range between 950 and 600°C; the plates were then annealed at 750°C for 1 h, followed by ordering treatment at 500°C for 13 d) a decrease in yield strength from 841 to 695 MPa, increase in elongation from 5.18 to 9.1% and ultimate tensile strength from 990 to 1084 MPa take place. Two large ingots weighing 269 or 104 kg, with the approximate composition of 5.5Cr–78.6Fe–15.9Al (at.%) and the presence (according to the conventional chemical analysis) of small amounts of C, Si, Mn, P and S, were prepared by [2004Hua] using vacuum induction melting and top cast. They had a satisfying surface appearance, and no crack was detected. Conventional thermomechanical processes were used to produce bars, sheets and seamless tubes. By controlling the thermomechanical treatment, a room temperature ductility with a value of more than 10% was achieved. The creep lifetime at 600°C and 200 MPa was more than 2000 h after annealing.

A high-temperature alloy Cr₅Fe_{82.5}Al_{12.5} (mass% or Cr_{4.7}Fe_{72.55}Al_{22.75} in at.%) has been developed for applications in the range from room temperature to 300°C. The billets of the alloy were obtained by [2013Nei] in two ways: using gas-atomized and water-atomized powders. Structural analysis shows that particles of the second phase in the water-atomized powders are finer and their number in the aluminum matrix is greater than that in the gas-atomized powders. The rods extruded from the water-atomized powders have much higher hardness, ultimate strength, and yield stress than those from the gas-atomized powders, plasticity being acceptable at all temperatures (20, 190, and 300°C). An additional powder metallurgy operation – pulsed hot pressing – does not increase the strength of billets from either the water-atomized or gas-atomized powders. The alloy based on the water-atomized 0–63 μ m powder shows the maximum strength: 483, 332, and 261 MPa at 20, 190, and 300°C, respectively.

Electrical resistance anomaly in Fe₃Al-based alloys, in particular with chromium, is analyzed in the review of [1998Nis]. It was noted that the electrical resistivity shows an anomalous temperature dependence: an appearance of a resistance maximum near the Curie point and a negative resistivity slope at higher temperatures.

It was noted by [2011Kim] that the alloy Cr₂₂Fe_{72.2}Al_{5.8} (mass%) or Cr_{21.9}Fe_{66.95}Al_{11.15} (at.%) has been drawing industrial attention for its outstanding high-thermal and oxidation resistance as well as for its applicability as a filter and support material.

The main modes of isothermal oxidation of Al–Cr–Fe, Al–Cr–Ni, and Al–Cr–Co alloys in oxygen at 1000 and 1200°C are summarized in [1971Sto]. It was noted that where protective $\alpha\text{Al}_2\text{O}_3$ scales always predominate, their ease of formation was in the order Al–Cr–Fe > Al–Cr–Ni > Al–Cr–Co, however, where catastrophic breakaway is possible, Al–Cr–Fe produces the most locally catastrophic breakaway. [2002Dem] concluded that resistance to oxidation in water as well as at high temperatures is significantly enhanced thanks to the addition of Cr. Electron energy loss spectroscopy measurements of the very thin Al–Cr–Fe films (10–30 nm) obtained by the flash evaporation technique show that all of them are not oxidized except for the presence of a native oxide layer that forms in an ambient atmosphere with a thickness that cannot exceed 0.3 nm [2004Dem]. It was concluded by [2005Zha] that the addition of chromium is obviously beneficial for the oxidation resistance of $\text{Fe}_{90}\text{Al}_{10}$ (at.%) by inhibiting the formation of fast-growing Fe-containing oxides and promoting the development of an exclusive alumina layer, however, the effect of chromium is different from the classical third-element effect.

The catalytic activity of the Al–Cr–Fe alloys was studied by [2008For]. As a whole, catalytic devices play a very important role in drastic reduction of the noxious contaminants released by combustion engines. Common devices consist of functionalized ceramic monoliths; an interesting alternative can be realized with a support material made of a high-temperature compatible metal alloy, like Al–Cr–Fe. In [2008For], the $\text{Cr}_{25}\text{Fe}_{70}\text{Al}_5$ (at.%) fibers used to make a device similar to the ceramic monolith were thermally treated to obtain alumina whiskers, which were homogeneously covered with alumina or ceria-zirconia-alumina washcoats. Pt or Pt and Pd have been loaded over the functionalized fibers obtaining an innovative oxidation catalyst. The good catalytic activity after severe aging treatments confirms the possibility of use of these innovative functionalized metallic stacks in air pollution control applications [2008For]. The Al–Cr–Fe alloys are proposed for use as a support for monolithic catalysts $\text{Cu}_x\text{Co}_{1-x}/\text{Al}_2\text{O}_3/\text{CrFeAl}$ for toluene catalytic combustion [2010Zha].

A review of the mechanical properties and application of the Al–Fe-based, particularly Al–Cr–Fe, alloys is presented by [2005Pal].

Miscellaneous

[1970Koz3] reported the solubility of C in liquid Al–Cr–Fe alloys at different temperatures. The formation and growth characteristics of iron-based aluminide diffusion layers at the Al–Fe interface have been analyzed by [1998Akd] in terms of interfacial interaction potentials based on the statistico-thermodynamical theory of multicomponent alloys combined with electronic theory in the pseudopotential approximation. The pairwise interatomic interaction potentials and partial ordering energies have been calculated to predict the effect of various alloying additions, in particular, of chromium, on the activity coefficient of Al atoms and considered up to 1 at.%. The calculation results show that chromium decreases the activity coefficient of Al atoms in (αFe). So as to reduce the thickness of the Al–Fe intermetallic diffusion layer. The influence of aluminium on the kinetics of the σ phase formation in alloys at the equiatomic Cr/Fe ratio with fine- and coarse-grained structures was studied by [2000Bla] using ^{57}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 the fine-grained samples. On the other hand, doping with 1 at.% Al resulted in significant retardation of the σ phase formation both in the fine-grained samples as well as in the coarse-grained samples.

[1989Aku] measured interdiffusion coefficients at 31 points in the ($\alpha\delta\text{Fe}$) phase at 900°C. The results indicate that $\bar{D}_{\text{CrCr}}^{\text{Fe}}$ falls quickly with increasing chromium concentration, with aluminium concentration more than 20 at.%, but is not a strong function of aluminium content. Conversely, $\bar{D}_{\text{AlAl}}^{\text{Fe}}$ is not a strong function of aluminium concentration but decreases with increasing chromium content.

According to [2010Air], *ab initio* calculations combined with experiments on the $\text{Cr}_{10}\text{Fe}_{80}\text{Al}_{10}$ (at.%) alloy show that the beneficial effect of Cr on the oxidation resistance is significantly related to bulk effects. The comparison of experimental and calculated results indicated a clear correlation between the Cr–Fe chemical potential difference and the formation of the protective oxide scales.

[2015Sus] have performed an experimental and theoretical study comparing the effects of Fe-doping of Cr_2Al , an antiferromagnet with a Neel temperature of 670 K, with known results on Fe-doping of antiferromagnetic *bcc* Cr. $(\text{Cr}_{1-x}\text{Fe}_x)_2\text{Al}$ materials are found to exhibit a rapid suppression of antiferromagnetic order with the presence of Fe, decreasing T_N to ≈ 170 K for $x = 0.10$. Antiferromagnetic behavior disappears entirely at $x = 0.125$, after which point increasing paramagnetic behavior is exhibited. This is unlike the effects of Fe doping of *bcc* antiferromagnetic Cr, in which T_N gradually decreases, followed by the appearance of a ferromagnetic state. Theoretical calculations explain that the Cr_2Al –Fe suppression of magnetic order originates from two causes: the first is band narrowing caused by doping of additional electrons from Fe substitution that weakens itinerant magnetism; the second is magnetic frustration of the Cr itinerant moments in Fe-substituted Cr_2Al . In pure-phase Cr_2Al , the Cr moments have an

antiparallel alignment; however, these are destroyed through Fe substitution and the preference of Fe for parallel alignment with Cr. This is unlike bulk Fe-doped Cr alloys in which the Fe anti-aligns with the Cr atoms, and speaks to the importance of the Al atoms in the magnetic structure of Cr_2Al and Fe-doped Cr_2Al .

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Table 1: Investigations of the Al–Cr–Fe Phase Relations, Structures and Thermodynamics

Reference	Method/Experimental Technique	Temperature/Composition/Phase Range Studied
[1932Tai1]	Thermal analysis	94-100 at.% Al, liquidus surface
[1932Tai2]	Thermal analysis	94-100 at.% Al, liquidus surface
[1935Gru]	Thermal analysis	$\text{Cr}_{29.97}\text{Fe}_{59.86}\text{Al}_{10.17}$ (at.%)
[1940Kor1]	Thermal analysis	Whole range of compositions, liquidus surface
[1940Kor2]	Thermal analysis	Whole range of compositions, liquidus surface
[1945Kor]	Thermal analysis	Whole range of compositions, liquidus surface, isothermal section at 1150°C
[1946Kor]	Optical microscopy, thermal analysis	800-1300°C, whole range of compositions, liquidus surface, isothermal section at 1150°C
[1951Pra]	Optical microscopy, X-ray diffraction (XRD), thermal analysis, chemical analysis	425°C, 600°C, the Al-rich corner
[1954Chi]	Thermal analysis, optical microscopy	0-50 at.% Al
[1955Tag]	XRD, optical microscopy, thermal analysis	500-1000°C; 20-35 at.% Cr, 0-4 at.% Al

Reference	Method/Experimental Technique	Temperature/Composition/Phase Range Studied
[1958Chu]	XRD, optical microscopy, thermal analysis	600-1000°C, whole range of compositions
[1958Tag]	XRD, optical microscopy, thermal analysis	500-1000°C; 20-35 at.% Cr, 0-4 at.% Al
[1960Zol1], [1960Zol2]	XRD, optical microscopy, thermal analysis	Al-rich corner
[1961Fel]	XRD, electron diffraction	Cr _{24.8} Fe _{75.02} Al _{0.18} (mass%) or Cr _{26.1} Fe _{73.54} Al _{0.36} (at.%)
[1968Bul], [1969Bul1], [1969Bul2]	XRD, dilatometry	≤ 1000°C; 0-25 at.% Cr, 50-100 at.% Fe
[1969Kal]	Neutron diffraction	700-1000°C, Cr _{2-x} Fe _x Al (x = 0 to 0.25)
[1969Sel]	High-temperature XRD	≤ 1000°C; 0-25 at.% Cr, 50-100 at.% Fe
[1970Koz1], [1970Koz2], [1970Koz3]	Optical microscopy, thermal analysis, XRD	0-70 mass% Fe, 0-40 mass% Al
[1971Sto]	Optical microscopy, XRD, scanning electron microscopy (SEM)	Cr _{12.9} Fe _{85.8} Al _{1.3} , Cr _{26.1} Fe ₇₃ Al _{0.9} , Cr _{11.5} Fe _{82.8} Al _{5.7} , Cr _{27.8} Fe _{67.3} Al _{4.9} (mass%)
[1971Yam]	Differential thermal analysis (DTA), Mössbauer absorption spectroscopy (Fe ⁵⁷ , Co ⁵⁷), optical microscopy	36-39 at.% Cr, 64-56 at.% Fe, 0-5 at.% Al
[1972Kaj]	XRD, neutron diffraction	25 at.% Al
[1974Niz]	XRD, neutron diffraction	25 at.% Al
[1975Lit]	XRD, neutron diffraction	25 at.% Al
[1976Vla]	XRD, optical microscopy	490°C, Cr _{0.6} Fe _{3.5} Al _{95.9} , Cr _{0.3} Fe _{3.5} Al _{96.2} , Cr _{0.8} Fe _{3.5} Al _{95.7} (at.%)
[1977Ost]	Solution calorimetry	1550-1600°C; aluminium solutions in Fe ₇₀ Cr ₃₀ (at.%) melt
[1977Tys]	XRD, neutron diffraction	25 at.% Al
[1981Bus]	XRD	800°C, Cr ₂₅ Fe ₅₀ Al ₂₅ (at.%)
[1982Nao]	XRD, optical microscopy, transmission electron microscopy (TEM)	10-50 at.% Cr, 5-40 at.% Al
[1983Bus]	XRD	800°C, Cr ₂₅ Fe ₅₀ Al ₂₅ (at.%)
[1985Okp]	XRD, neutron diffraction, optical microscopy, electron microscopy	830°C, Cr _{0.5} FeAl _{0.5} , Cr _{0.4} FeAl _{0.6}
[1986Sme]	Optical microscopy, SEM, EDXD	1050°C, Cr _{25.24} Fe _{71.37} Al _{3.39} (mass%)
[1987Wou]	Angular dispersive XRD (ADX), EDXD, TEM, Mössbauer spectroscopy	Cr _{0.7} Fe _{0.3} Al ₆
[1988Man]	XRD	850-900°C, > 92 at.% Al
[1988Sch]	ADX, TEM, EDXD	50 at.% Al
[1989Law1]	XRD, DTA, TEM, electron diffraction	86 at.% Al
[1989Law2]	XRD, DTA	86 at.% Al
[1989Man]	XRD	80 at.% Al
[1989McK]	Optical microscopy, SEM, TEM	Fe ₇₂ Al ₂₈ (at.%) with additions 2-6 at.% Cr
[1990Ioa]	XRD, optical microscopy, TEM	Cr _{2.13} Fe _{0.5} Al _{97.37} (at.%)
[1991Pra]	SEM, EDXD, wavelength dispersive X-ray spectrometry (WDS)	50-80 at.% Fe, ≤ 20 at.% Cr
[1991Tre]	XRD, optical microscopy, DTA	≤ 1800°C, Cr-FeAl section
[1992Hil]	Knudsen effusion mass spectroscopy (KEMS)	1040-1283°C, Cr _{19.96} Fe _{70.72} Al _{9.32} (at.%)
[1993Kni]	XRD, SEM, TEM, electron energy loss spectroscopy (EELS)	Fe ₃ Al with 2 or 5 mass% Cr
[1993Sta]	XRD, DSC, Mössbauer spectroscopy	Cr ₈ Fe ₆ Al ₈₆ (at.%)

Reference	Method/Experimental Technique	Temperature/Composition/Phase Range Studied
[1994Hyd]	Electrical resistivity measurements	$\text{Cr}_{1.8}\text{Fe}_{72.69}\text{Al}_{25.51}$, $\text{Cr}_{4.29}\text{Fe}_{69.74}\text{Al}_{25.97}$ (at.%)
[1994Mor]	XRD, TEM, DSC	$\text{Cr}_5\text{Fe}_{28}\text{Al}_{67}$ (at.%)
[1995Ant]	XRD, high-temperature DTA, differential scanning calorimetry (DSC)	$\text{Cr}_1\text{Fe}_{73}\text{Al}_{26}$, $\text{Cr}_2\text{Fe}_{72}\text{Al}_{26}$, $\text{Cr}_4\text{Fe}_{70}\text{Al}_{26}$ (at.%)
[1995Sta]	XRD, DTA, EDXD	$\text{Cr}_8\text{Fe}_6\text{Al}_{86}$ (at.%)
[1995Sui]	XRD, TEM	$\text{CrFe}_2\text{Al}_{12}$
[1995Yos]	Electrical resistivity measurements, TEM	$\text{Cr}_2\text{Fe}_{73}\text{Al}_{25}$, $\text{Cr}_2\text{Fe}_{70}\text{Al}_{28}$ (at.%)
[1995Zia]	XRD, SEM, TEM, DSC	$\text{Cr}_3\text{Al}_{97}$, $\text{Cr}_3\text{Fe}_1\text{Al}_{96}$, $\text{Cr}_3\text{Fe}_3\text{Al}_{94}$ (at.%)
[1997Nis1], [1997Nis2]	Vickers hardness measurements, electrical resistivity measurements, XRD	$(\text{Fe}_{1-x}\text{Cr}_x)_3\text{Al}$ series
[1997Pal]	XRD, electron microprobe analysis (EPMA)	1000°C, 40-100 at.% Al
[1997Rud]	DSC, EPMA	20-700°C, Fe_3Al -5 at.% Cr
[1997Sat]	XRD, neutron diffraction, Mössbauer studies	10-300 K, $\text{Cr}_x\text{Fe}_{3-x}\text{Al}$
[1997Sui]	XRD, high-resolution electron microscopy (HREM)	$\text{CrFe}_2\text{Al}_{12}$
[1998Kim]	Neutron diffractometry, XRD, TEM	25-1100°C, $\text{Cr}_5\text{Fe}_{67}\text{Al}_{28}$ (at.%)
[1998Lia]	Electron diffraction, HREM	$\text{CrFe}_2\text{Al}_{12}$
[1998Sun]	Neutron diffractometry, XRD, SEM, TEM	500°C, Fe_3Al + 5 at.% Cr
[1999Sui]	Electron diffraction, TEM	$\text{CrFe}_2\text{Al}_{12}$
[1999Wit]	TEM, EDXD, atomic force microscopy (AFM), lateral force microscopy (LFM)	0-18 at.% Cr, 7-25 at.% Al
[2000Bla]	EPMA, Mössbauer spectroscopy	1200°C, ≤ 1 at.% Al
[2000Dem]	DTA, TEM, SEM, EMPA	$\text{Cr}_{11}\text{Fe}_8\text{Al}_{81}$
[2000Mo]	TEM, HREM, XRD	$\text{CrFe}_2\text{Al}_{12}$
[2000Spi]	XRD, TEM	9.3-18 at.% Cr, 7.6-25.5 at.% Al
[2001Alo]	XRD, Mössbauer spectroscopy	830°C, $\text{Cr}_x\text{Fe}_{0.7-x}\text{Al}_{0.3}$ ($x \leq 0.35$)
[2001Dem]	DTA, TEM, SEM, EPMA	$\text{Cr}_{11}\text{Fe}_8\text{Al}_{81}$
[2002Ban]	Calculation based on the Bragg-Williams theory of order-disorder transformation	Atomic ordering in $(\text{Cr,Fe})\text{Al}$
[2003Zou]	High-resolution TEM, electron diffraction	$\text{CrFe}_2\text{Al}_{12}$
[2004Dem]	TEM, EDXD, EPMA	25-584°C, thin films $\text{Cr}_{23.3}\text{Fe}_{9.1}\text{Al}_{67.6}$, $\text{Cr}_{22}\text{Fe}_8\text{Al}_{70}$, $\text{Cr}_{19.5}\text{Fe}_8\text{Al}_{72.5}$, $\text{Cr}_{15.8}\text{Fe}_{8.7}\text{Al}_{75.5}$, $\text{Cr}_{14.5}\text{Fe}_8\text{Al}_{77.5}$ (at.%)
[2004Den]	XRD (on the single crystal), EPMA	$\text{CrFe}_2\text{Al}_{12}$
[2004Wu]	X-ray Laue back reflection technique	400°C, $\text{Cr}_3\text{Fe}_{57}\text{Al}_{40}$ (at.%)
[2004Zha]	XRD	$\text{Cr}_{25}\text{Fe}_{50}\text{Al}_{25}$ (at.%)
[2005Bel]	XRD, SEM, backscattered electron (BSE) imaging, EDXD	$\text{Cr}_{16.5}\text{Fe}_6\text{Al}_{77.5}$ (at.%)
[2005Reg1]	SEM	500°C, 14.5 and 19 at.% Al, 1, 2 and 5 at.% Cr
[2005Reg2]	SEM	500°C, 14.5 and 19 at.% Al, 1, 2 and 5 at.% Cr
[2005Zha]	XRD, SEM, EDXD	1000°C, $\text{Cr}_5\text{Fe}_{85}\text{Al}_{10}$ and $\text{Cr}_{10}\text{Fe}_{80}\text{Al}_{10}$ (at.%)
[2006Bih]	XRD, SEM, optical microscopy, EDXD, BSE imaging	$\text{Cr}_{19.5}\text{Fe}_8\text{Al}_{72.5}$, $\text{Cr}_{21.5}\text{Fe}_6\text{Al}_{72.5}$, $\text{Cr}_{23.7}\text{Fe}_{9.1}\text{Al}_{67.6}$ (at.%)
[2006Dem]	TEM, electron diffraction	65-81 at.% Al
[2006Gol1], [2006Gol2]	Inductively coupled plasma optical emission spectroscopy (ICPOES), TEM, SEM, optical microscopy, XRD, DSC	Fe_3Al + (2.5-25) at.% Cr
[2006Kar]	Melt spinning, high-temperature XRD	$\text{Cr}_2\text{Fe}_4\text{Al}_{94}$, $\text{Cr}_{3.4}\text{Fe}_8\text{Al}_{88.6}$ (at.%)
[2006Sha]	TEM, SEM, optical microscopy	600-1000°C, $\text{Cr}_3\text{Fe}_{69}\text{Al}_{28}$ (at.%)

Reference	Method/Experimental Technique	Temperature/Composition/Phase Range Studied
[2007Chi]	Chemical analysis, optical microscopy	$\text{Cr}_5\text{Fe}_{67}\text{Al}_{28}$, $\text{Cr}_2\text{Fe}_{70}\text{Al}_{28}$ (at.%)
[2007Cho]	SEM, EDXD, optical microscopy	$\text{Cr}_6\text{Fe}_{69}\text{Al}_{25}$ (at.%)
[2007Pad]	XRD, Mössbauer spectroscopy	400°C, $\text{Cr}_{22.5}\text{Fe}_{52.5}\text{Al}_{25}$, $\text{Cr}_{25}\text{Fe}_{50}\text{Al}_{25}$, $\text{Cr}_{27.5}\text{Fe}_{47.5}\text{Al}_{25}$ (at.%)
[2007Pan]	Auger electron spectroscopy (AES), XRD	300°C, 400°C, 500°C, Cr/Al/Fe thin films
[2008For]	SEM	Fibers $\text{Cr}_{25}\text{Fe}_{70}\text{Al}_5$ (at.%)
[2008Jac]	KEMS, EDXD, SEM	877-1277°C, $\text{Cr}_{15.1}\text{Fe}_{45.1}\text{Al}_{39.8}$, $\text{Cr}_{30.2}\text{Fe}_{49.9}\text{Al}_{19.9}$ (at.%)
[2008Lu]	XRD, EPMA, SEM, EDXD	600°C, 5-20 at.% Cr, 10 at.% Al
[2008Pav1]	TEM, DSC	$\text{Cr}_5\text{Fe}_{69}\text{Al}_{26}$ (at.%)
[2008Pav2]	EDXD-SEM, electron diffraction	1000°C, 70-81 at.% Al
[2008Pav3]	SEM, EPMA, TEM, DTA	800°C, 80-90 at.% Al, 5-15 at.% Cr
[2008Pin]	SEM, EPMA	900-1000°C, 10-19 at.% Al, 1-20 at.% Cr
[2008Shr]	XRD	$\text{Cr}_{25}\text{Fe}_{50}\text{Al}_{25}$ (at.%)
[2009Bau]	Czochralski method, neutron diffraction	$\text{Cr}_{19}\text{Fe}_3\text{Al}_{78}$ (at.%)
[2009Dea]	Combustion-infrared absorbance, inert gas fusion-thermal conductivity, inductively-coupled plasma analysis, Netzsch STA 409 high-temperature thermogravimetric analysis (TGA), SEM, EDXD	$\text{Cr}_5\text{Fe}_{85}\text{Al}_{10}$, $\text{Cr}_5\text{Fe}_{82.5}\text{Al}_{12.5}$ (mass%)
[2009Gol]	XRD, TEM, DSC	25-28 at.% Al, 3-25 at.% Cr
[2009Pav]	XRD, SEM, EDXD, TEM, DTA	700-1000°C, $\sim\text{Cr}_{16}\text{Fe}_{12}\text{Al}_{72}$ (at.%)
[2010Bau], [2011Bau]	Bridgman method, Czochralski method, optical microscopy, neutron diffraction measurement, EPMA, single crystal XRD, DTA, X-ray topography	75-81 at.% Al, 1-11 at.% Cr
[2010Bra]	SEM, EPMA, high angle annular dark field (HAADF) scanning transmission electron microscopy (STEM)	$\text{Cr}_{20}\text{Fe}_{70}\text{Al}_{10}$ (at.%)
[2010Gal]	XRD, TEM, DSC	$\text{Cr}_{2.8}\text{Fe}_{4.2}\text{Al}_{93.0}$ (at.%)
[2010Kob]	Optical microscopy, SEM, TEM	475°C, ≤ 20 at.% Al, 10-30 at.% Cr
[2010Kra]	SEM, TEM, secondary ion mass spectrometry (SIMS), AES	Water-atomized powders, 5-8 at.% Cr, 1.5-5 at.% Fe
[2010Pav]	XRD, SEM, EDXD, TEM, DTA	700-980°C, 78.0-82.3 at.% Al, ≤ 4.9 at.% Fe
[2010Sch]	XRD, SEM, BSE imaging, energy dispersive spectroscopy (EDS)	$\text{Cr}_{4.0}\text{Fe}_{69.6}\text{Al}_{26.4}$ (at.%)
[2011Kho1]	Optical microscopy, XRD, DTA, SEM, EPMA	600-1165°C, 58-100 at.% Al
[2011Kho2]	Optical microscopy, XRD, DTA, SEM, TEM, EPMA	58-100 at.% Al
[2011Kim]	Optical microscopy, XRD, SEM, field emission-scanning electron microscopy (FE-SEM), EPMA	$\text{Cr}_{22}\text{Fe}_{72.2}\text{Al}_{5.8}$ (mass%) or $\text{Cr}_{21.9}\text{Fe}_{66.95}\text{Al}_{11.15}$ (at.%)
[2011La]	Optical microscopy, XRD, EPMA, TEM	$\text{Fe}_3\text{Al} + 5$ (10, 15) mass% Cr
[2011Tom]	Optical microscopy, XRD, SEM	44.8-48.0 at.% Al, 1-11.7 at.% Cr
[2012Lam]	ICPOES, optical microscopy, DSC, mechanical spectroscopy (MS), DTA	$\text{Cr}_8\text{Fe}_{67}\text{Al}_{25}$, $\text{Cr}_{25}\text{Fe}_{50}\text{Al}_{25}$ (at.%)
[2012Sah]	EDXD, SEM, XRD	1000°C, CrFe_2Al
[2012Ume]	Optical microscopy, EPMA, DSC, XRD, electron diffraction, TEM	600°C, 400°C, $\text{Cr}_{25}\text{Fe}_{50}\text{Al}_{25}$ (at.%)
[2012Yil]	EDXD, SEM-EPMA, XRD, DSC	400°C, $\text{Cr}_1\text{Fe}_{50}\text{Al}_{49}$ (at.%)

Reference	Method/Experimental Technique	Temperature/Composition/Phase Range Studied
[2013Bau]	Czochralski method, XRD, neutron diffraction	Al _{79.1} Cr _{17.8} Fe _{3.1} (at.%)
[2013Mar]	KEMS, wavelength dispersive X-ray (WDX) analysis	961-1335°C, 11-31 at.% Al, 13-35 at.% Cr
[2013Nei]	Melt atomization, pulsed hot pressing (PHP), hot extrusion (HE), XRD, SEM	20, 190, and 300°C, Cr ₅ Fe _{82.5} Al _{12.5} (mass%) or Cr _{4.7} Fe _{72.55} Al _{22.75} (at.%)
[2014Gas]	XRD, EPMA, X-ray topography, TEM, HAADF STEM	Cr _{17.8} Fe _{3.1} Al _{79.1} (at.%) single crystal
[2014Pav]	XRD, SEM, EDXD, TEM, DTA	700-1160°C, 50-100 at.% Al
[2015Sus]	XRD	1050°C, 33.3 at.% Al, ≤ 33.3 at.% Cr
[2015Zho]	XRD, SEM-EDXD, BSE imaging	700°C, 70-100 at.% Al
[2016Li1]	XRD, SEM, EPMA, DTA	As-cast, 1000°C, Cr ₂ Fe ₃₇ Al ₆₁ (at.%)
[2016Sve]	XRD, SEM, EDXD, EBSD technique	As-cast, 460-1200°C, Cr ₂ Fe ₇₂ Al ₂₆ (at.%)
[2017Kra]	XRD, TEM	26 at.% Al, 0 to 8 at.% Cr
[2019Cha]	XRD, EDXD	Magnetron-sputtered films, 60-75 at.% Fe
[2019Eze]	XRD, SEM, DTA, EPMA	81-99.6 at.% Al
[2019Ran], [2020Ran]	XRD, SEM-EDXD, EPMA, ICPOES, carrier gas hot extraction (CGHE), DSC, DTA, dilatometry, diffusion couples (DC) technique	10-70 at.% Al
[2019Wan]	Kohn-Sham equations of the density-functional theory, cluster variation method, cluster expansion method	FeAl, Fe ₃ Al, 327-2727°C
[2020Ma]	TEM, HAADF STEM, selected-area electron diffraction, energy dispersive X-ray spectrometry	1000°C, Cr ₁₅ Fe ₁₁ Al ₇₄ (at.%)
[2020Ran]	Calphad-type assessment	Calculated isothermal sections between 700 and 1160°C, isopleth at 47.5 at.% Cr, liquidus surface

Table 2: Crystallographic Data of Solid Phases

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments/References
(Al) < 660.452	<i>cF4</i> <i>Fm$\bar{3}m$</i> Cu	$a = 404.96$	pure Al at 25°C [Mas2] solubility of Cr: < 0.39 at.% [2015Wit] (Al–Cr) solubility of Fe: 0.023 at.% [2019Ran] (Al–Fe) dissolves up to 0.08 at.% Fe at 0.3 at.% Cr (Al–Cr–Fe) [2019Eze]
(Cr, $\alpha\delta$ Fe) < 1863 Cr < 1863 α Fe < 912 δ Fe 1538-1394	<i>cI2</i> <i>Im$\bar{3}m$</i> W	$a = 288.48$ $a = 286.65$ $a = 293.15$	Strukturbericht designation: <i>A2</i> pure Cr at 25°C [Mas2] at 25°C [Mas2] [Mas2] solubility of Al in ($\alpha\delta$ Fe): 45.0 at.% [1993Kat, 2007Ste] (Al–Fe) solubility of Al in (Cr): up to 53 at.% [2014Ste] (Al–Cr)
(γ Fe) 1394-846	<i>cF4</i> <i>Fm$\bar{3}m$</i> Cu	$a = 364.67$	at 915°C [V-C2, Mas2] solubility of Al: 1.35 at.% [1993Kat] (Al–Fe) solubility of Cr: < 11.9 at.% [2010Xio] (Cr–Fe)

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments/References
CrAl ₇ < 794	<i>m</i> C104 <i>C</i> 2/ <i>m</i> V ₇ Al ₄₅	$a = 2065.0 \pm 0.2$ $b = 759.78 \pm 0.08$ $c = 1096.74 \pm 0.11$ $\beta = (107.308 \pm 0.002)^\circ$ $a = 2060.28$ $b = 758.50$ $c = 1093.85$ $\beta = 107.33^\circ$	sometimes named Cr ₂ Al ₁₃ , Cr ₇ Al ₄₅ , θ -CrAl ₇ or θ from 86.6 to 86.9 at.% Al [2013Khv] single crystal [2020Bou] (denoted as Cr ₇ Al ₄₅) for Cr _{11.3} Fe _{2.4} Al _{86.3} (at.%) [2019Eze] solubility of Fe: < 2.5 at.% [2019Eze] (Al–Cr–Fe)
Cr ₂ Al ₁₁ (913 < <i>T</i> < 985)–(~500–~600)	<i>m</i> C616 <i>C</i> 2/ <i>c</i> Cr ₂ Al ₁₁	$a = 1773.48 \pm 0.10$ $b = 3045.55 \pm 0.17$ $c = 1773.44 \pm 0.10$ $\beta = (91.052 \pm 0.012)^\circ$ $a = 1771.5 \pm 1.2$ $b = 3069 \pm 3$ $c = 1773.8 \pm 2.5$ $\beta = (90.39 \pm 0.05)^\circ$	sometimes named CrAl ₅ , η -Cr ₂ Al ₁₁ or η from 83.5 to 84 at.% Al [2013Khv] single crystal [2008Cao] for Cr _{16.8} Fe _{2.9} Al _{80.3} (at.%) at 910°C [2010Pav] solubility of Fe: up to ~3 at.% at around 80 at.% Al [2010Pav] (Al–Cr–Fe)
CrAl ₄ < 1040	<i>h</i> P574 <i>P</i> 6 ₃ / <i>mmc</i> MnAl ₄	$a = 2019.11 \pm 0.15$ $c = 2485.40 \pm 0.19$ $a = 2013.79 \pm 0.04$ $c = 2482.92 \pm 0.09$	sometimes named μ -CrAl ₄ or μ from 78.7 to 81.3 at.% Al [2013Khv] single crystal [2017Cao] single crystal Cr _{20.6} Fe _{0.7} Al _{78.7} (at.%) [2010Bau] Solubility of Fe: < 1.7 at.% [2011Kho1] (Al–Cr–Fe)
Cr ₄ Al ₁₁ < 829	<i>a</i> P15 <i>P</i> $\bar{1}$ Mn ₄ Al ₁₁	$a = 508.9 \pm 0.5$ $b = 903.3 \pm 0.8$ $c = 504.4 \pm 0.2$ $\alpha = (91.84 \pm 0.08)^\circ$ $\beta = (100.77 \pm 0.07)^\circ$ $\gamma = (107.59 \pm 0.09)^\circ$	sometimes named ν [2006Gru]
α Cr ₅ Al ₈ (r) < 1138	<i>h</i> R78 <i>R</i> $\bar{3}m$ Cr ₅ Al ₈	$a = 1272.8$ $c = 794.2$ $a = 1271.5 \pm 0.1$ to 1281.3 ± 0.1 $c = 792.8 \pm 0.1$ to 795.1 ± 0.1 $a = 1253.7$ $c = 779.1$	Strukturbericht designation: <i>D</i> 8 ₁₀ sometimes named Cr ₅ Al ₈ (l), γ_2 -Cr ₅ Al ₈ or γ_2 [V–C2] 58.0 to 67.9 at.% Al [1989Ell] for 31.2 at.% Fe at 1000°C [1997Pal] solubility of Fe: up to ~35 at.% [2014Pav] (Al–Cr–Fe)

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments/References
Cr ₂ Al < 910	<i>tI</i> 6 <i>I4/mmm</i> MoSi ₂	$a = 300.86 \pm 0.02$ $c = 865.31 \pm 0.11$	Strukturbericht designation: <i>C</i> 11 _b ~28.6 to ~35.5 at.% Al [2013Khv] [2021Mil] Solubility of Fe: up to 22 at.% Fe [2019Ran, 2020Ran] (Al–Cr–Fe)
σ , CrFe 820-(~500~510)	<i>tP</i> 30 <i>P</i> 4 ₂ / <i>mm</i> CrFe	$a = 879.95 \pm 0.04$ $c = 454.42 \pm 0.02$	~50.2 to ~57.3 at.% Fe [2010Xio] single crystals [1954Ber] solubility of Al: up to 3 at.% [1958Chu] (Al–Cr–Fe)
Fe ₃ Al < 545	<i>cF</i> 16 <i>Fm</i> $\bar{3}$ <i>m</i> BiF ₃	$a = 579.30$ $a = 578.86$	sometimes named α_1 phase Strukturbericht designation: <i>D</i> 0 ₃ ~24 to ~34 at.% Al at 400°C [1993Kat] at 23.1 at.% Al, water-quenched from 250°C [1958Tay] at 35.0 at.% Al, water-quenched from 250°C [1958Tay]
FeAl < 1318	<i>cP</i> 2 <i>Pm</i> $\bar{3}$ <i>m</i> CsCl	$a = 289.53$ to 290.90	sometimes named α_2 phase Strukturbericht designation: <i>B</i> 2 23.5 to ~53 at.% Al [2007Ste] at 36.2 to 50.0 at.% Al, water-quenched from 250°C [1958Tay]
FeAl ₂ < 1146	<i>aP</i> 18 <i>P</i> $\bar{1}$ FeAl ₂	$a = 487.45$ $b = 645.45$ $c = 873.61$ $\alpha = 87.930^\circ$ $\beta = 74.396^\circ$ $\gamma = 83.062^\circ$ $a = 486.3$ $b = 645.4$ $c = 880.1$ $\alpha = 91.92^\circ$ $\beta = 72.95^\circ$ $\gamma = 96.87^\circ$	sometimes named ζ phase 64.7 to 66.7 at.% Al [2022Ste] at 66.4 at.% Al [2010Chu] at 4.5 at.% Cr at 1000°C [1997Pal] solubility of Cr: up to 4.5 at.% [1997Pal] (Al–Cr–Fe)
Fe ₂ Al ₅ 1159 - ~331	<i>oC</i> 24 <i>Cmcm</i> Fe ₂ Al ₅	$a = 765.59 \pm 0.08$ $b = 641.54 \pm 0.06$ $c = 421.84 \pm 0.04$ $a = 769.4$ $b = 644.3$ $c = 422.7$	sometimes named η phase 68.4 to 72.5 at.% Al [2022Ste] at 71.5 at.% Al [1994Bur] at 6.2 at.% Cr at 1000°C [1997Pal] solubility of Cr: up to 6.2 at.% [1997Pal] (Al–Cr–Fe)

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments/References
Fe ₄ Al ₁₃ < 1150	<i>mC</i> 102 <i>C2/m</i> Fe ₄ Al ₁₃	$a = 1548.8 \pm 0.1$ $b = 808.66 \pm 0.05$ $c = 1247.69 \pm 0.08$ $\beta = (107.669 \pm 0.004)^\circ$	referred to as FeAl ₃ in old literature before ~1995 sometimes named θ phase 74.5 to 76.9 at.% Al [2022Ste] single crystal grown by Czochralski technique [2008Gil, 2010Pop]
		$a = 1554.3$ $b = 802.9$ $c = 1245.0$ $\beta = 107.47^\circ$	at 6.4 at.% Cr at 1000°C [1997Pal] solubility of Cr: up to 7 at.% [2019Ran, 2020Ran] (Al–Cr–Fe)
FeAl ₆	<i>oC</i> 28 <i>Cmc</i> 2 ₁ FeAl ₆	$a = 744.0$ $b = 646.4$ $c = 877.9$	metastable single crystal [1965Wal]
(Cr,Fe) ₅ Al ₈ < 1185 β Cr ₅ Al ₈ (h) 1321–1060	<i>cI</i> 52 <i>I</i> $\bar{4}3m$ Cu ₅ Zn ₈	$a = 909.0 \pm 0.1$	Strukturbericht designation: <i>D</i> 8 ₂ Continuous solid solution at 1160°C [2014Pav] sometimes named Cr ₅ Al ₈ (h), γ_1 -Cr ₅ Al ₈ or γ_1 (Al–Cr) 59.2 to 68.4 at.% Al [2013Khv, 2015Wit] at 67.3 at.% Al [1992Bra]
		$a = 910.4 \pm 0.1$ to 904.7 \pm 0.1	58.0 to 70.0 at.% Al [1989Ell]
Fe ₅ Al ₈ 1231–1095		$a = 897.57 \pm 0.02$	sometimes named ε phase (Al–Fe) 56.0 to 64.5 at.% Al [2016Li2] at 1120°C, 59.4 at.% Al [2010Ste]
* ε -(Cr,Fe)Al ₄ < 1055	<i>oC</i> 584 <i>Cmcm</i>	$a = 1252.1 \pm 0.1$ $b = 3470.5 \pm 0.2$ $c = 2022.3 \pm 0.1$	sometimes named as ε -Al ₄ Cr or ε single crystal [1997Li] (metastable in Al–Cr).
		$a = 1249.841 \pm 0.03$ $b = 3473.73 \pm 0.09$ $c = 2021.29 \pm 0.05$	for Cr _{19.3} Fe _{1.8} Al _{78.9} (at.%), single crystal [2010Bau]
			This phase is metastable in Al–Cr. It is stabilized in Al–Cr–Fe at around 2–3 at.% Fe and 78–77 at.% Al [2010Bau, 2011Bau, 2011Kho1]
* σ -(Cr,Fe)Al ₄ <~ 1026	<i>oP</i> * <i>Pmm</i> 2	$a = 1248.0 \pm 0.1$ $b = 2502.9 \pm 0.1$ $c = 3058.1 \pm 0.1$	Compound possesses a highly modulated structure [2013Bau] Homogeneity range extends between 3 and 6 at.% Fe at around 78 at.% Al [2010Bau, 2011Bau]
*O ₁ < 1087	<i>o</i> *	$a \approx 3270$ $b \approx 1240$ $c \approx 2340$	Stoichiometry is unknown. sometimes named as O ₁ or C _{3,I} -Al–Cr–Fe [2008Pav2] Homogeneity range extends between ca. Cr _{15.0} Fe _{11.0} Al _{74.0} to Cr _{19.7} Fe _{4.3} Al _{76.0} and Cr _{15.0} Fe _{6.9} Al _{78.1} to Cr _{18.3} Fe _{8.9} Al _{72.8} (at.%) [2011Kho1, 2011Kho2, 2014Pav]

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments/References
*H < 998	$hR1512$ $R\bar{3}$	$a = 1772.28 \pm 0.03$ $c = 8068.1 \pm 0.2$	Stoichiometry is unknown. Also named v, H-(Al-Fe-Cr) or H-Al ₄ (Cr,Fe) for Cr _{13.35} Fe _{6.63} Al _{80.02} (at.%), single crystal [2010Bau, 2011Bau] Large homogeneity extends between approximately Cr _{12.0} Fe _{8.0} Al _{80.0} to Cr _{19.7} Fe _{4.3} Al _{76.0} and Cr _{11.0} Fe _{6.3} Al _{82.7} to Cr _{13.5} Fe _{7.0} Al _{79.4} (at.%) [2011Kho1, 2019Eze]
*D < 1096	- $P10_5/mmc$ -	$n \approx 1230$ along the 10-fold symmetry axis	Stoichiometry is unknown. Cr ₁₅ Fe ₁₁ Al ₇₄ (at.%) single crystal [2020Ma] Homogeneity range may extend from 70 to 72 at.% Al and from 14 to 18 at.% Cr [2011Kho1]
i (m)	simple icosahedral-type	$a_{6D} = 654.2 \pm 0.2$	metastable phase emerging at high cooling rates Proposed composition is Cr _{12±1} Fe _{12±1} Al _{75±0.5} (at.%) [1995Zia] [1995Sta]

Table 3: Invariant Equilibria

Reaction	T (°C)	Type	Phase	Composition (at.%)		
				Al	Cr	Fe
$L + (Cr, Fe)_5Al_8 \rightleftharpoons \alpha Cr_5Al_8$	1185	p ₃ , max	L	~69.5	~17.7	~12.8
$L \rightleftharpoons \alpha Cr_5Al_8 + Fe_2Al_5$	1136	e ₂ , max	L	~67.2	~10.2	~22.6
$L \rightleftharpoons (Cr, Fe)_5Al_8 + \alpha Cr_5Al_8 + Fe_2Al_5$	1125	E ₁	L	66	10	24
			(Cr, Fe) ₅ Al ₈	63.1	13.0	23.9
			αCr_5Al_8	63.4	13.7	22.8
			Fe ₂ Al ₅	70.2	4.3	25.5
$L \rightleftharpoons \alpha Cr_5Al_8 + Fe_4Al_{13}$	1115	e ₃ , max	L	~70.4	~10.7	~18.9
$L \rightleftharpoons Fe_4Al_{13} + \alpha Cr_5Al_8 + Fe_2Al_5$	1105	E ₂	L	69.2	10.0	20.8
			Fe ₄ Al ₁₃	74.0	4.5	21.5
			αCr_5Al_8	64.8	18.4	16.8
			Fe ₂ Al ₅	71.2	5.3	23.5
$L + \alpha Cr_5Al_8 \rightleftharpoons D$	1096	p ₅ , max	L	~72.1	~13.6	~14.3
$L \rightleftharpoons D + Fe_4Al_{13}$	1093	e ₄ , max	L	~73.2	~11.4	~15.4
$L + \alpha Cr_5Al_8 \rightleftharpoons O_1$	1087	p ₆ , max	L	~76.2	~15.7	~8.1
$L \rightleftharpoons D + Fe_4Al_{13} + \alpha Cr_5Al_8$	1085	E ₃	L	71	11	18
			D	69.8	16.4	13.8
			Fe ₄ Al ₁₃	74.0	5.2	20.8
			αCr_5Al_8	66.0	21.9	12.1
$L + \alpha Cr_5Al_8 \rightleftharpoons O_1 + D$	1085	U ₁	L	74.3	14.5	11.2
			αCr_5Al_8	67.0	23.8	9.2
			O ₁	~72.8	~18.3	~8.9
			D	71.4	18.0	10.6
$L + D \rightleftharpoons O_1 + Fe_4Al_{13}$	~1075	U ₂	L	74.8	13.0	12.2
			D	72.4	15.3	12.3
			O ₁	74.0	15.0	11.0
			Fe ₄ Al ₁₃	75.5	6.0	18.5
$L + \alpha Cr_5Al_8 \rightleftharpoons \varepsilon-(Cr,Fe)Al_4$	1055	p ₇ , max	L	~82.6	~15.0	~2.4

Reaction	T (°C)	Type	Phase	Composition (at.%)		
				Al	Cr	Fe
$L + \alpha\text{Cr}_5\text{Al}_8 \rightleftharpoons \varepsilon\text{-(Cr,Fe)Al}_4 + \text{O}_1$	1045	U_3	L	82.4	14.3	3.3
			$\alpha\text{Cr}_5\text{Al}_8$	~70	~27	~3
			$\varepsilon\text{-(Cr,Fe)Al}_4$	~77	~20	~3
			O_1	~76	~20	~4
$L + \alpha\text{Cr}_5\text{Al}_8 \rightleftharpoons \varepsilon\text{-(Cr,Fe)Al}_4 + \text{CrAl}_4$	1035	U_4	L	83.0	15.0	2.0
			$\alpha\text{Cr}_5\text{Al}_8$	~70	~28	~2
			$\varepsilon\text{-(Cr,Fe)Al}_4$	~77	~21	~2
			CrAl_4	~78	~20	~2
$L + \varepsilon\text{-(Cr,Fe)Al}_4 + \text{O}_1 \rightleftharpoons \text{o-(Cr,Fe)Al}_4$	~1026	P_1	L	~84	~13	~3
$L + \text{O}_1 + \text{Fe}_4\text{Al}_{13} \rightleftharpoons \text{H}$	998	P_2	L	84.0	9.0	7.0
			O_1	77.1	14.7	8.2
			$\text{Fe}_4\text{Al}_{13}$	76.7	4.8	18.4
			H	80.0	12.0	8.0
$L + \varepsilon\text{-(Cr,Fe)Al}_4 \rightleftharpoons \text{CrAl}_4 + \text{o-(Cr,Fe)Al}_4$	~985	U_5	L	~85	~13	~2
$L + \text{O}_1 \rightleftharpoons \text{o-(Cr,Fe)Al}_4 + \text{H}$	~980	U_6	L	~85	~9	~6
$L + \text{CrAl}_4 + \text{o-(Cr,Fe)Al}_4 \rightleftharpoons \text{Cr}_2\text{Al}_{11}$	$913 < T < 985$	P_3	-	-	-	-
$L + \text{o-(Cr,Fe)Al}_4 \rightleftharpoons \text{Cr}_2\text{Al}_{11} + \text{H}$	$900 < T < 980$	U_7	-	-	-	-
$L + \text{Cr}_2\text{Al}_{11} \rightleftharpoons \text{CrAl}_7 + \text{H}$	750	U_8	L	96.8	2.3	0.9
			$\text{Cr}_2\text{Al}_{11}$	~83.0	~15.5	~1.5
			CrAl_7	~86.0	~13.0	~1.0
			H	~82.3	~14.2	~3.5
$L + \text{H} \rightleftharpoons \text{CrAl}_7 + \text{Fe}_4\text{Al}_{13}$	660	U_9	L	97.6	0.6	1.8
			H	82.7	11.0	6.3
			CrAl_7	86.0	11.5	2.5
			$\text{Fe}_4\text{Al}_{13}$	~77	~4	~19
$L + \text{CrAl}_7 \rightleftharpoons \text{Fe}_4\text{Al}_{13} + (\text{Al})$	657	U_{10}	L	98.0	0.3	1.7
			CrAl_7	86.6	11.0	2.4
			$\text{Fe}_4\text{Al}_{13}$	~77	~1	~22
			(Al)	99.7	0.2	0.1

* Compositions of liquid phase for the maxima in the monovariant lines are as-read from the original figure by [2011Kho2]

Table 4: Thermodynamic Properties of the (Cr, $\alpha\delta\text{Fe}$) Phase

Phase	Temperature (°C)	Property per mole of atoms (J, mol, K)	Comments
(Cr, $\alpha\delta\text{Fe}$)	1227	$a_{\text{Al}} = (3.3 \pm 1.4) \cdot 10^{-3}$ $a_{\text{Cr}} = 0.28 \pm 0.4$ $a_{\text{Fe}} = 0.50 \pm 0.07$ $^{\text{ex}}\mu_{\text{Al}} = -42.0 \pm 7.0$ $^{\text{ex}}\mu_{\text{Cr}} = 4.3 \pm 1.9$ $^{\text{ex}}\mu_{\text{Fe}} = -4.4 \pm 2.0$	$\text{Cr}_{19.8}\text{Fe}_{71.2}\text{Al}_9$ (at.%), Knudsen effusion mass spectrometry [1992Hil]
(Cr, $\alpha\delta\text{Fe}$)	1177	$a_{\text{Al}} = 0.11$ $a_{\text{Cr}} = 0.19$ $a_{\text{Fe}} = 0.33$ $\Delta G_f = -18.4$ $a_{\text{Al}} = 0.07$ $a_{\text{Cr}} = 0.23$ $a_{\text{Fe}} = 0.35$ $\Delta G_f = -19.1$	[2013Mar], Knudsen effusion mass spectrometry $\text{Cr}_{13}\text{Fe}_{56}\text{Al}_{31}$ (at.%) $\text{Cr}_{17}\text{Fe}_{54.5}\text{Al}_{28.5}$ (at.%)

Phase	Temperature (°C)	Property per mole of atoms (J, mol, K)	Comments
(Cr, $\alpha\delta$ Fe) (continued)	1177 (continued)	$a_{\text{Al}} = 0.048$	Cr ₁₉ Fe ₅₅ Al ₂₆ (at.%)
		$a_{\text{Cr}} = 0.26$	
		$a_{\text{Fe}} = 0.38$	
		$\Delta G_f = -19.0$	
		$a_{\text{Al}} = 0.16$	Cr ₂₁ Fe ₄₄ Al ₃₅ (at.%)
		$a_{\text{Cr}} = 0.23$	
		$a_{\text{Fe}} = 0.19$	
		$\Delta G_f = -20.2$	
		$a_{\text{Al}} = 0.031$	Cr _{24.4} Fe ₅₅ Al _{20.5} (at.%)
		$a_{\text{Cr}} = 0.28$	
		$a_{\text{Fe}} = 0.41$	
		$\Delta G_f = -18.2$	
		$a_{\text{Al}} = 0.028$	Cr ₃₁ Fe ₄₈ Al ₂₁ (at.%)
		$a_{\text{Cr}} = 0.34$	
		$a_{\text{Fe}} = 0.35$	
		$\Delta G_f = -19.2$	
		$a_{\text{Al}} = 0.009$	Cr ₃₅ Fe ₅₄ Al ₁₁ (at.%)
		$a_{\text{Cr}} = 0.43$	
		$a_{\text{Fe}} = 0.53$	
		$\Delta G_f = -14.0$	
(Cr, $\alpha\delta$ Fe)	1027	$\Delta H_{\text{mix}} = -22.74 \pm 2.0$	[2008Jac], Knudsen effusion mass spectrometry
		$\Delta H_{\text{mix}} = -11.05 \pm 1.1$	Cr _{15.1} Fe _{45.1} Al _{39.8} (at.%)
			Cr _{30.2} Fe _{49.9} Al _{19.9} (at.%)

Table 5: Investigations of the Al–Cr–Fe Materials Properties

Reference	Method/Experimental Technique	Type of Property
[1940Kor2]	Electrical measurements	Electrical resistivity
[1946Kor]	Brinell indentation, electrical measurements, dilatometry	Hardness, electrical resistivity, thermal expansion RT to 1000°C
[1955Tag], [1958Tag]	Rockwell indentation	Hardness
[1968Bul]	Brinell hardness test, electrical measurements	Hardness, electrical resistivity RT to 950°C
[1969Kal]	Magnetic measurements, neutron diffraction	Magnetic susceptibility RT to 500°C, magnetic moment, Néel temperature
[1971Sto]	TGA in O ₂ atmosphere	Oxidation behaviour at 1000°C and 1200°C
[1974Niz], [1975Lit]	Magnetic measurements, neutron diffraction	Magnetic susceptibility -170°C to 500°C, magnetic moment
[1981Bus]	VSM	Curie temperature, magnetization at RT
[1982Nao]	Vickers indentation, tensile tests, bending tests, electrical measurements	Microhardness, yield stress, UTS, elongation, and electrical resistivity at RT; temperature coefficient of resistivity RT to 500°C
[1983Bus]	VSM, Kerr rotation measurements	Curie temperature, saturation moment at -269°C, magnetization at RT, Kerr rotation
[1985Okp]	VSM	Magnetization and magnetic susceptibility -196°C to RT
[1986Sme]	Oxidation tests in air	Oxidation behaviour at 1050°C
[1989McK]	Tensile tests	(0.2%) yield stress at RT and 600°C
[1991Pra]	Knoop indentation on melt-spun ribbons	Microhardness
[1991Sik1]	Tensile tests	0.2% yield stress, UTS, elongation, creep behaviour 450 to 704°C

Reference	Method/Experimental Technique	Type of Property
[1993Kni]	Tensile tests	Yield stress and elongation 700 to 850°C
[1994Hyd]	Electrical measurements	Electrical resistivity RT to 1200°C
[1995Sta]	VSM	Magnetic susceptibility -273 to -73°C
[1996Jim]	Compression tests	Creep behaviour 750°C to 1000°C
[1997Sat]	Magnetic balance, neutron diffraction	Magnetization at -196°C and RT, magnetic moments at -263°C, -196°C and RT
[1998Su]	Tensile tests	0.2% yield stress, UTS and elongation at RT
[1998Sun]	Tensile tests	UTS and elongation at RT
[2000Spi]	Compression tests	Compressive yield stress, work-hardening behavior
[2002Zho]	Torsion measurements	Internal friction RT-620°C
[2004Dem]	Optical measurements and wetting of thin films	Reflectivity, absorption and contact-angle
[2004Hua]	Tensile tests	0.2% yield stress and elongation at RT & 600°C, creep behaviour at 600°C
[2004Wu]	VSM	Magnetization -196°C to RT
[2004Zha]	SQUID, electrical measurements	Magnetic susceptibility, magnetization, and electrical resistivity -273°C to RT, DOS
[2005Bel]	SQUID, electrical measurements, NMR spin-lattice relaxation, SXES	Magnetic susceptibility and electrical resistivity -273°C to RT, relaxation rates -196°C to RT, DOS
[2005Reg1], [2005Reg2]	TGA	Oxidation, sulfidation and oxidation/sulfidation behaviour at 500°C
[2005Zha]	TGA in O ₂ atmosphere	Oxidation behaviour and mass gain at 1000°C
[2006Bih]	SQUID, electrical measurements, heat flow	Magnetization, electrical resistivity -269°C to RT, thermal conductivity -265°C to 42°C
[2006Gol1], [2006Gol2]	Mechanical spectroscopy, DSC, VSM, Vickers indentation	Curie temperature, magnetization RT to 650°C, internal friction RT to 600°C, microhardness
[2006Sha]	Tensile tests	Yield stress 600°C to 1000°C
[2007Chi]	TIG weldability study, Vickers indentation, four-point bending	Microhardness, time-to-failure in humid air and WD40 oil
[2007Cho]	Electrochemical corrosion tests	E_{corr} , E_{trans} , E_{pp} , I_a , I_p in 0.1M H ₂ SO ₄ and 0.1 M H ₂ SO ₄ + 0.001M KSCN; pitting corrosion in 0.1 M HCl
[2007Pad]	Magneto balance, SQUID	Curie temperature, magnetization -273°C to 70°C, magnetic saturation & magnetic moment at -269°C
[2007Pan]	Nanoindentation, electrical measurements	Nanohardness, electrical conductivity
[2008For]	Catalytic activity measurements	Hydrocarbon and CO conversion ability
[2008Lu]	Corrosion tests in H ₂ -CO ₂ and H ₂ -HCl-H ₂ S-CO ₂	Corrosion behavior at 600°C
[2008Pav1]	Magnetometer, mechanical spectroscopy	Curie temperature, magnetization RT to 650°C, internal friction -180°C to 650°C
[2008Pin]	Cyclic oxidation tests in air	Oxidation behaviour and mass gain 700°C to 1000°C
[2009Dea]	Sulfidation-oxidation tests	Corrosion behaviour at 500°C and 700°C, mass change
[2009Gol]	Mechanical spectroscopy, VSM	Internal friction 400°C to 650°C
[2010Air]	Oxidation tests in O ₂	Oxidation behavior at 1000°C
[2010Bra]	Sulfidation-oxidation tests in H ₂ S-H ₂ -H ₂ O-Ar	Corrosion behaviour at 600°C
[2010Gal]	Tensile tests	UTS RT to 355°C

Reference	Method/Experimental Technique	Type of Property
[2010Kob]	Vickers indentation	Microhardness at 475°C
[2010Kra]	Tensile tests	Tensile strength
[2010Sch]	Tensile tests, fatigue tests	0.2% yield stress, UTS, Young's modulus, LCF at RT & 300°C
[2011Hei]	Oxidation, XPS, DFT-EMTO	Initial stages of oxidation
[2011Kim]	Oxidation tests in air	Oxidation behavior 900-1100°C
[2011La]	Vickers indentation, compression tests	Hardness, compressive 0.2% yield stress at RT
[2011Tom]	Electrochemical corrosion tests in 0.1 mol/L HCl	Anodic polarization curves, mass change
[2012Lam]	Mechanical spectroscopy, DSC	Internal friction, Curie temperature
[2012Ume]	SQUID, VSM	Magnetization, thermomagnetization -273°C to 100°C, magnetic moment, Curie temperature
[2013Nei]	Vickers indentation, tensile tests	Microhardness; yield stress, UTS, and elongation RT to 300°C
[2015Sus]	Physical property measurements, SQUID	Magnetic susceptibility -273°C to 100°C, magnetic ordering, DOS
[2016Li1]	Vickers indentation, four-point bending tests, compression tests	Martens microhardness, brittle-to-ductile transition temperature (BDTT), compressive 0.2% yield stress at 600°C to 1000°C
[2016Sve]	Dilatometry	Thermal expansion
[2017Kra]	Compression tests	Compressive 0.2% yield stress at 800°C
[2019Cha]	Nanoindentation	Hardness, Young's modulus

Fig. 1: Al–Cr–Fe.
Assessed Al–Cr phase diagram

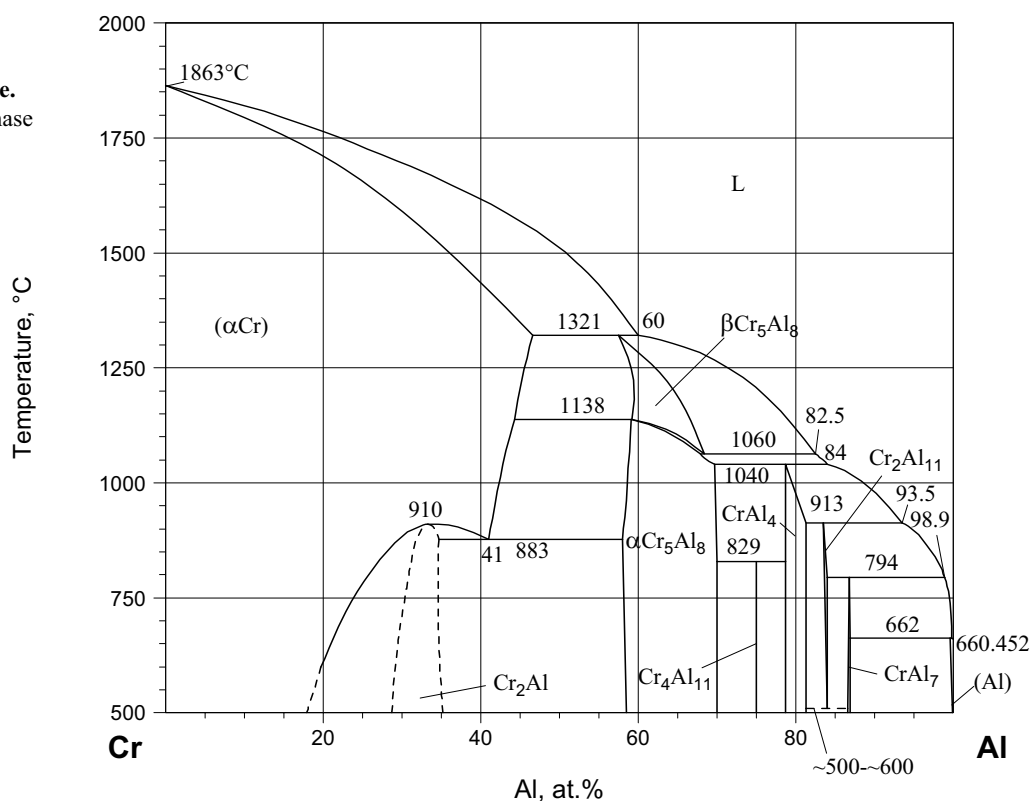


Fig. 2a: Al-Cr-Fe.
Lattice constant a_0 of
the $\text{Cr}_5\text{Al}_8(\text{r})$ phase in
dependence of Fe
content (Al content is
55 to 58 at.%)

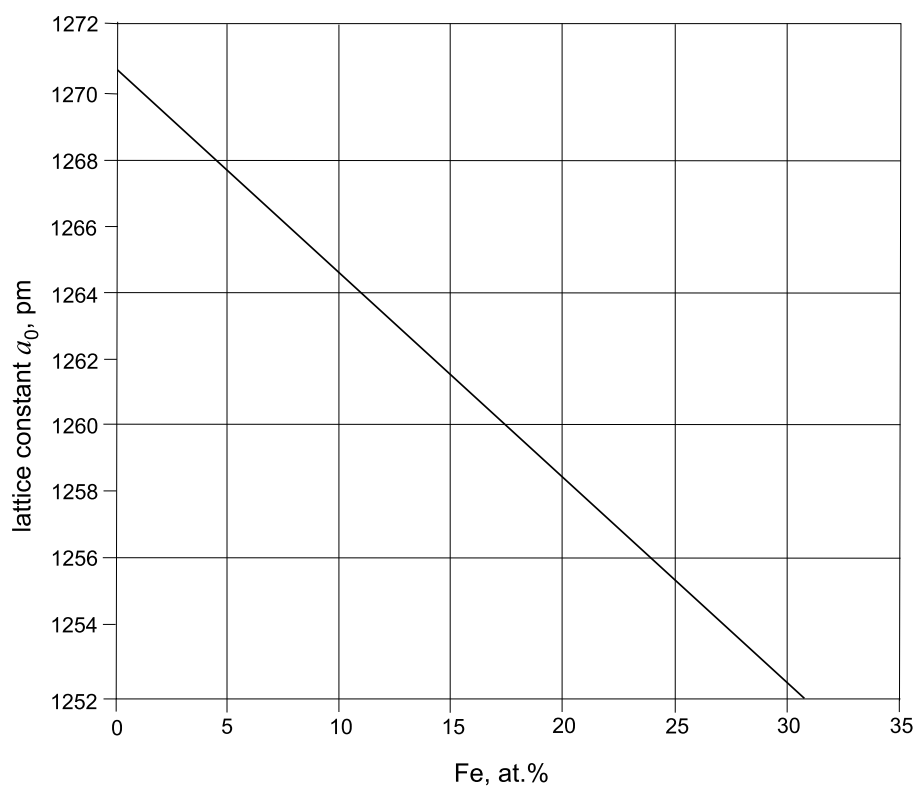
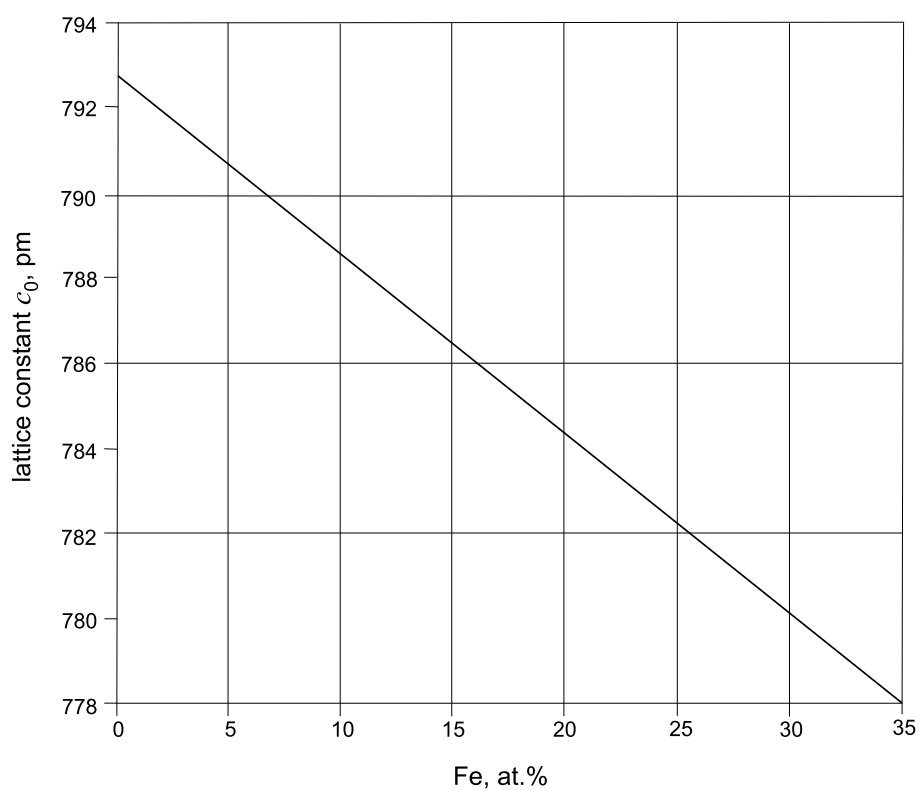


Fig. 2b: Al-Cr-Fe.
Lattice constant c_0 of
the $\text{Cr}_5\text{Al}_8(\text{r})$ phase in
dependence of Fe
content (Al content is
55 to 58 at.%)



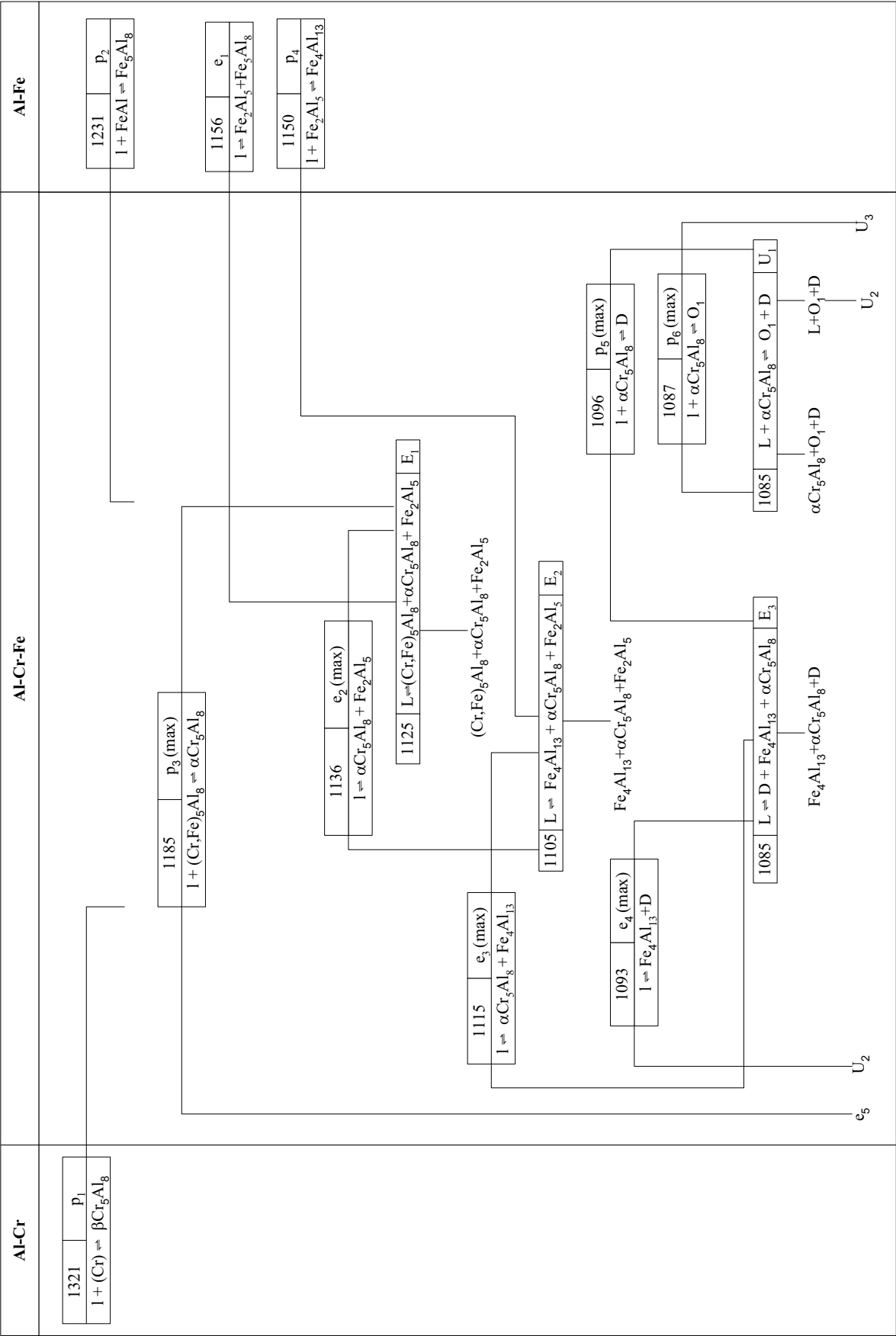


Fig.3a: Al-Cr-Fe. Reaction scheme

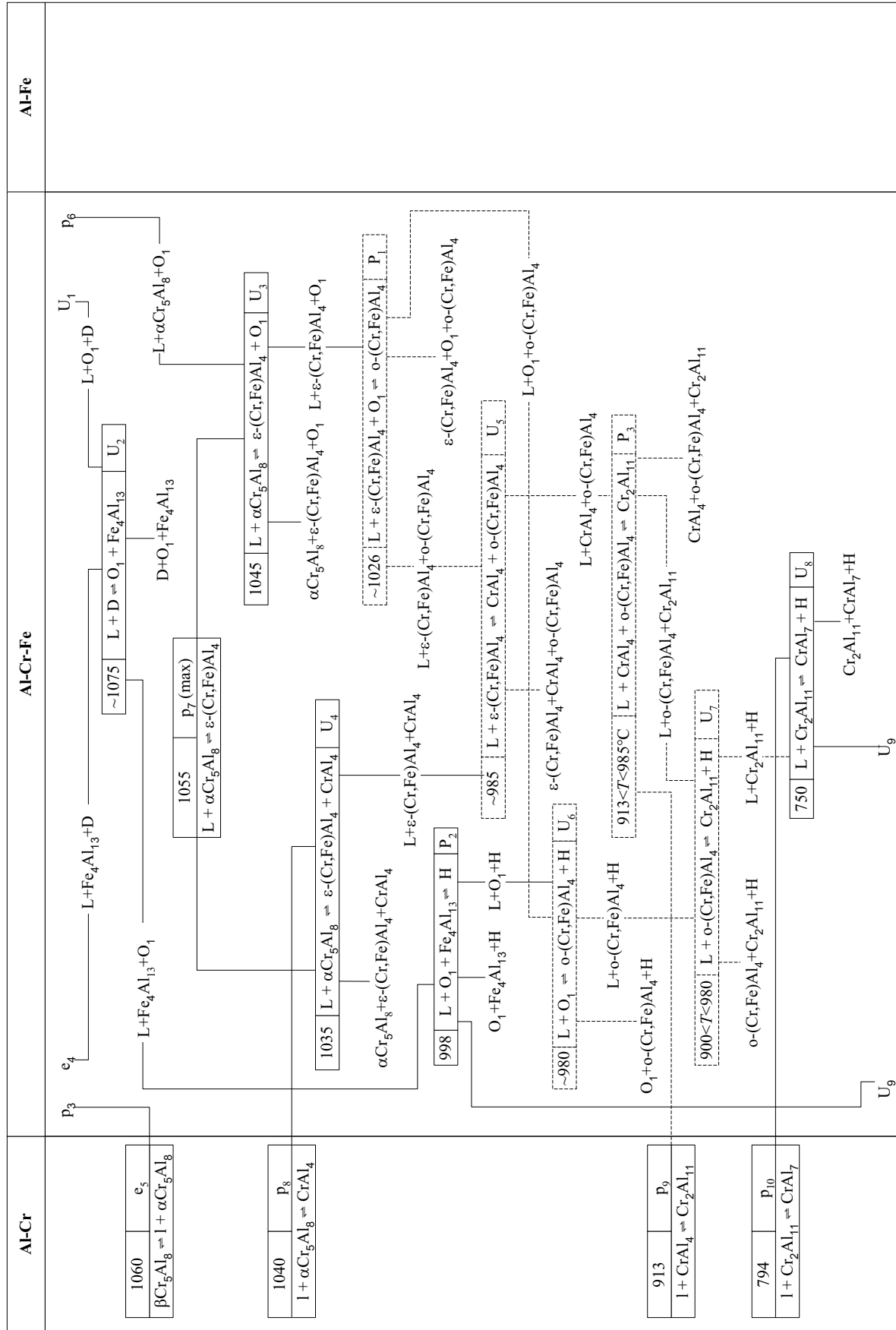


Fig. 3b: Al-Cr-Fe. Reaction scheme

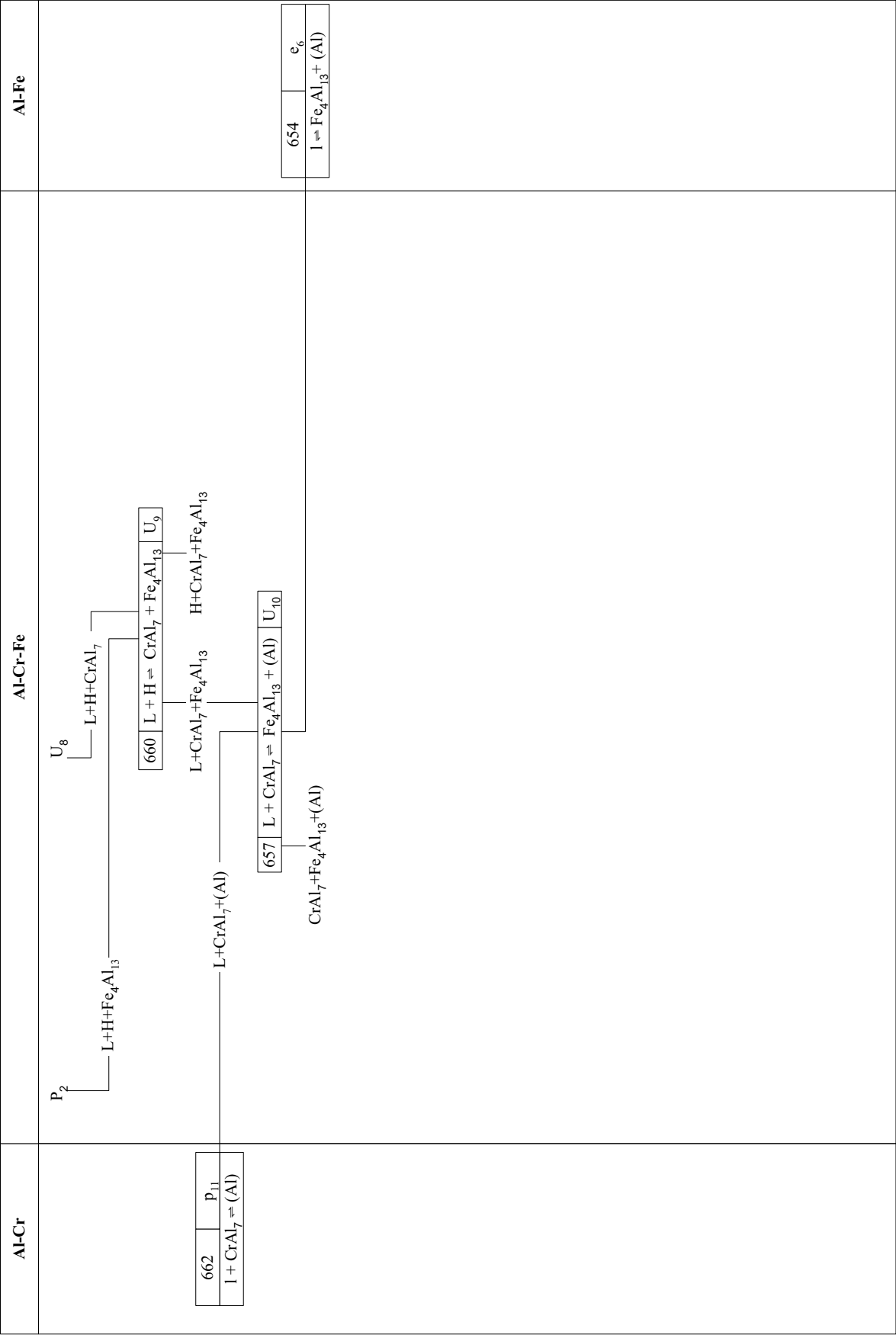


Fig. 3c: Al-Cr-Fe. Reaction scheme

Fig. 4a: Al-Cr-Fe.
Liquidus surface
projection

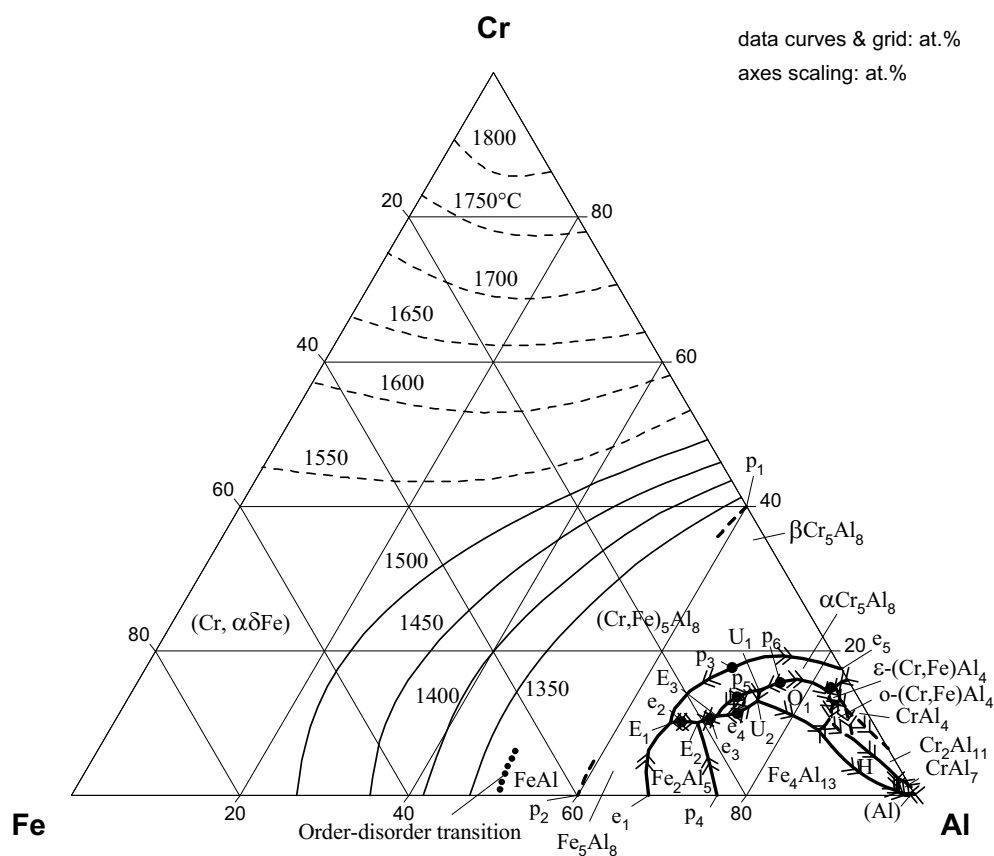


Fig. 4b: Al-Cr-Fe.
Liquidus surface
projection at
50-100 at.% Al

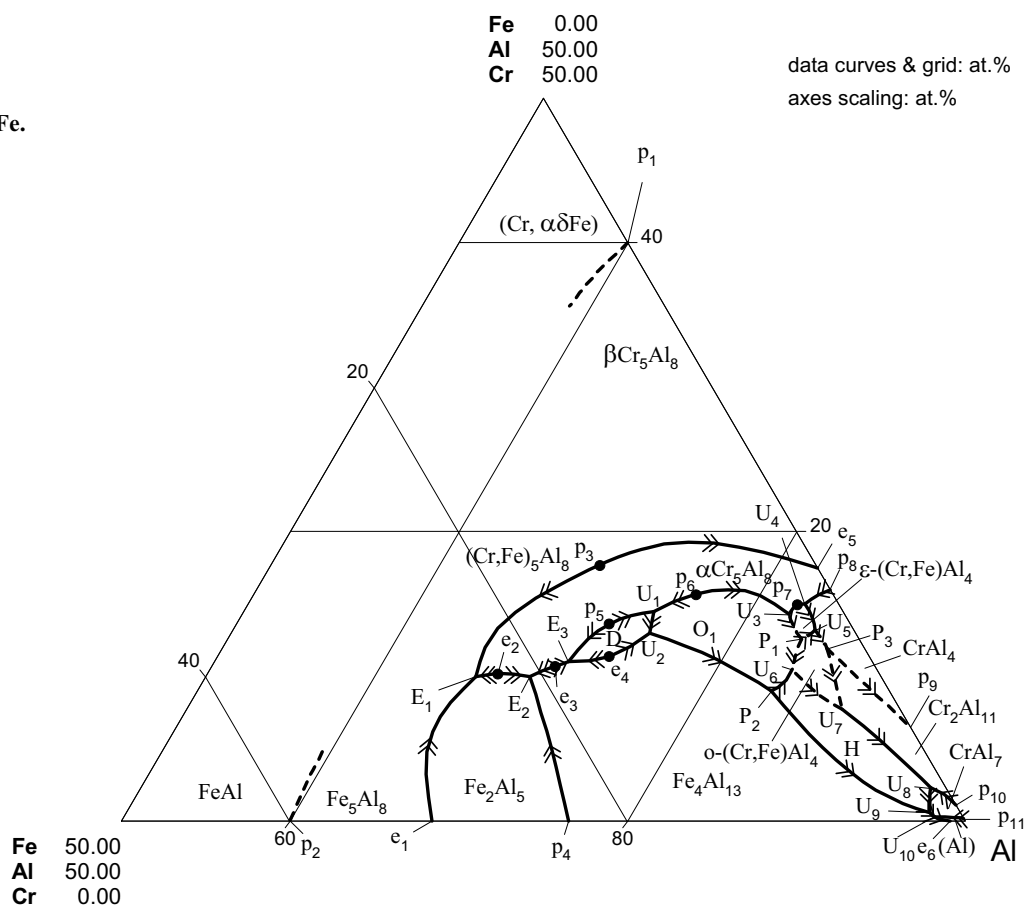


Fig. 5: Al-Cr-Fe.
Solidus surface
projections in the
range of compositions
60-100 at.% Al

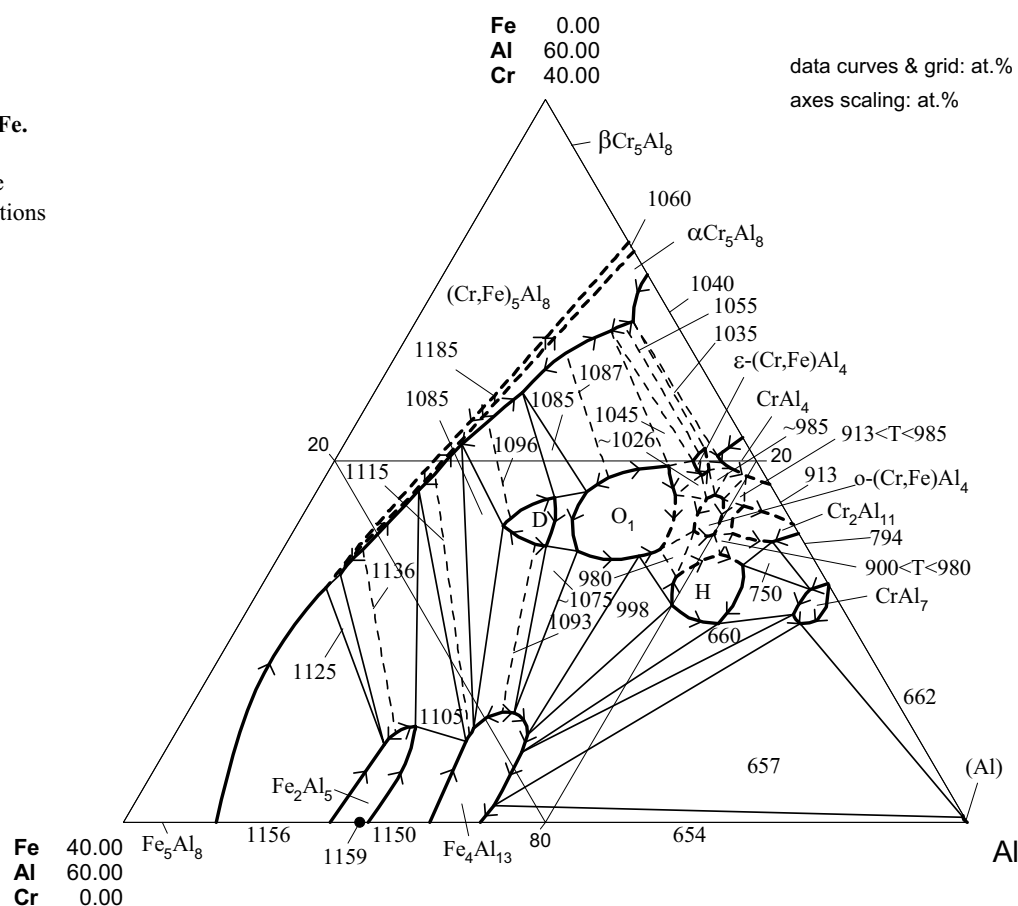


Fig. 6: Al-Cr-Fe.
Isothermal section at
1160°C

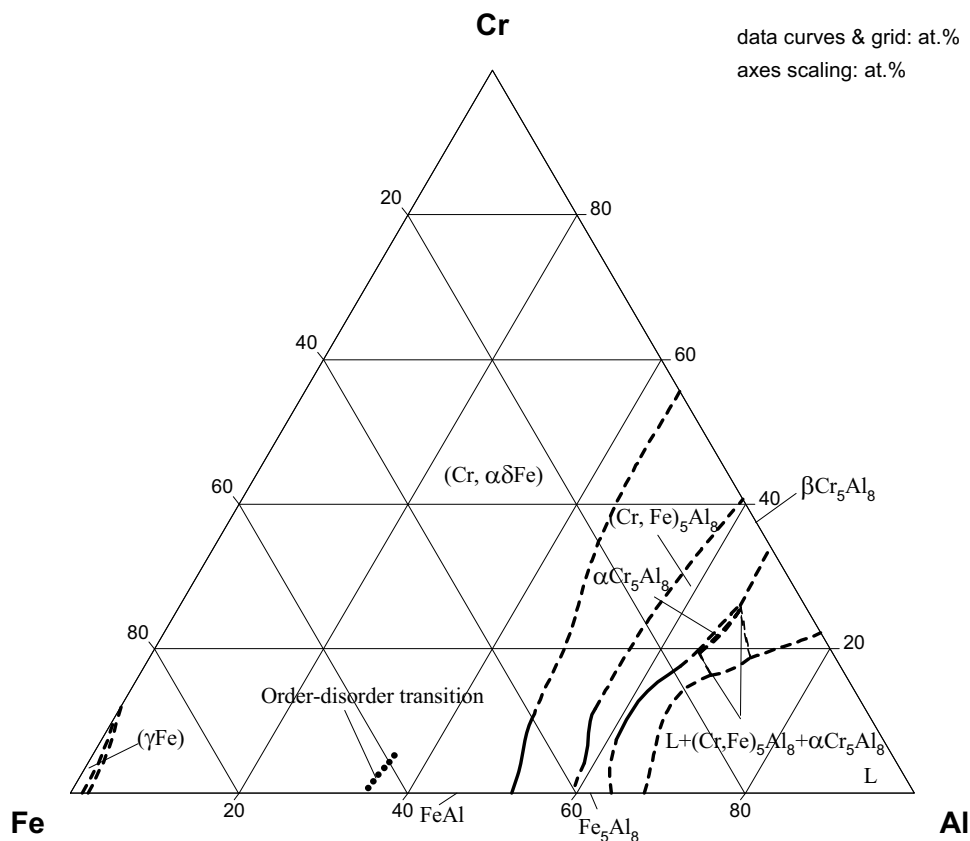


Fig. 7: Al-Cr-Fe.
Isothermal section at
1100°C

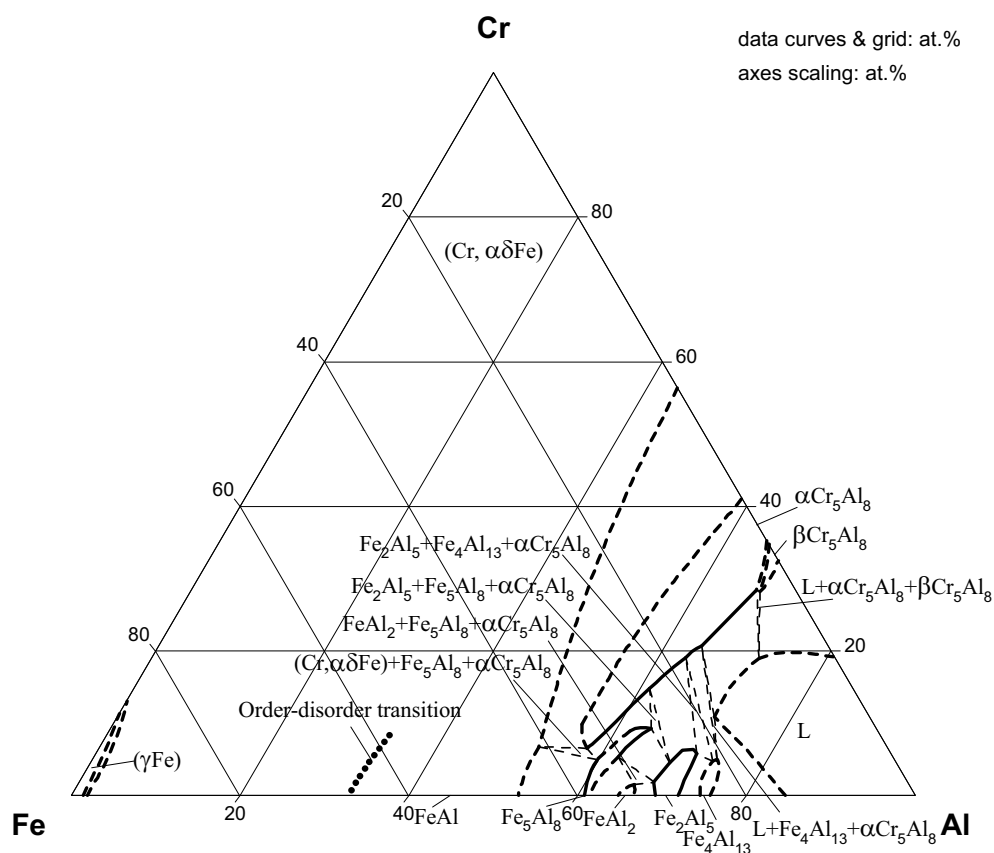


Fig. 8: Al-Cr-Fe.
Isothermal section at
1075°C

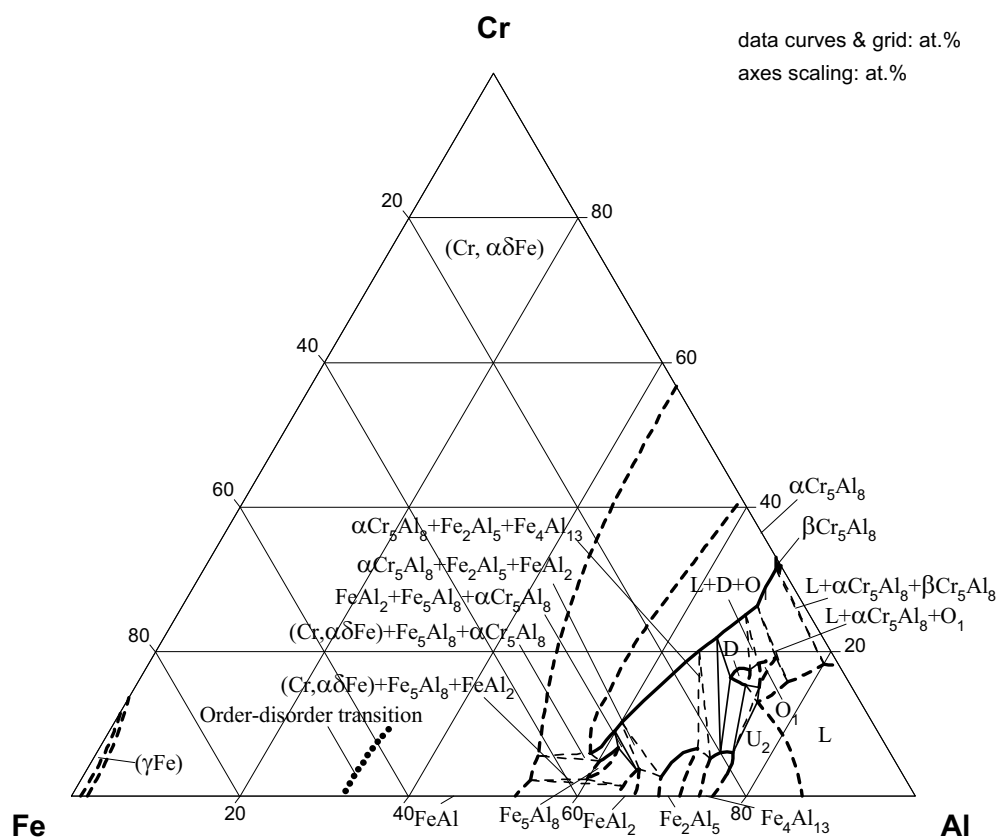


Fig. 9: Al-Cr-Fe.
Isothermal section at
1042°C

- 1: $\alpha\text{Cr}_5\text{Al}_8 + \text{O}_1 + \varepsilon\text{-(Cr,Fe)Al}_4$
- 2: $\text{L} + \text{O}_1 + \varepsilon\text{-(Cr,Fe)Al}_4$
- 3: $\text{L} + \text{O}_1 + \varepsilon\text{-(Cr,Fe)Al}_4$
- 4: $\text{O}_1 + \text{D} + \text{Fe}_4\text{Al}_{13}$

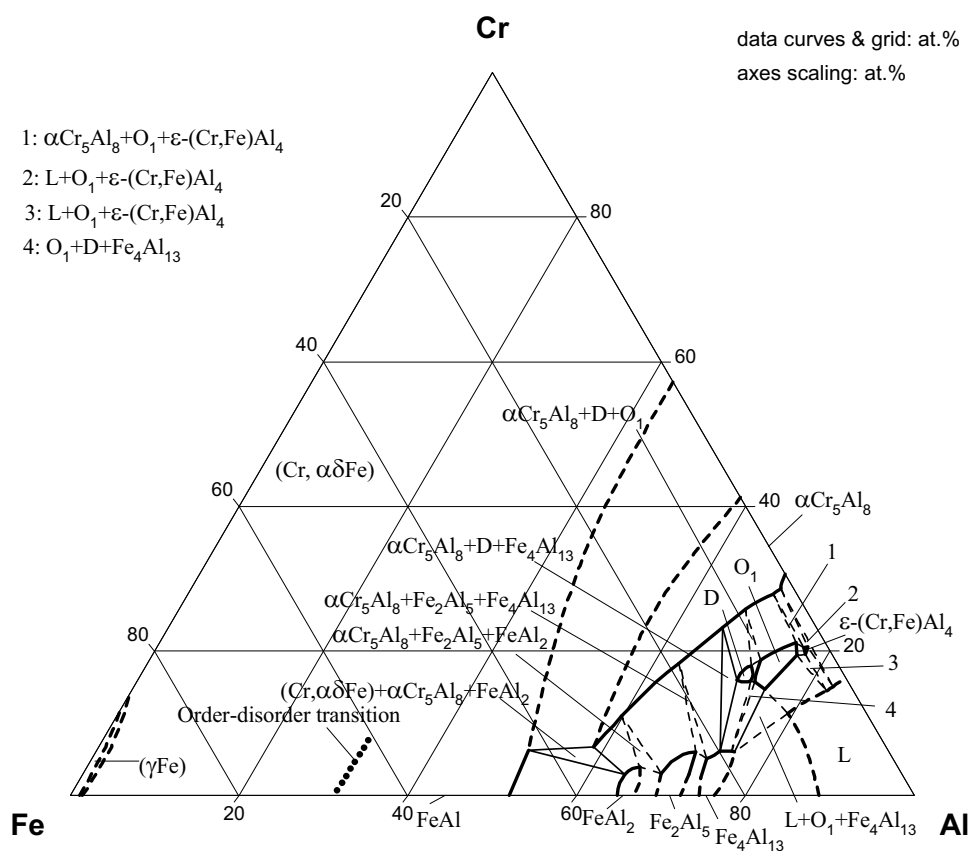


Fig. 10a: Al-Cr-Fe.
Isothermal section at
1000°C

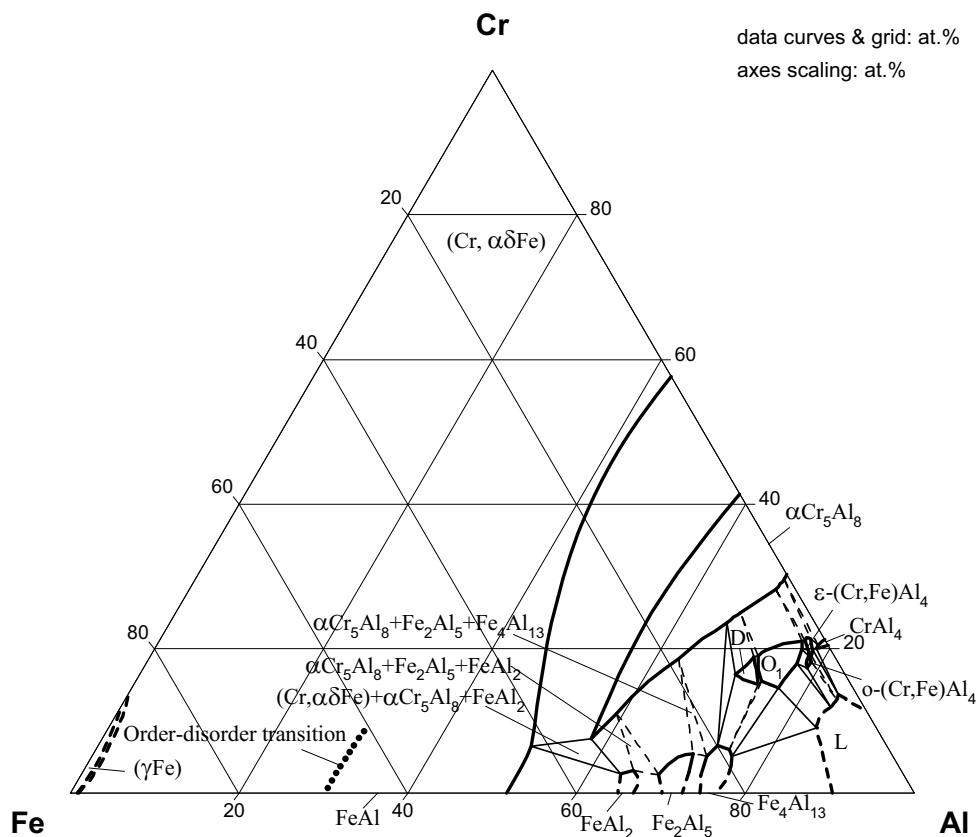


Fig. 10b: Al-Cr-Fe.
Enlarged portion of
isothermal section at
1000°C

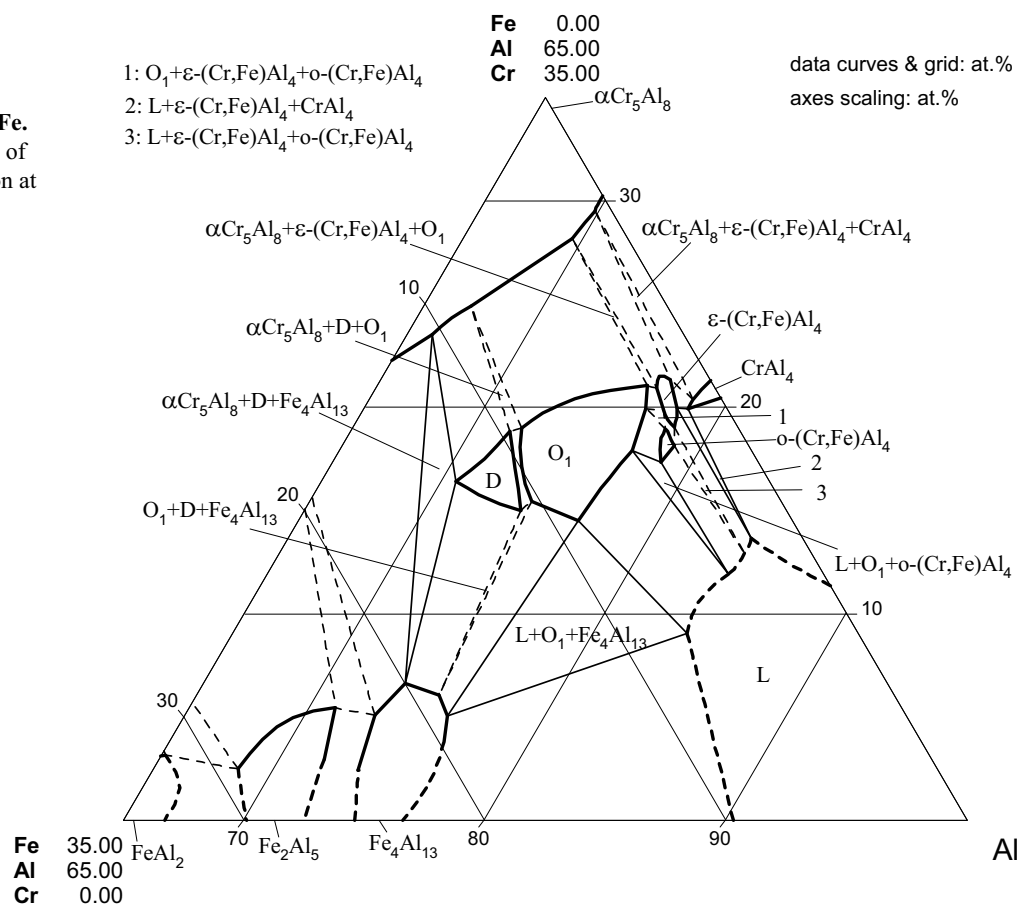


Fig. 11a: Al-Cr-Fe.
Isothermal section at
900°C

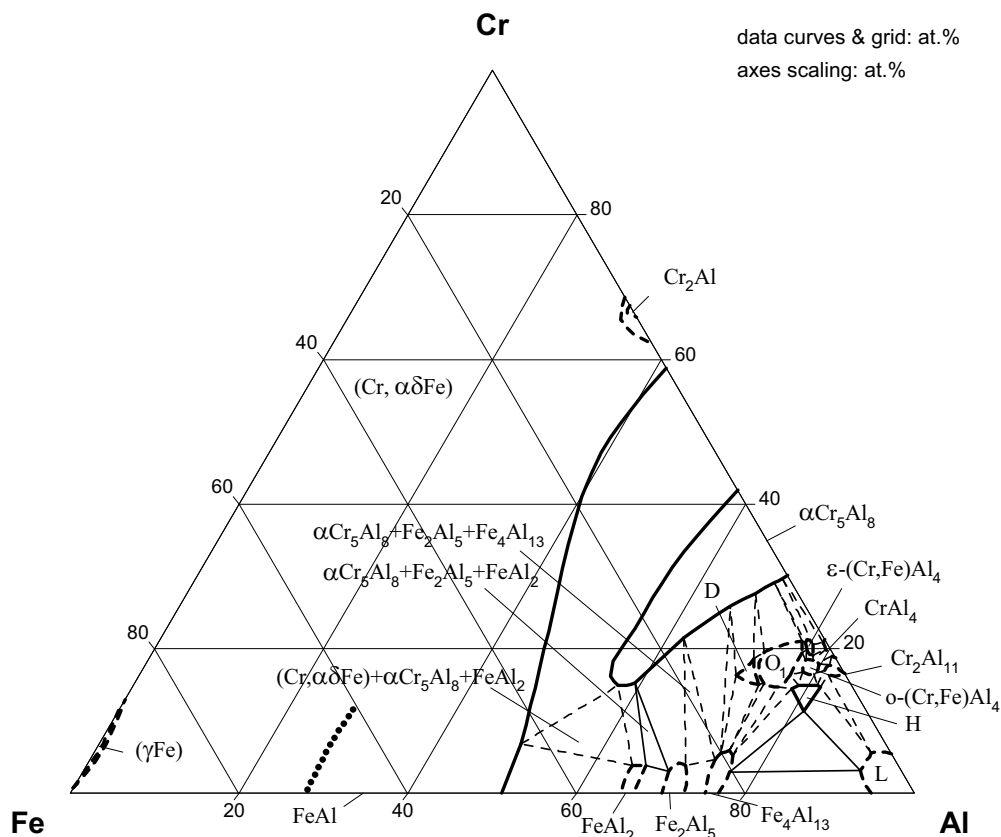


Fig. 11b: Al-Cr-Fe.
Enlarged portion of
isothermal section at
900°C

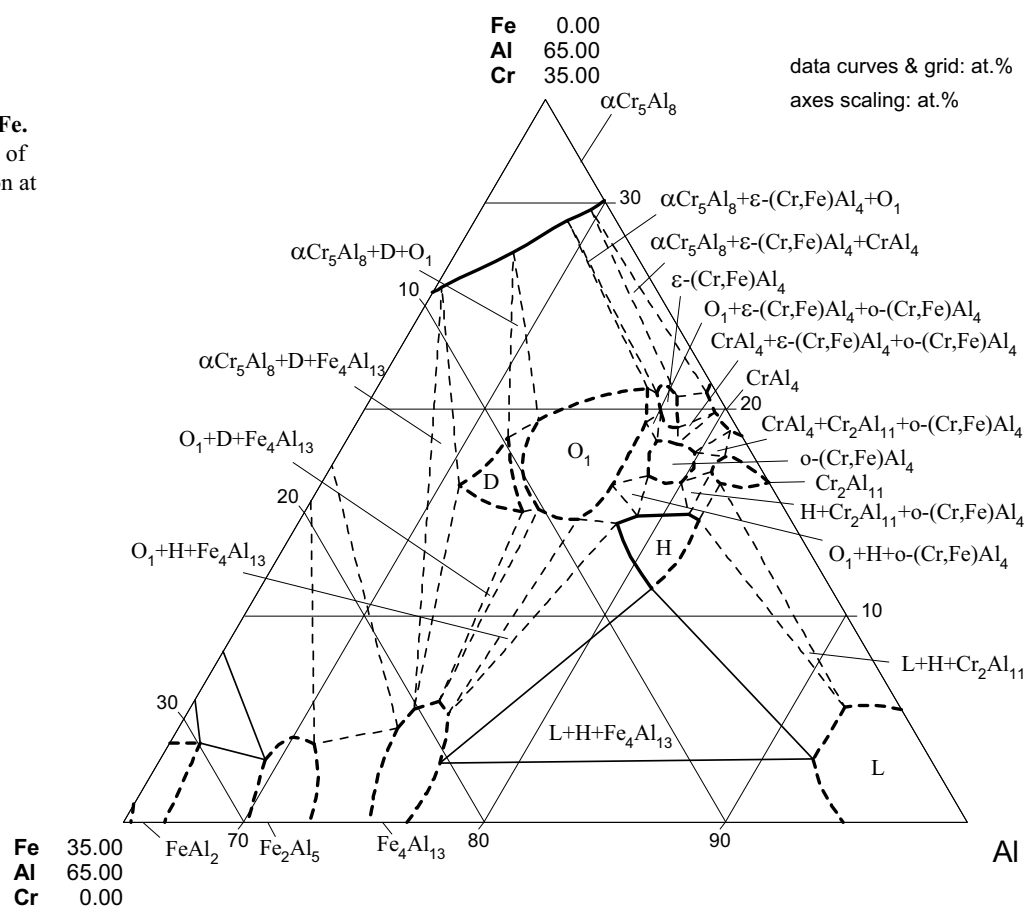


Fig. 12a: Al-Cr-Fe.
Isothermal section at
700°C

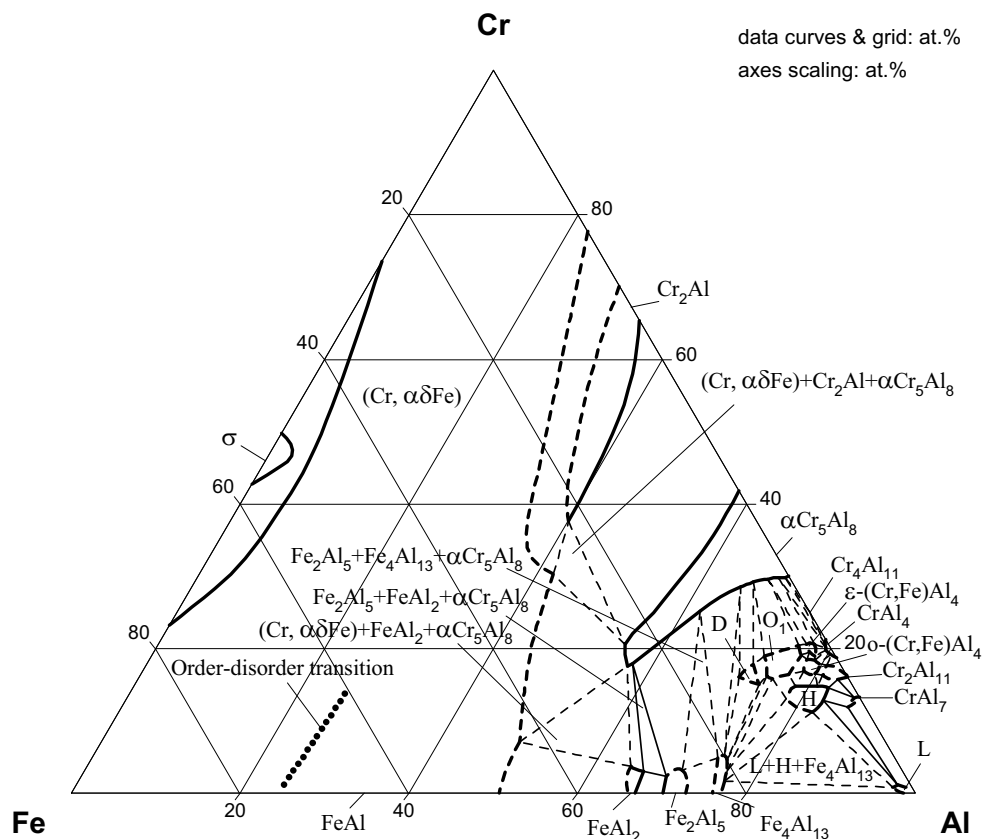


Fig. 12b: Al-Cr-Fe.
Enlarged portion of
isothermal section at
700°C

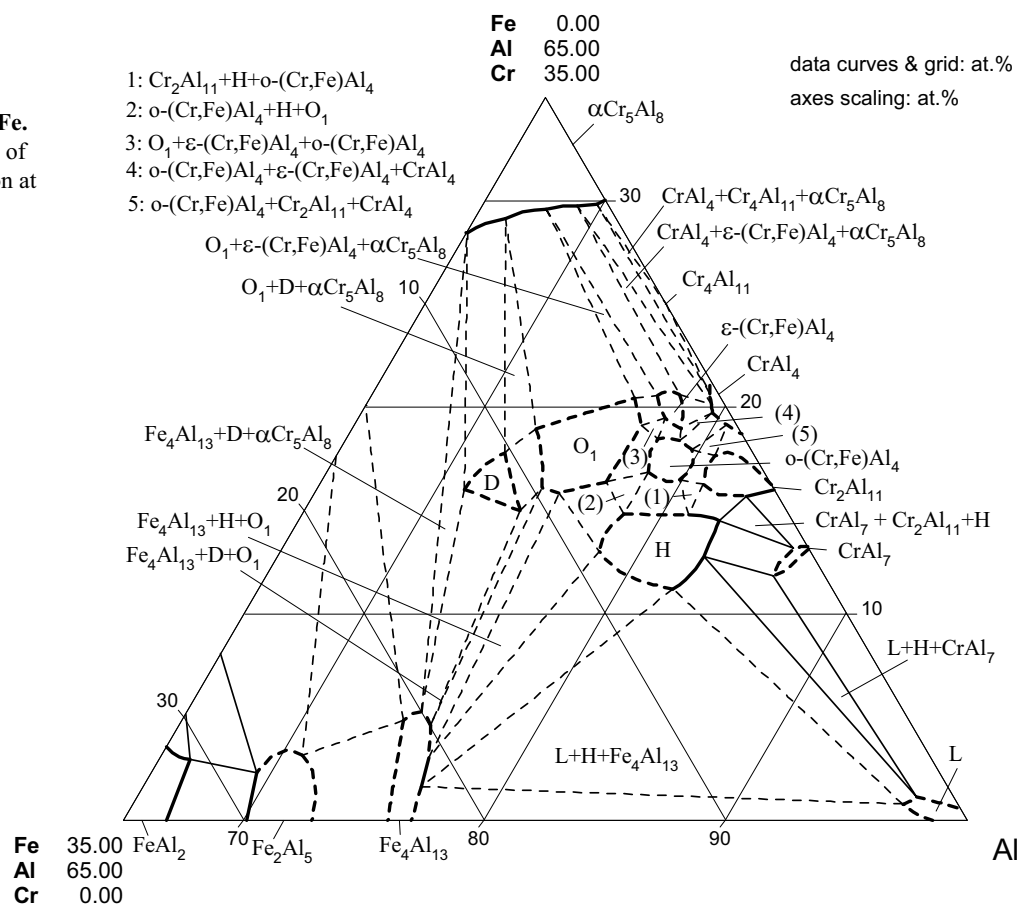


Fig. 13a: Al-Cr-Fe.
Isothermal section at
650°C

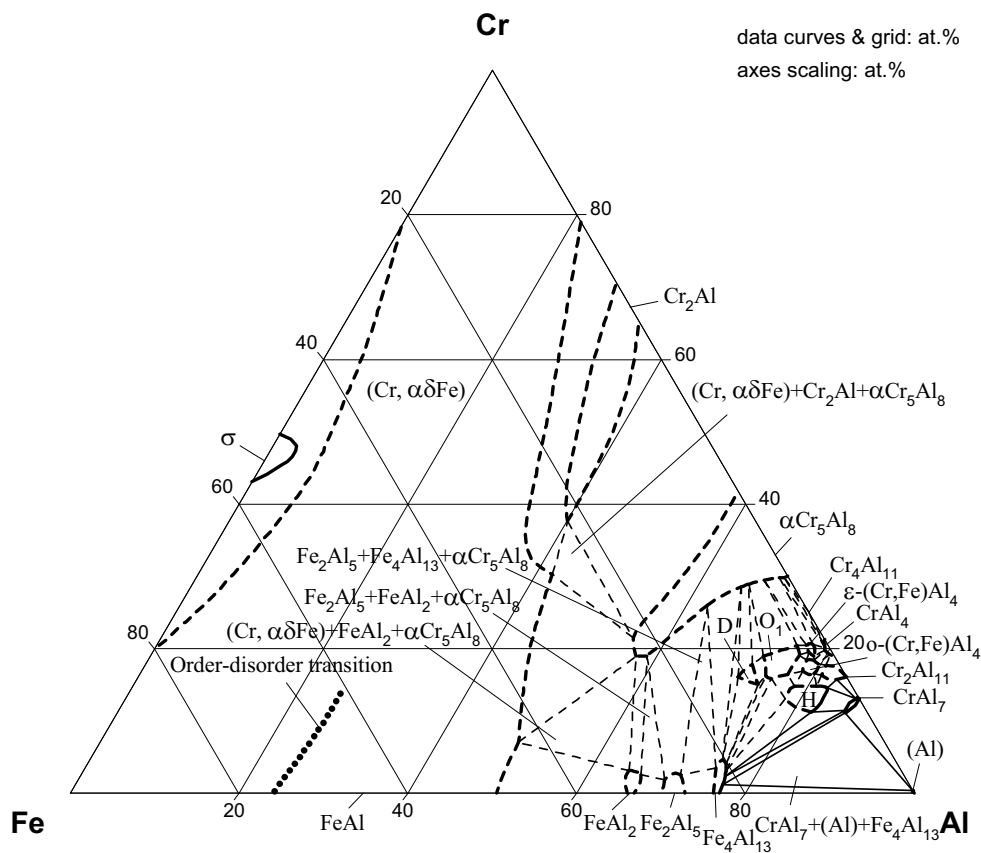


Fig. 13b: Al-Cr-Fe.
Enlarged portion of
isothermal section at
650°C

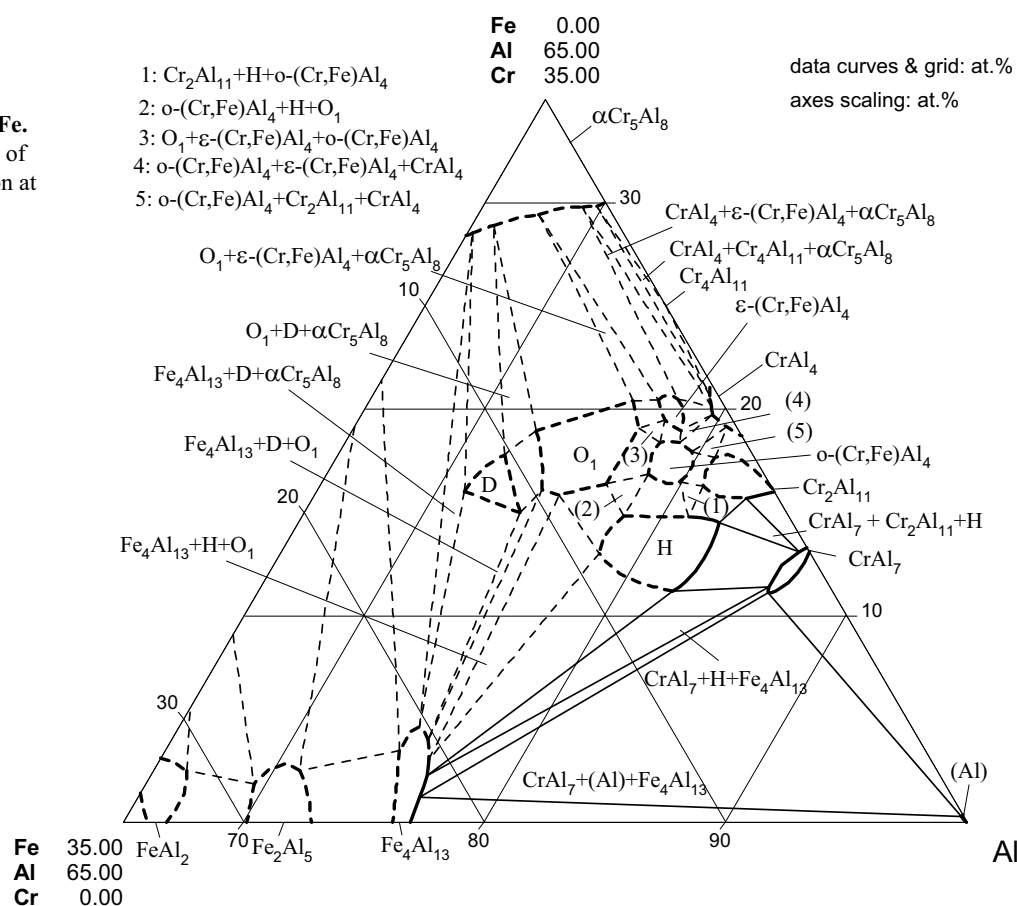


Fig. 14: Al-Cr-Fe.
Partial vertical section
at molar ratio of Fe:Al
as 1:1

