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Metallurgy

On the influence of iron and silicon content on the phase composition of the Al-Fe-Si system

***Andreyachshenko V.A., Toleuova A.R.**

Abylkas Saginov Karaganda Technical University, Karaganda, Kazakhstan

**Corresponding author email: Vi-ta.z@mail.ru*

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ABSTRACT
Increasing interest in intermetallic phases of the Al-Fe-Si system is associated with their high specific strength, corrosion and wear resistance, as well as the low cost of their production. To exhibit the most successful combination of properties, it is necessary to impart a specific compact morphology to the precipitated intermetallic phases. It is important to create an alloy with a composition capable of accepting plastic deformation. The purpose of the work is to develop the composition of an Al-Fe-Si system alloy capable of withstanding plastic deformation and determining the corresponding deformation interval. Based on computer modeling, an alloy composition capable of accepting plastic deformation was developed and the corresponding deformation interval was determined. The simulation was carried out in the ThermoCalc software package, TCAL8 database. It has been revealed that alloys with a high content of both silicon and iron are not characterized by the formation of a single-phase region, however, with a certain combination of alloy components, it is possible to achieve a quasi-single-phase structure, when the content of one phase is observed to be more than 90%. The solidus temperatures for different alloy compositions and the boundary conditions for the existence of phases have been determined. The α phase is present in the system from a temperature of 770°C up to a temperature of 446°C. In composition, it is found in the range from 5 to 35% iron with an amount of silicon of 10% and from 0 to 15% silicon with an iron content of 30%. The maximum amount of α phase was obtained for the Al60-65 alloy; Fe30-32; and Si5-10%, deformation temperature range is 600-450°C. Deformation in this region will ensure processing in a quasi-single-phase region without melting.

Keywords: Al-Fe-Si, ThermoCalc software, intermetallic phases, phase diagram, α phase.

Information about authors:

Andreyachshenko Violetta Alexandrovna
PhD, associate professor, Head of the Testing Laboratory Engineering Profile "Comprehensive Development of Mineral Resources". Abylkas Saginov Karaganda Technical University, N. Nazarbayev Ave., 56, Karaganda, Kazakhstan. E-mail: Vi-ta.z@mail.ru

Toleuova Ainagul Rymkulovna
PhD, associate professor, docent of the Department of Nanotechnology and Metallurgy. Abylkas Saginov Karaganda Technical University, N. Nazarbayev Ave., 56, Karaganda, Kazakhstan. Email: rymkul.ainagul@mail.ru

Introduction

In recent years, many studies have been devoted to the processing and processing of aluminum alloys with a high iron content [1]. At the same time, it is the processing of iron-enriched alloys that claims to be a leader in the field of light metallurgy. The main problem that scientists may encounter when developing technological schemes for processing aluminum alloys is the high iron content, which significantly reduces all the properties of the alloys [2]. In works devoted to the processing of aluminum alloys, attention is paid to alloys containing an increased amount of iron, i.e. 1, 3, 5 and even 10% [[3], [4], [5], [6], [7]]. At the same time, many researchers see a promising direction in applying efforts to transform the needle-shaped β phase into the α phase, which has a more compact morphology [[8], [9], [10], [11]]. It is noted that in alloys with such an iron content, the α phase is the main strengthening phase, and a general increase in strength and thermal stability is realized due to dispersion strengthening. At the same time, there is information that the α phase has very high Vickers hardness values, including in comparison with the β phase. An effective way to suppress the α↔β transformation is also doping with transition metals such as Cr, Mn, Cu, etc., accelerated cooling and exposure to deformation [[12], [13], [14], [15], [16], [17], [18], [19], [20]].

Although Al–Si alloys are the most commonly used aluminum alloys in the foundry industry [21], it is often necessary to use specific processing methods to meet the increasing demands on the performance and properties of these alloys. One of the processing methods is injection molding methods [[22], [23]], while porosity can be successfully controlled by modifying the traditional process with the transition to Two-stage super vacuum (19 mbar) assisted high-pressure die casting (HPDC) [24] or the use of An air-cooled stirring rod (ACSR) process technology [25]. Selective laser melting makes it possible to effectively process aluminum alloys, including those containing high amounts of iron [26]. In addition, additive technologies, which have been intensively developing in recent decades, have proven themselves well. With the high variability of technological conditions, it is possible to obtain both porous and practically monolithic alloys with a wide chemical range of composition [[27, [28], [29], [30]]. Depending on the strengthening mechanism, aluminum alloys are divided into two main groups: heat-strengthening and non-heat-strengthening [31]. Depending on the group, additional post-processing is usually used to increase and stabilize the final properties of the alloy, such as [[32], [33], [34], [35], [36]] and others.

Experimental part

Numerical modeling to study the phase composition of the three-component system was carried out using ThermoCalc software. As part of the study, the Al-Fe-Si system under study was specified for calculation. An important element of the calculations is the identification and assessment of the interaction of the main components of the system. Aluminum was chosen as the base material, because its quantity in the system is maximum. ThermoCalc software version 2024a, TCAL8 database, and version v8.2 were used for modeling. The tools Phase diagram, One Axis, Scheil Solidification, and Ternary calculation were used for the calculation.

Modeling the phase composition of a system begins with the formulation of the problem. The Al-Fe-Si system containing aluminum ≥50% (by weight %) was chosen as the object of study. To build an isothermal section, we performed the following steps: My project→Ternary. Next, we selected the required elements from the table of elements: Al, Fe, Si. The temperature is set to 660°C. After setting the parameters, we moved on to setting the boundary conditions. The iron content is located along the X-axis, from 0 to 50% wt., the silicon content along the Y-axis, from 0 to 50% wt.

To construct polythermal sections, the Phase diagram tool was used: My project → Phase diagram. The required elements are also selected from the table, their quantity is specified in mass percent. When constructing phase diagrams of multicomponent systems, the number of elements other than 2 is constant for calculation. In our case, Si-const=10% and Fe-const=10%. The calculation was carried out using the following parameters: Temperature, °C – 1200°; Pressure, Pascal – 100000; Size of the system, mol – 1.

Estimation of the number of formed phases under given modeling conditions was carried out in a combination of the One Axis and Scheil Solidification tools according to the following scheme: My project → One Axis → Selection of elements and their content in weight % → setting modeling conditions (similar to the previous task) → Interpretation of results.

My project→Scheil Solidification→Selection of elements and their content in weight %→setting modeling conditions→Interpretation of results.

The choice of compositions is explained by the peculiarities of alloy production technology - the fact that the combination of iron and silicon can neutralize the negative impact on mechanical properties with the formation of intermetallic compounds of various types. Therefore, it is necessary to know which iron-containing phases will be formed during the production process. Variation of iron and silicon is necessary to better understand the crystallization intervals and phase transformation of each composition. The simulation was implemented using the ThermoCalc Software 2024a software in the Testing Laboratory Engineering Profile "Comprehensive Development of Mineral Resources" of the Abylkas Saginov Karaganda Technical University, Karaganda, Kazakhstan.

Discussion the results

The literature presents a sufficient number of casting alloys containing silicon and iron, as well as a number of wrought aluminum alloys with these elements. Increasing the level of mechanical properties, heat resistance, wear resistance and a number of other properties is achieved, as a rule, by alloying with various elements, including rare earth ones. Another way to improve the properties of the alloy is by using heat treatment, including thermomechanical treatment. Often the desired level of properties can only be achieved through a combination of chemical alloying and exposure to temperature. At the same time, the main efforts of materials scientists are aimed at purifying the alloy from harmful iron impurities and stabilizing the composition of silicon. Alloys of the Al-Fe-Si system with equiatomic and/or quasi-equiatomic composition have not been sufficiently studied in the literature. We believe that alloys of the Al-Fe-Si system have sufficient potential for use as a structural material capable of being subjected to deformation treatments. However, to ensure the possibility of plastic deformation, a number of conditions must be met, such as:

-increased deformation temperature for transition to a single-phase region, or a region with a predominant one-phase;

- rational composition, which will ensure the formation of a phase with the most compact morphology, or a type of crystal lattice capable of accepting plastic deformation;

- the use of heat treatment, which makes it possible to consolidate or enhance the effect of plastic deformation of an alloy with a rational composition.

At this stage of the work, the authors concentrated their efforts on selecting an alloy composition capable of withstanding plastic deformation and determining the appropriate deformation interval.

Alloys of the Al-Fe-Si system are considered in this work as alloys based on aluminum, i.e. Σ Fe+Si≤50 wt%. In this system, aluminum has the lowest melting point, which is 660°C; an assessment of the phase composition under these conditions (Fig.1) shows that liquid is observed for almost any composition. First of all, crystallization begins with an iron content of more than 40% and a minimum amount of silicon with the release of the primary high-temperature phase θ, which has a monoclinic crystal lattice. This phase exists only when there is a lack of silicon, which is dissolved in the liquid phase

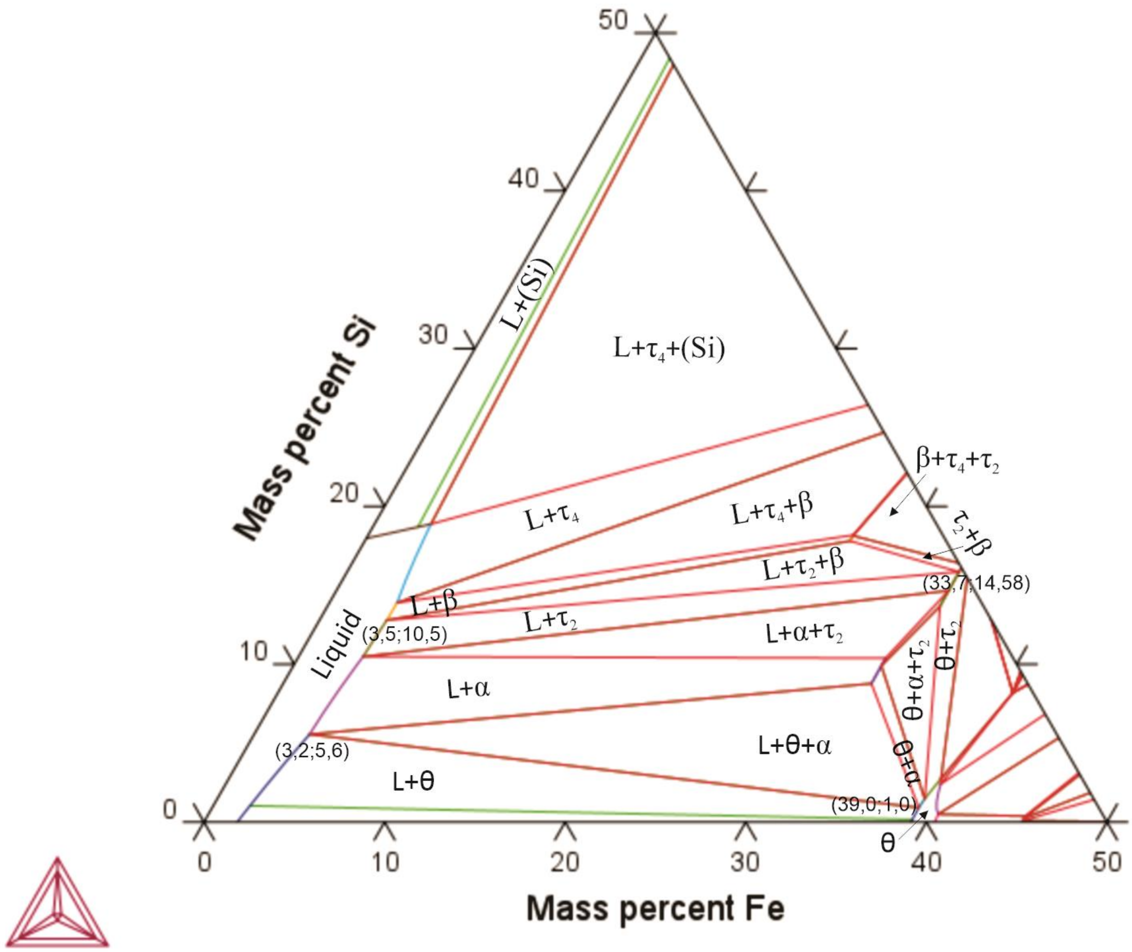

Figure 1 - Isothermal section diagram Al-Si-Fe at 660°C

and in the θ phase, while the solubility in the latter does not exceed 1.5 mol%.

As silicon increases, conditions are created for the formation of ternary intermetallic phases, such as α, then τ2, β and τ4. With an iron content of up to 5%, structurally free silicon is released directly from the melt at a silicon content of 18%. With an increase in the amount of iron, in addition to silicon, the τ4 phase is also formed, the amount of which increases with the amount of iron in the ternary system.

The range of formation of the ternary intermetallic phase α at a temperature of 660°C is limited by the content of iron and silicon as shown in Table 1.

Table 1 - The content of iron and silicon

Phase composition	Composition, wt.%	
	Fe	***Si***
L+α+θ	up 39	from 1
L+α+ $τ_2$	up 33.7	up 14.58
L+α	from 3.5	up 10.5
L+α+θ	from 3.2	from 5.6

In this case, the composition of the α phase remains quite constant and is Al 0.59:Fe 0.32:Si 0.09 wt%, Al 0.70:Fe 0.19:Si 0.11 at%. It is logical to assume that the maximum amount of α phase can be achieved with alloy compositions close to the composition of the α phase.

It is worth noting that the equilibrium α-phase is released only at relatively high temperatures with its further decomposition. To understand the mechanism of formation and decomposition of the α phase, phase diagrams with the base composition Al60-Fe30-Si10 were studied. Two main polythermal sections with fixed values of iron and silicon of 30 and 10%, respectively, are considered (Fig.2 and Fig.3.).

It was revealed that the α phase is present in the system from a temperature of 770°C up to a temperature of 446°C. In composition, it is found in the range from 5 to 35% iron with a fixed amount of silicon of 10% and from 0 to 15% silicon with an iron content of 30%.

Let us consider in more detail the phase transformations in the indicated composition ranges.

Alloys of the Al-Fe-Si system are very sensitive to composition, which manifests itself in a significant change in the phase composition, which, in turn, causes a change in the final properties of the metal. Alloys with a high iron content are particularly sensitive. From the point of view of the level of mechanical properties, the phases formed in a given

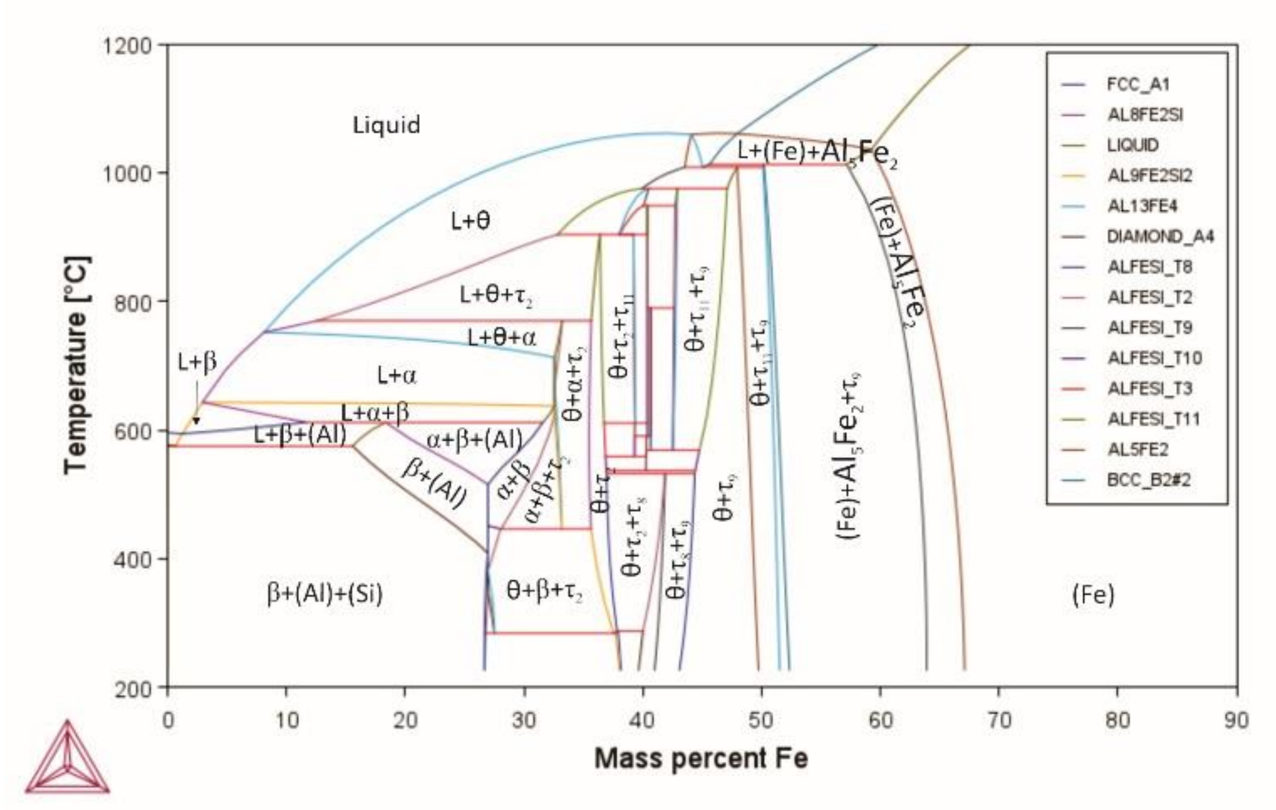

Figure 2 - Polythermal section diagram Al-Si-Fe with Si-const=10%

metal can be divided into harmful and useful. Solid solutions of silicon and iron in aluminum (indicated as (Al) in the figure), silicon and aluminum in iron (indicated as (Fe) in the figure) and the α phase, which exists only at elevated temperatures, can be considered useful. The morphology of the α phase typically has a “Chinese script” shape and is characterized by a hexagonal crystal lattice. With slow cooling, the α phase is transformed into the β phase, which is classified as “harmful” due to its morphology. The β phase is represented predominantly by tube-shaped or needle-shaped particles and is monoclinic. The remaining intermetallic compounds formed have monoclinic, triclinic and orthorhombic crystal lattices. In addition to the indicated phases, a monoclinic double phase θ and structurally free silicon are formed.

With an iron content of less than 26% and 10% silicon at room temperature, the alloy consists of a mechanical mixture of the β phase, an fcc solid solution of aluminum and excess silicon, which is present in the form of structurally free silicon precipitated as inclusions. But in this region, complex processes of dissolution and separation of individual phases are observed at higher temperatures.

When the iron content is less than 44%, the primary high-temperature phase, crystallizing at temperatures below 1065°C, is the monoclinic, iron-depleting liquid θ phase. After sufficient purification of the liquid from iron, the formation of ternary intermetallic phases becomes possible as the temperature decreases. At a high iron content, the intermetallic phase τ11 is released; for this composition, the solidus temperature is 904°C. In this case, the residual liquid after crystallization of the θ phase disintegrates simultaneously with the formation of phases τ2 and τ11, with further rectistallization of the τ11 phase into the τ8 phase. When the amount of iron decreases to 36%, only phases θ and τ2 are formed. When the iron content is 12-36%, in addition to the θ phase, the τ2 phase immediately begins to separate from the liquid, which, with a decrease in temperature and through interaction with the remaining liquid, transforms into the α phase at a temperature of 770°C. In this case, the α phase becomes dominant as the composition of the alloy approaches the composition of the α phase up to 32.5% iron. A decrease in the amount of iron leads to an increase in the proportion of fluid in this area.

For an alloy with a large amount of iron, a temperature of 770°C is the solidus temperature,

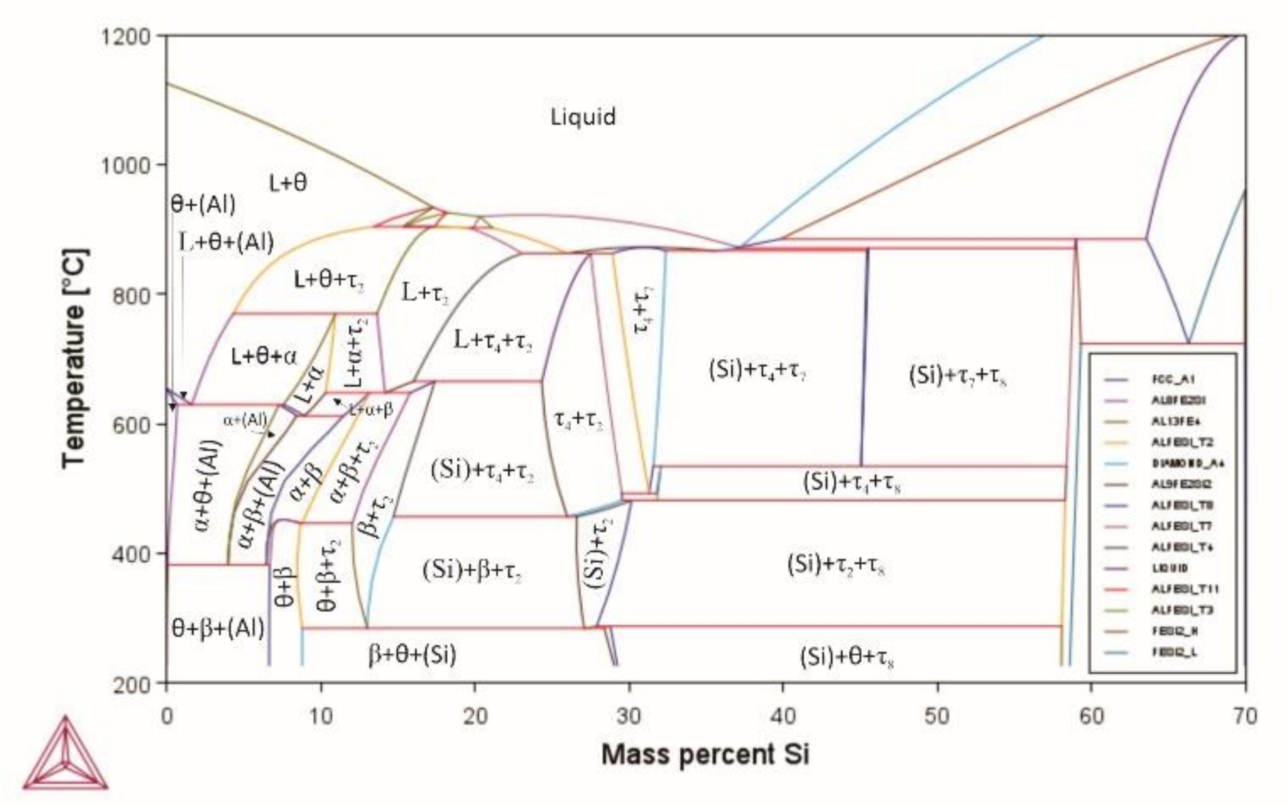

Figure 3 - Polythermal section diagram Al-Si-Fe with Fe-const=30%

and the entire liquid ends up with the composition of the α phase, into which it crystallizes. Subsequently, the α↔β transition occurs at a temperature of 446°C. This is the boundary of the existence of phase α. With iron content in the range of 8-12%, i.e. If the iron/silicon ratio = 1 is observed, phases α and θ are released directly from the liquid. For alloys with an iron content of less than 35% and temperatures below 715°C, the θ phase either does not form or completely dissolves. Alloys with an iron content of 1-3% are characterized by the release of β phase crystals directly from the liquid at temperatures below 642 ° C; with a further decrease in temperature, crystallization of the fcc solid solution of silicon and iron in aluminum begins.

An iron content of less than 1% with a silicon amount of 10% leads to the formation of a minimum melting temperature, which is 595°C, which is lower than the melting point of pure aluminum, with the crystallization of the aluminum fcc solid solution immediately. When the solubility limit of silicon in aluminum is reached with a further decrease in temperature, structurally free silicon precipitates in the form of inclusions (at temperatures below 580°C). In this case, the release of silicon particles is observed in up to 40% of iron.

When examining the phase diagram with an amount of iron of 30% (Fig.3), it is clear that structurally free silicon will be present in the microstructure of the metal already at a silicon content of 11.5%, and even at high temperatures it will not be completely dissolved. The θ phase is released when there is an excess of iron. It crystallizes from liquid primarily at iron/silicon ratios >2. As the amount of silicon increases, intermetallic compounds are formed that bind both silicon and iron. At room temperature, the θ phase is observed at silicon contents up to 11.5. The aluminum solid solution completely transforms into intermetallic compounds when the silicon content is more than 8%. The solidus temperatures were as follows: 629°C with a silicon content of 0.5-7.5, 613°C with a silicon content of 8.5-11.5%, 646°C with a silicon content of 13-16%, 665°C, with a silicon content of 17-24%, 862°C with a silicon content of 27-29% and 872°C with an iron/silicon ratio of 1:1, with 30% silicon.

The α phase is observed in the alloy containing 4.3-13.5 in the temperature range below 770°C, while the lower temperature limit of the α phase in the range of 8-12% is 446°C, and for the range of 0.06-6.7% silicon –382°C. It can be seen that the α phase for all compositions is present together with other phases, such as aluminum solid solution, β, τ2 phases and liquid.

In order to provide the alloy with the greatest ductility, it is preferable to carry out deformation in a single-phase region, or with a minimum amount of the second phase. Therefore, to optimize the composition, modeling was performed with a quantitative assessment of the phases formed when the temperature changes with varying number of alloy components. The variation was carried out with a step of 5. The variation conditions, temperature parameters and modeling results are shown in Table 2.

Analysis of the data obtained indicates that the determining factor in the formation of the phase composition is the content of elements, while a significant amount of α-phase is observed at an aluminum content of 60-65%, iron ~30%, and silicon 5-10%. It is noted that for the Al60-Fe30-Si10 composition the maximum concentration of the α phase is observed at a temperature of 662°C and reaches a concentration of 87%, and for the Al65-Fe30-Si5 composition the maximum concentration reaches 89% at a temperature of 510°C. Thus, reducing the amount of silicon to 5% while increasing aluminum leads to a decrease in the lower limit by 65° and an increase in the upper limit by 50°C.

Table 2 - Batch parameters and quantitative assessment

№	**Content of main elements, %**			**α-phase quantity, %**	**Temperature conditions, °C**
	Al	***Fe***	***Si***		
1	60	30	10	87	725-450
2	60	20	20	-	
3	60	10	30	-	
4	60	35	5	60	780-450
5	60	25	15	15	640-620
6	60	29	1	20	620-380
7	50	30	20	-	
8	50	20	30	-	
9	50	35	15	-	
10	50	25	15	15	640-620
11	50	35	5	65	760-450
12	55	35	10	25	780-450
13	50	35	15	-	
14	65	30	5	89	775-385
15	70	25	5	70	745-385

In this case, a further increase in aluminum concentration to 70%, on the contrary, causes a decrease in the amount of α phase.

When the silicon content exceeds 15% or more, a sharp decrease in the amount of the α phase is observed, but a decrease in silicon of less than 5% also leads to a decrease in its amount. It is worth noting that iron and silicon have a complex effect, and their amount should be close to the composition of the α phase. Oscillations of even 5% already have a significant impact on the phase relationship.

Thus, the composition of the Al60-65 alloy was adopted as the most optimal; Fe30-32; Si5-10%, deformation temperature range is 600-450°C. Deformation in this region will provide processing in a quasi-single-phase region without melting.

Conclusions

By constructing diagrams of the Al-Fe-Si system, the phase composition and kinetics of phase separation were revealed, the boundary conditions for the existence of phases were determined for a wide range of compositions, and the liquidus, solidus and solvus temperatures were identified. With an aluminum content of 60-65%, iron ~30%, and silicon 5-10%, the amount of α-phase reaches 87-89%. An increase in aluminum content to more than 70% causes a decrease in the amount of α phase in favor of an fcc solid solution of silicon and iron in aluminum. In this case, the aluminum solid solution completely transforms into intermetallic compounds with a silicon content of more than 8% in the presence of iron. A quasi-single-phase region with a phase composition that provides susceptibility to plastic deformation has been found. The temperature range of deformation is 600-450°C without melting. The most optimal composition of the alloy is Al60-65; Fe30-32; Si5-10%.

Conflict of interest. On behalf of all authors, the corresponding author declares that there is no conflict of interest.

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Al-Fe-Si жүйесінің фазалық құрамына темір мен кремний құрамының әсері туралы

Андреященко В.А., Толеуова А.Р.

Әбілқас Сағынов атындағы Қарағанды техникалық университеті, Қарағанды, Қазақстан

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ТҮЙІНДЕМЕ

Al-Fe-Si жүйесінің интерметалдық фазаларына қызығушылықтың артуы олардың жоғары меншікті беріктігімен, коррозияға және тозуға төзімділігімен, сондай-ақ оларды өндірудің төмен құнымен байланысты. Қасиеттердің ең сәтті комбинациясын көрсету үшін тұндырылған интерметалдық фазаларға нақты ықшам морфологияны беру қажет. Пластикалық деформацияны қабылдауға қабілетті құрамы бар қорытпаны жасау маңызды. Жұмыстың мақсаты - пластикалық деформацияға төтеп беруге қабілетті Al-Fe-Si жүйесі қорытпасының құрамын жасау және сәйкес деформация аралығын анықтау. Компьютерлік модельдеу негізінде пластикалық деформацияны қабылдауға қабілетті қорытпа композициясы әзірленді және сәйкес деформация аралығы анықталды. Модельдеу ThermoCalc бағдарламалық пакетінде, TCAL8 деректер базасында жүргізілді. Құрамында кремнийдің де, темірдің де мөлшері жоғары қорытпалар бір фазалы аймақтың түзілуімен сипатталмайтыны анықталды, алайда қорытпа компоненттерінің белгілі бір комбинациясы кезінде бір фазаның мөлшері 90% -дан жоғары болған кезде квази-бірфазалы құрылымға қол жеткізуге болады. Әртүрлі қорытпалар құрамы үшін солидус температуралары және фазалардың болуының шекаралық шарттары анықталды. α фазасы жүйеде 770°C температурадан 446°C температураға дейін болады. Құрамында кремний мөлшері 10% болатын 5-тен 35%-ға дейін темір және 30% темір мөлшерімен 0-15% кремний аралығында кездеседі. α фазасының максималды мөлшері Al60-65 қорытпасы үшін алынды; Fe30-32; Si5-10% қорытпаларында деформация температурасының диапазоны 600-450°C болады. Бұл аймақтағы деформация балқымай-ақ квази-бірфазалы аймақта өңдеуді қамтамасыз етеді.

Түйін сөздер: Al-Fe-Si, ThermoCalc бағдарламалық қамтамасыз ету, металаралық фазалар, фазалық диаграмма, α фаза.

Авторлар туралы ақпарат:

Андреященко Виолетта Александровна — *PhD, қауымдастырылған профессор, "Минералдық шикізат қазбаларды кешенді игеру" инженерлік бейіндегі сынақ зертханасының басшысы. Әбілқас Сағынов атындағы Қарағанды техникалық университеті, Н. Назарбаев даңғылы, 56, Қарағанды, Қазақстан. Email: Vi-ta.z@mail.ru*

Толеуова Айнагуль Рымкуловна — *PhD, қауымдастырылған профессор, Нанотехнология және металлургия кафедрасының доценті, Әбілқас Сағынов атындағы Қарағанды техникалық университеті, Н.Назарбаев даңғылы, 56, Қарағанды, Қазақстан. Email: rymkul.ainagul@mail.ru*

О влиянии содержания железа и кремния на фазовый состав системы Al-Fe-Si

Андреященко В.А., Толеуова А.Р.

Карагандинский технический университет имени Абылкаса Сагинова, Караганда, Казахстан

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АННОТАЦИЯ

Возрастающий интерес к интерметаллидным фазам системы Al-Fe-Si связан с их высокой удельной прочностью, коррозионной и износостойкостью, а также низкой стоимостью их изготовления. Для проявления наиболее удачного сочетания свойств необходимо придание специфической компактной морфологии выделяющимся интерметаллидным фазам. Актуально создание сплава с составом, способным воспринимать пластическую деформацию. Цель работы разработать состав сплава системы Al-Fe-Si, способного воспринимать пластическую деформацию и определить соответствующий интервал деформирования. На основе компьютерного моделирования разработан состав сплава, способного воспринимать пластическую деформацию и определен соответствующий интервал деформирования. Моделирование осуществлялось в программном комплексе ThermoCalc, база данных TCAL8. Выявлено, что для сплавов с высоким содержанием как кремния, так и железо не характерно формирование однофазной области, однако при определенном сочетании компонентов сплава удается достичь квази однофазной структуры, когда наблюдается содержание одной фазы более чем на 90%. Определены температуры солидуса для различного состава сплава, граничные условия существования фаз. α фаза присутствует в системе с температуры 770°C вплоть до температуры 446°C. По составу она обнаруживается в диапазоне от 5 до 35 % железа при количестве кремния 10% и от 0 до 15% кремния при содержании железа 30%. Максимальное количество α фазы получено для сплава Al60-65; Fe30-32; Si5-10%, температурный интервал деформирования составляет 600-450°C. Деформирование в данной области обеспечит обработку в квазиоднофазной области без оплавления.

Ключевые слова: Al-Fe-Si, программное обеспечение ThermoCalc, интерметаллидные фазы, фазовая диаграмма, α-фаза.

Информация об авторах:

Андреященко Виолетта Александровна — *PhD, ассоциированный профессор, руководитель испытательной лаборатории инженерного профиля «Комплексное освоение ресурсов минерального сырья», Карагандинский технический университет имени Абылкаса Сагинова, пр. Н. Назарбаева, 56, Караганда, Казахстан. Email: Vi-ta.z@mail.ru*

Толеуова Айнагуль Рымкуловна — *PhD, ассоциированный профессор, доцент каф. нанотехнологии и металлургии. Карагандинский технический университет имени Абылкаса Сагинова, пр. Н. Назарбаева, 56, Караганда, Казахстан. Email: rymkul.ainagul@mail.ru*

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