Ternary Alloys

Volume 21

MSI
Science Simplified

Ternary Alloys Series

A Comprehensive Compendium of Evaluated Constitutional Data and Phase Diagrams

critically evaluated by MSIT®

"Ternary Alloys" is the result of an international assessment program performed by Materials Science International Services GmbH and its international Team (MSIT®).

The phase diagram evaluations in this publication have been carefully reviewed by the MSIT® review board on behalf of Materials Science International Services GmbH, and are presented as the most accurate and reliable information available on the subject.

The first 15 volumes of the Ternary Alloys series were published originally by VCH (1988-1995). In 1999, all rights and the previously published volumes were transferred to MSI GmbH, whose team (MSIT®) had produced the content. A new ISBN has been assigned to each of these volumes. From volume 16, MSI GmbH continues as publisher of the series.

List of published Ternary Alloys volumes:

Ag-X-Y category (vols. 1 & 2)
Vol. 1: Ag-Al-Au to Ag-Cu-P
Vol. 2: Ag-Cu-Pb to Ag-Zn-Zr

Al-X-Y category (vols. 3 to 8)
Vol. 3: Al-Ar-O to Al-Ca-Zn
Vol. 4: Al-Cd-Ce to Al-Cu-Ru
Vol. 5: Al-Cu-S to Al-Gd-Sn
Vol. 6: Al-Gd-Tb to Al-Mg-Sc
Vol. 7: Al-Mg-Se to Al-Ni-Ta
Vol. 8: Al-Ni-Tb to Al-Zn-Zr

As-X-Y category (vols. 9 to 11)
Vol. 9: As-Au-Ca to As-Zn-Zr
Vol. 10: As-Cr-Fe to As-I-Zn
Vol. 11: As-In-Ir to As-Yb-Zn

Au-X-Y category (vols. 12 & 13)
Vol. 12: Au-B-Co to Au-Ge-La
Vol. 13: Au-Ge-Li to Au-Tl-Zn

Li-X-Y category (vols. 14 & 15)
Vol. 14: Ag-Al-Li to Ge-Li-Nd
Vol. 15: Ge-Li-Ni to Li-V-Zr

Mg-X-Y category (vols. 16 to 18)
Vol. 16: Ag-Al-Mg to Bi-Mg-Zr
Vol. 17: Br-Cs-Mg to Ge-Mg-Yb
Vol. 18: H-K-Mg to Mg-Zn-Zr

Vol. 19: Selected Systems for Nuclear Applications.
Vol. 20: Selected Systems for Lead-free Soldering and Brazing Applications
Vol. 21: Selected Al-Fe-X Ternary Systems for Industrial Applications

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

Editors
Frank Stein, Martin Palm

Associate Editors
Liya Dreval, Oleksandr Dovbenko, Svitlana Iljenko

Authors
Materials Science International Team, MSIT®

MSI
Science Simplified

Editors: Frank Stein,
Martin Palm
Associate Editors: Liya Dreval
Oleksandr Dovbenko
Svitlana Iljenko

ISBN 978-3-932120-51-0

Vol. 21. Selected Al-Fe-X Ternary Systems for Industrial Applications. – 2022

This volume is part of the book series:
Ternary Alloys: A Comprehensive Compendium of Evaluated Constitutional Data and Phase Diagrams/
Materials Science International Services GmbH, Stuttgart, Germany

Group ISBN for the Ternary Alloys book series: 978-3-932120-41-1

Published by
MSI, Materials Science International Services GmbH, Stuttgart (Federal Republic of Germany)
Am Wallgraben 100, D-70565 Stuttgart, Germany
Postfach 800749, D-70507, Stuttgart, Germany
http://www.msiport.com
http://www.msi-eureka.com/

Printed on acid-free paper.

Printing and binding:
WIRmachenDRUCK GmbH, Mühlbachstraße 7, 71522 Backnang

Printed in the Federal Republic of Germany

Authors: Materials Science International Team, MSIT®

This volume results from collaborative evaluation programs performed by MSI and authored by MSIT®. In this program, data and knowledge are contributed by many individuals and have accumulated over almost thirty five years, up to the present day. The content of this volume is a subset of the ongoing MSIT® Evaluation Programs. Authors of this volume are:

Nataliya Bochvar, Moscow, Russia
Anatoliy Bondar, Kyiv, Ukraine
Gabriele Cacciamani, Genova, Italy
Lesley Cornish, Johannesburg, South Africa
Oleksandr Dovbenko, Stuttgart, Germany
Liya Dreval, Stuttgart, Germany
Yong Du, Changsha, China
Kiyaasha Dyal Ukabhai, Johannesburg, South Africa
Olga Fabrichnaya, Freiberg, Germany
Lorenzo Fenocchio, Genova, Italy
Sergio Gama, Campinas, Brasil
Gautam Ghosh, Evanston, USA
Bernd Grieb, Tübingen, Germany
Kiyohito Ishida, Sendai, Japan
Hermann A. Jehn, Stuttgart, Germany
Kostyantyn Korniyenko, Kyiv, Ukraine
Mario J. Kriegel, Freiberg, Germany
Ortrud Kubaschewski†, Aachen, Germany
K.C. Hari Kumar, Chennai, India
Bernard Legendre, Paris, France
Xiaojing Li, Changsha, China
Shuhong Liu, Changsha, China
Xing Jun Liu, Sendai, Japan
Annelies Malfliet, Heverlee, Belgium
Niraja Moharana, Chennai, India
Martin Palm, Düsseldorf, Germany
Jian Peng, Wuhan, China
Pierre Perrot, Lille, France
Alexander Pisch, Grenoble, France
Qingsheng Ran, Stuttgart, Germany
Maximilian Rank, Karlsruhe, Germany
Peter Rogl, Vienna, Austria
Lazar Rokhlin, Moscow, Russia
Rainer Schmid-Fetzer, Clausthal-Zellerfeld, Germany
Frank Stein, Düsseldorf, Germany
Vasyl Tomashyk, Kyiv, Ukraine
Lyudmila Tretyachenko†, Kyiv, Ukraine
Mikhail Turchanin, Kramatorsk, Ukraine
Oksana Tymoshenko, Kyiv, Ukraine
Thomas Vaubois, Chatillon, France
Alexander Walnsch, Freiberg, Germany
Chuanbin Wang, Wuhan, China
Cui Ping Wang, Sendai, Japan
Junjun Wang, Wuhan, China
Andrew Watson, Chesterfield, UK
Liming Zhang, München, Germany

Institutions

The content of this volume is produced by MSI, Materials Science International Services GmbH and the international team of materials scientists, MSIT®. Contributions to this volume have been made from the following institutions:

Baikov Institute of Metallurgy and Materials Science, Russian Academy of Science, Moscow, Russia

Central South University, Research Institute of Powder Metallurgy, State Key Laboratory for Powder Metallurgy, Changsha, China

Donbas State Engineering Academy, Department of Technology and Equipment of Foundry, Kramatorsk, Ukraine

Hampton Thermodynamics Ltd, Basingstoke, UK

I.M. Frantsevich Institute for Problems of Materials Science, National Academy of Sciences, Kyiv, Ukraine

Indian Institute of Technology Madras, Department of Metallurgical Engineering, Chennai, India

Institute for Semiconductor Physics, National Academy of Sciences, Kyiv, Ukraine

Katholieke Universiteit Leuven, Department Metaalkunde en Toegepaste Materiaalkunde, Heverlee, Belgium

Karlsruher Institut für Technologie (KIT), Institut für Angewandte Materialien - Angewandte Werkstoffphysik (IAM-AWP), Karlsruhe, Germany

Université Paris-Sud, Faculté de Pharmacie, Chatenay-Malabry, Paris, France

Magnequench Europe, Tübingen, Germany

Materials Science International Services GmbH, Stuttgart, Germany

Max-Planck-Institut für Eisenforschung GmbH, Department of Structure and Nano/Micromechanics of Materials, Düsseldorf, Germany

Max-Planck-Institut für Metallforschung, Institut für Werkstoffwissenschaften, Stuttgart, Germany

Northwestern University, Department of Materials Science and Engineering, Evanston, USA

ONERA - The French Aerospace Lab, Departement Materiaux et Structures Metalliques, Unite Materiaux et Microstructures (MMS), Chatillon, France

RWTH Aachen, Metallurgie der Kernbrennstoffe und Theoretische Hüttenkunde, Aachen, Germany

SIMaP (UMR5266-UGA/CNRS/Grenoble INP), Thermodynamics and Process Optimization Department, Grenoble, France

Technische Universität Clausthal, Institut für Metallurgie, Clausthal-Zellerfeld, Germany

TU Bergakademie Freiberg, Institut für Werkstoffwissenschaft, Freiberg, Germany

Tohoku University, Department of Materials, Science Graduate School of Engineering, Sendai, Japan

Universidade Estadual de Campinas Insituto de Fisica “Gleb Wataghin” DFESCM Campinas – SP, Brazil

Universität München, Institut für Kristallographie und Angewandte Mineralogie, München, Germany

Universita di Genova, Dipartimento di Chimica, Genova, Italy

Universität Wien, Institut für Physikalische Chemie, Wien, Austria

University of the Witwatersrand, DST/NRF Centre of Excellence in Strong Materials, Johannesburg, South Africa

Wuhan Institute of Technology, Engineering Research Center of Environmental Materials and Membrane Technology of Hubei Province, School of Materials Science and Engineering, Wuhan, China

Wuhan University of Technology, State Key Lab of Advanced Technology for Materials Synthesis and Processing, Wuhan, China

About the *Ternary Alloys* book series

The book series *Ternary Alloys* provides reliable and comprehensive descriptions of materials constitution, based on the critical and intellectual evaluation of all relevant data available at the time. Data from different sources are carefully compared and assessed, and their compatibility with the accepted edge binary systems is checked in order to produce a single set of information that is internally consistent and represents the state of knowledge of that ternary system. Ternary systems are chosen mainly for their application in alloy development, but others are chosen because they have gained scientific interest in their own right. In any one ternary material system, however, one may find a number of alloys that can be used for a variety of different applications, depending on the chosen composition.

Reliable phase diagrams provide scientists and engineers with basic information of critical importance for fundamental research and for the development and optimization of materials. So, collections of such diagrams are extremely useful, if the data on which they are based have been subjected to critical evaluation, as in these volumes. Critical evaluation means: where contradictory information is published, data and conclusions are analyzed, broken down into firm facts and re-interpreted in the light of all present knowledge. Depending on the information available this can be a very difficult task. Critical evaluation establishes descriptions of phase configurations and related data that are reliable.

The evaluations are performed by MSIT®, the Materials Science International Team, a group of scientists working together since 1984. Within this team, skilled expertise is available covering a broad range of methodologies, materials and applications. This joint competence is employed in the critical evaluation of the often-conflicting literature data. A particularly useful tool at the disposal of the MSIT is the ability to perform targeted thermodynamic and atomistic calculations for individual equilibria, driving forces and also for complete phase diagram sections, that can provide additional insight when trying to reconcile conflicting data.

Conclusions on phase equilibria may be drawn from direct observations, *e.g.* by microscopy, from monitoring caloric or thermal effects, or measuring properties such as electrical resistivity, electro-magnetic or mechanical properties. Other examples of useful methods in materials chemistry are mass-spectrometry, thermo-gravimetry, the measurement of electro-motive forces, and X-ray and microprobe analyses. In each published case the applicability of the chosen methodology has to be validated, the way of actually performing the experiment or computer modeling has to be assessed as well and the interpretation of the results with regard to the material chemistry. Thus, an understanding of the materials constitution and phase reactions is gained from many distinctly different types of experiments, calculations and observations. Intellectual critical evaluations which interpret all data simultaneously reveal the chemistry of the materials system best.

An additional degree of complexity is introduced by the material itself, as the state of the material under observation depends heavily on its history, in particular with regard to homogenization, thermal and mechanical treatments. All of this is taken into account in an MSIT® expert evaluation.

To include binary data in a ternary evaluation is mandatory. Each of the three-dimensional ternary phase diagrams has edge binary systems as boundary planes; their data have to match the ternary data smoothly. At the same time each of the edge binary systems A-B is a boundary plane for many other ternary A-B-X systems. Therefore, combining systematically binary and ternary evaluations increases confidence and reliability in both ternary and binary phase diagrams. This began systematically for the first time in the frame of the MSIT® Evaluation Program. The degree of success, however, depends on both the nature of materials and scientists!

The multitude of correlated or inter-dependent data requires that special care be taken. Within MSIT® an evaluation routine has been established that is knowledge driven, and applies both human based expertise and electronically formatted data together with software tools. MSIT® internal discussions take place during almost all of the evaluations. In this way, the efforts of the individual are supplemented with the expertise of a team. In some cases,

the authors of earlier publications have contributed to the whole knowledge base by making their original data records available for re-interpretation. All evaluation reports published here have undergone a thorough peer-review process in which the reviewers had access to all the original data.

In its publications, MSIT® has adopted a standard format that presents the reader with the data for each ternary system in a concise and consistent manner, as applied in the MSI Eureka data base. The standard format and special features of the *Ternary Alloys* compendium are explained in the Introduction to this volume.

In spite of the skill and labor that have been put into this volume, it will not be faultless. All criticisms and suggestions that can help us to improve our work are very welcome. Please contact us via evaluation@msiport.com. We hope that this volume will prove to be as useful for materials scientists and engineers as the other volumes of *Ternary Alloys* and all previous works of MSIT® have been. We hope that this volume will be well received by our colleagues in research and industry.

Starting with the Volume 19, MSI has changed slightly the concept of the series "*Ternary Alloys*". Instead of exploring alphabetically all ternary systems based on one chemical element, such as Al-X-Y or Mg-X-Y, the subsequent volumes are dedicated to particular classes of materials or particular application areas, as volume 21 - "Selected Al-Fe-X Ternary Systems for Industrial Applications" with the guest editors Dr. Frank Stein and Dr. Martin Palm.

Preface

Fe-Al-based materials are an economic alternative to Cr-Ni steels and Ni-based superalloys for structural applications. They are also the basis of corrosion- and wear-resistant coatings and magnetic materials, *e.g.* Heusler alloys. In addition, they are applied in catalysis and hydrogen generation and storage, and in many systems quasicrystalline phases form, which exhibit remarkable properties. This volume of the MSI book series Ternary Alloys summarizes and critically analyses the knowledge on phase equilibria and phase transitions of 22 ternary application-related iron-aluminium-based systems that are of interest for the development of Fe-Al-based alloys for industrial use. It also includes a new critical assessment of the binary Fe-Al system.

Fe-Al-based materials have been of interest for structural applications for more than a century. Interest started about 1900 with the discovery of their outstanding oxidation resistance. Application-oriented alloy developments can be traced back to the 1930´s and major efforts towards industrialization of Fe-Al-based alloys were performed in the 1950´s and 1980´s. However, insufficient strength at elevated temperatures and lack in ductility at room temperature were major drawbacks, which ended those efforts. As at that time even phase equilibria in the binary Al-Fe system had not been settled and only little information about phase equilibria and phase transformations in ternary Al-Fe-X systems was available, a targeted improvement of these shortcomings was not possible.

Materials based on intermetallic phases can offer a high ratio of strength in relation to their density. Therefore, specifically the Al-containing intermetallics with Ni, Ti, and Fe became of interest from the 1970´s onwards, when energy saving became a crucial issue. In the wake of these developments, research on phase equilibria of respective systems intensified, which led to more aimed alloy developments, *i.e.* by designing specific microstructures to enhance strength at high temperature or for improving ductility.

The outcome of those "phase-diagram-based" alloy developments were Fe-Al-based materials, whose strength matches those of high-strength steels or even some Ni-based superalloys. Besides their satisfactory strength, these alloys are also characterized by low density, high wear resistance, good tribological properties, and an outstanding corrosion resistance. These improved properties and the demand for more sustainable materials lead to widespread industrial activities in exploiting the potential of iron aluminides. As iron and aluminium are the most abundant metals in the earth´s crust and as properties can already be tuned by comparable small alloying additions, the resulting low materials costs are specifically attractive for looking at these materials in more detail.

Knowledge of Al-Fe-X systems plays also an important role in the development of various coatings. Understanding the complex phase equilibria and kinetics in the Al-Fe-Zn system is the basis for galvanizing of steels. For corrosion resistant coatings for higher temperatures the Al-Cr-Fe system is of great importance and the low coefficients of friction make iron aluminides also interesting candidates for the developments of wear-resistant coatings.

In view of functional applications, Heusler phases are an important class of intermetallic phases because of their magnetic and thermoelectric properties or their spintronic behavior. Heusler phases are stable or metastable in many Al-Fe-X systems, *e.g.* with X = Ti, V, Mn, Co, Ni, Cu, Nb, Ta…, and specifically Fe_2CuAl has achieved a widespread usage. Quasicrystals, which form in the Al corner of many of the Al-Fe-X systems discussed here, also exhibit a wide range of beneficial properties, including low electrical and thermal conductivity, good oxidation resistance, and high hardness.

Catalytic properties, *e.g.* of Fe_4Al_{13}, the possibilities for hydrogen generation (Al-Fe-Sn), absorption or desorption (Al-Fe-Ti), and extended solid solubility ranges in many systems, *e.g.* with Ti, Cr, Co, Ni…, which are the basis for the development of so-called chemically complex alloys (CCAs, also termed high-entropy alloys HEAs) are other features that are already exploited.

The current compendium critically evaluates and summarizes all the available knowledge on phase equilibria, phase transformations, crystallographic details of the phases and their known properties and applications of 22 Al-Fe-X systems, which are important for industrial applications.

The editors are indebted to all authors and reviewers who made it possible to realize this volume. Specific thanks are due to MSI, who granted, organized the review, and managed the publication.

Frank Stein and Martin Palm August 2022

Contents

Ternary Alloys
A Comprehensive Compendium of Evaluated Constitutional Data and Phase Diagrams

Volume 21
Selected Al-Fe-X Ternary Systems for Industrial Applications

Introduction
- General . . . XII
- Structure of a System Report . . . XII
  - Introduction . . . XII
  - Binary Systems . . . XII
  - Solid Phases . . . XII
  - Quasibinary Systems . . . XIII
  - Invariant Equilibria . . . XIII
  - Liquidus, Solidus, Solvus Surfaces . . . XIV
  - Isothermal Sections . . . XIV
  - Temperature – Composition Sections . . . XIV
  - Thermodynamics . . . XIV
  - Notes on Materials Properties and Applications . . . XIV
  - Miscellaneous . . . XIV
  - References . . . XIV
- General References . . . XVIII

Ternary Systems
- Al – Fe (Aluminium – Iron) . . . 1
  Frank Stein
- Al – B – Fe (Aluminium – Boron – Iron) . . . 39
  Peter Rogl
- Al – C – Fe (Aluminium – Carbon – Iron) . . . 51
  Gautam Ghosh, updated by Oksana Tymoshenko, Anatolii Bondar, Oleksandr Dovbenko
- Al – Co – Fe (Aluminium – Cobalt – Iron) . . . 73
  Hari K.C. Kumar, Martin Palm, Maximilian Rank, Alexander Walnsch, Andy Watson; updated by Martin Palm
- Al – Cr – Fe (Aluminium – Chromium – Iron) . . . 100
  Kostyantyn Korniyenko, Liya Dreval
- Al – Cu – Fe (Aluminium – Copper – Iron) . . . 147
  Cui Ping Wang, Xing Jun Liu, Liming Zhang, Kiyohito Ishida, updated by Niraja Moharana and K C Hari Kumar
- Al – Fe – Hf (Aluminium – Iron – Hafnium) . . . 180
  Frank Stein
- Al – Fe – Mn (Aluminium – Iron – Manganese) . . . 188
  Qingsheng Ran, Alexander Pisch, updated by Alexander Walnsch and Mario J. Kriegel
- Al – Fe – Mo (Aluminium – Iron – Molybdenum) . . . 213
  Junjun Wang, Jian Peng, Chuanbin Wang
- Al – Fe – N (Aluminium – Iron – Nitrogen) . . . 227
  Hermann A. Jehn, Pierre Perrot, updated by Vasyl Tomashyk
- Al – Fe – Nb (Aluminium – Iron – Niobium) . . . 240
  Annelies Malfliet, Frank Stein, Thomas Vaubois, K.C. Hari Kumar; updated by Frank Stein
- Al – Fe – Ni (Aluminium – Iron – Nickel) . . . 266
  Gabriele Cacciamani, Lorenzo Fenocchio, Liya Dreval
- Al – Fe – O (Aluminium – Iron – Oxygen) . . . 315
  Ortrud Kubaschewski†, Rainer Schmid-Fetzer, Lazar Rokhlin, Lesley Cornish, Olga Fabrichnaya updated by Liya Dreval

Al – Fe – P (Aluminium – Iron –Phosphorus) 352
Rainer Schmid-Fetzer, updated by Vasyl Tomashyk and Liya Dreval
Al – Fe – S (Aluminium – Iron – Sulfur) 368
Natalie Bochvar, Bernard Legendre, Ortrud Kubaschewski†, updated by Lesley Cornish, Kiyaasha Dyal Ukabhai, Andy Watson
Al – Fe – Si (Aluminium – Iron – Silicon) 381
Gautam Ghosh, updated by Xiaojing Li, Shuhong Liu, Yong Du, Mikhail Turchanin and Liya Dreval
Al – Fe – Sn (Aluminium – Iron – Tin) 437
Sergio Gama, Bernd Grieb and Lyudmila Tretyachenko†, updated by Martin Palm
Al – Fe – Ta (Aluminium – Iron – Tantalum) 447
Anatolii Bondar, Oksana Tymoshenko, Oleksandr Dovbenko
Al – Fe – Ti (Aluminium – Iron – Titanium) 474
Frank Stein, Kostyantyn Korniyenko
Al – Fe – V (Aluminium – Iron – Vanadium) 516
Gautam Ghosh, updated by Kostyantyn Korniyenko
Al – Fe – W (Aluminium – Iron – Tungsten) 537
Frank Stein
Al – Fe – Zn (Aluminium – Iron – Zinc) 541
Gautam Ghosh, updated by Martin Palm
Al – Fe – Zr (Aluminium – Iron – Zirconium) 569
Frank Stein