

Determination of the Partial Structure Factors of the Metallic Glass $\text{Fe}_{58}\text{B}_{22}$

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By X-ray diffraction and neutron diffraction using the isotopic substitution method, the partial structure factors S_{FeFe} , S_{FeB} , and S_{BB} as well as S_{FeC} , S_{FeC} , and S_{BC} were determined for the metallic glass $\text{Fe}_{58}\text{B}_{22}$. The Fourier-transforms yielded the pair correlation functions C_{ij} from which the atomic distances and the partial coordination numbers were calculated. The partial coordination numbers are in good agreement with those of the metastable Fe_2B -phase, which is the first crystallization product formed during annealing of the metallic glass $\text{Fe}_{58}\text{B}_{22}$. The chemical short range order parameter amounts to 100%, thus indicating perfect chemical order.

Introduction

It is the aim of the present paper to investigate by means of diffraction experiments the mutual distribution of the components in the metallic glass $\text{Fe}_{58}\text{B}_{22}$. For this purpose three independent diffraction experiments have to be performed, in each of which the ratio of the scattering powers of Fe and B must be different. This can be achieved either by applying different radiations or by using isotopes with different scattering lengths in preparing samples with the same chemical composition for neutron scattering experiments. In the present work both methods have been combined.

Theoretical Fundamentals

We will only present a short compilation of the equations needed for the evaluation of the three partial structure factors. For a comprehensive presentation see Refs. [1] to [4]. The scattering behaviour of an isotropic binary molten or amorphous alloy can be described by three partial structure factors $S_{ij}(Q)$, where $S_{ij}(Q) = S_{ji}(Q)$. From these partial functions the total function can be obtained

$$\begin{aligned} S(Q) &= \frac{c_A^2 b_A^2}{\langle b \rangle^2} S_{AA}(Q) + \frac{c_B^2 b_B^2}{\langle b \rangle^2} S_{BB}(Q) \\ &+ \frac{2 c_A c_B b_A b_B}{\langle b \rangle^2} S_{AB}(Q) \\ &= W_{AA} S_{AA}(Q) + W_{BB} S_{BB}(Q) \\ &+ W_{AB} S_{AB}(Q) \end{aligned} \quad (1)$$

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with c_i concentration of component i in atomic fractions, b_i scattering length of the atoms of component i , $\langle b \rangle = c_A b_A + c_B b_B$.

The total structure factor $S(Q)$ is obtained from the coherently scattered intensity per atom $I_n(Q)$ which follows from the measured intensity by a correction- and normalization-procedure. The following equation stands according to the Faber-Ziman definition [5]:

$$S(Q) = \frac{I_n(Q) - \text{LMS}}{\langle b \rangle^2}. \quad (2)$$

The Laue monotonic scattering LMS

$$\text{LMS} = \langle b^2 \rangle - \langle b \rangle^2 = c_A c_B \langle b \rangle^2 \quad (3)$$

is regarded as part of the coherent scattering and is subtracted in (2). The LMS is observed in the unmodulated form given by (3) if the atoms of both components with their different scattering lengths are distributed statistically within the global structure (see for example [6]).

According to Ashcroft and Langreth [7] a total structure factor for a binary system can also be defined in the following way:

$$S_{\text{AL}}(Q) = I_n(Q)/\langle b^2 \rangle. \quad (4)$$

By this procedure the LMS is not subtracted and there is a normalization to $\langle b^2 \rangle$ and not to $\langle b \rangle^2$ as in (3).

In neutron diffraction experiments with materials containing atoms M with a magnetic moment an additional scattering contribution $I_m(Q)$ will occur which has its origin in the interaction of the magnetic moments of neutrons and the atoms M :

$$I_m(Q) = P^2(Q) S_{MM}(Q) \sin^2 \alpha \quad (5)$$

Methods In The Determination Of Partial Structure Factors

Pavel Ivanovich Bystrov

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Methods in the Determination of Partial Structure Factors,1993 [Determination of Organic Structures by Physical Methods V3](#) F.C. Nachod,2012-12-02 Determination of Organic Structures by Physical Methods Volume 3 is a seven chapter text that describes the refinements of some established physical methods for organic structure determination Each chapter of this book examines specific physical method including photoelectron spectroscopy X ray diffraction optical rotary dispersion circular dichroism mass spectrometry and electron spin resonance and NMR spectroscopies The historical developments instrumentation and applications to organic chemistry of these methods are discussed This work will be of value to organic and analytical chemists and researchers

Methods In The Determination Of Partial Structure Factors Of Disordered Matter By Neutron And Anomalous X-ray Diffraction - Proceedings Of The Ill/esrf Workshop

Jens-boie Suck,Christian Riekel,D Raoux,P Chieux,1993-08-12 [Neutron Scattering in Earth Sciences](#) Hans Rudolf Wenk,2018-12-17

Volume 63 of Reviews in Mineralogy and Geochemistry provides an introduction for those not yet familiar with neutrons by describing basic features of neutrons and their interaction with matter as well illustrating important applications The volume is divided into 17 Chapters The first two chapters introduce properties of neutrons and neutron facilities setting the stage for applications Some applications rely on single crystals Chapter 3 but mostly powders Chapters 4 5 and bulk polycrystals Chapters 15 16 are analyzed at ambient conditions as well as low and high temperature and high pressure Chapters 7 9 Characterization of magnetic structures remains a core application of neutron scattering Chapter 6 The analysis of neutron data is not trivial and crystallographic methods have been modified to take account of the complexities such as the Rietveld technique Chapter 4 and the pair distribution function Chapter 11 Information is not only obtained about solids but about liquids melts and aqueous solutions as well Chapters 11 13 In fact this field approached with inelastic scattering Chapter 10 and small angle scattering Chapter 13 is opening unprecedented opportunities for earth sciences Small angle scattering also contributes information about microstructures Chapter 14 Neutron diffraction has become a favorite method to quantify residual stresses in deformed materials Chapter 16 as well as preferred orientation patterns Chapter 15 The volume concludes with a short introduction into neutron tomography and radiography that may well emerge as a principal application of neutron scattering in the future Chapter 17

Spectroscopic Methods in Mineralogy and Material Sciences

Grant Henderson,Daniel Neuville,Robert Downs,2014-11-21 Spectroscopic Methods in Mineralogy and Material Science covers significant advances in the technological aspects and applications of spectroscopic and microscopic techniques used in the Earth and Materials Sciences The current volume compliments the now classic Volume 18 Spectroscopic Methods in Mineralogy and Geology which became an essential resource to many scientists and educators for the past two decades This volume updates techniques covered in Volume 18 and introduces new techniques available for probing the secrets of Earth materials such as X ray Raman and Brillouin spectroscopy Other important topics including

Transmission Electron Microscopy TEM and Atomic Force Microscopy AFM are also covered *Proceedings of the ILL/ESRF Workshop on Methods in the Determination of Partial Structure Factors of Disordered Matter by Neutron and Anomalous X-Ray Diffraction, Grenoble, France, 10-11 September 1992* J. B. Suck, 1993 **Modern Diffraction Methods** E. J. Mittemeijer, U. Welzel, 2013-02-04 The role of diffraction methods for the solid state sciences has been pivotal to determining the micro structure of a material. Particularly the expanding activities in materials science have led to the development of new methods for analysis by diffraction. This book offers an authoritative overview of the new developments in the field of analysis of matter by in particular X-ray electron and neutron diffraction. It is composed of chapters written by leading experts on modern diffraction methods. The focus in the various chapters of this book is on the current forefront of research on and applications for diffraction methods. This unique book provides descriptions of the state of the art and at the same time identifies avenues for future research. The book assumes only a basic knowledge of solid state physics and allows the application of the described methods by the readers of the book either graduate students or mature scientists.

Amorphous Structures Dietrich Schulze, 1990 Treatise on Process Metallurgy, Volume 1: Process Fundamentals, 2013-11-20 Process metallurgy provides academics with the fundamentals of the manufacturing of metallic materials from raw materials into finished parts or products. Coverage is divided into three volumes entitled Process Fundamentals encompassing process fundamentals extractive and refining processes and metallurgical process phenomena. Processing Phenomena encompassing ferrous processing, non-ferrous processing and refractory reactive and aqueous processing of metals and Industrial Processes encompassing process modeling and computational tools, energy optimization, environmental aspects and industrial design. The work distils 400 years combined academic experience from the principal editor and multidisciplinary 14 member editorial advisory board providing the 2 608 page work with a seal of quality. The volumes will function as the process counterpart to Robert Cahn and Peter Haasen's famous reference family Physical Metallurgy 1996 which excluded process metallurgy from consideration and which is currently undergoing a major revision under the editorship of David Laughlin and Kazuhiro Hono publishing 2014. Nevertheless process and extractive metallurgy are fields within their own right and this work will be of interest to libraries supporting courses in the process area. Synthesizes the most pertinent contemporary developments within process metallurgy so scientists have authoritative information at their fingertips. Replaces existing articles and monographs with a single complete solution saving time for busy scientists. Helps metallurgists to predict changes and consequences and create or modify whatever process is deployed **Amorphous Metals and Semiconductors** P. Haasen, R. I. Jaffee, 2013-10-22 Amorphous Metals and Semiconductors contains the proceedings of an international workshop held at Coronado California USA on May 12-18 1985. Organized into five parts this book first looks into the historical perspective on semiconductors and metals. This book then explains the glass formation, magnetic glasses and amorphous semiconductors. The mechanical and chemical properties of these materials are also given.

Microscopic Methods in Metals Ulrich Gonser, 2012-12-06 Methods of scientific investigation can be divided into two categories they are either macroscopic or microscopic in nature The former are generally older classical methods where the sample as a whole is studied and various local properties are deduced by differentiation The microscopic methods on the other hand have been discovered and developed more recently and they operate for the most part on an atomistic scale Glancing through the shelves of books on the various scientific fields and in particular on the field of physical metallurgy we are surprised at how little consideration has been given to the microscopic methods How these tools provide new insight and information is a question which so far has not attracted much attention Similar observations can be made at scientific conferences where the presentation of papers involving microscopic methods is often pushed into a far corner This has led users of such methods to organize their own special conferences The aim of this book is to bridge the present gap and encourage more interaction between the various fields of study and selected microscopic methods with special emphasis on their suitability for investigating metals In each case the principles of the method are reviewed the advantages and successes pointed out but also the shortcomings and limitations indicated

Treatise on Process Metallurgy Roderick Guthrie, Alexander McLean, Sridhar Seetharaman, H. Y. Sohn, 2024-01-25 Treatise on Process Metallurgy Volume One Process Fundamentals provides academics with the fundamentals of the manufacturing of metallic materials from raw materials into finished parts or products In these fully updated volumes coverage is expanded into four volumes including Process Fundamentals encompassing process fundamentals structure and properties of matter thermodynamic aspects of process metallurgy and rate phenomena in process metallurgy Processing Phenomena encompassing interfacial phenomena in high temperature metallurgy metallurgical process phenomena and metallurgical process technology Metallurgical Processes encompassing mineral processing aqueous processing electrochemical material and energy processes and iron and steel technology non ferrous process principles and production technologies and more The work distills the combined academic experience from the principal editor and the multidisciplinary four member editorial board Provides the entire breadth of process metallurgy in a single work Includes in depth knowledge in all key areas of process metallurgy Approaches the topic from an interdisciplinary perspective providing broad range coverage on topics

Structural Studies of Liquids and Glasses Using Aerodynamic Levitation Thomas Farmer, 2014-07-07 This thesis presents neutron scattering data that contribute to the understanding of four distinct areas of condensed matter physics including iso compositional liquid liquid phase transitions and the glass formation in rare earth doped BaTi₂O₅ In situ aerodynamic levitation with laser heating was combined with neutron scattering in order to study both liquid liquid phase transitions in Y₂O₃ x Al₂O₃ 1 x and the atomic and magnetic ordering in liquid Invar Among several significant results obtained in this case from small angle neutron scattering was the absence of a phase transition across a range of temperatures and compositions in the yttria aluminates As these are a principal system in which liquid liquid phase transitions have been hypothesized this is an important contribution in a

contentious area *Zeitschrift für Naturforschung*, 1985 *Structural Evolution in Materials* Naohiro Igata, Omourtague Dimitrov, 1995 *Structure and Motion in Molecular Liquids*, 1978 Liquid-metal Coolants for Heat Pipes and Power Plants Pavel Ivanovich Bystrov, 1990 This work on liquid metal coolants contains knowledge concerning heat pipe properties and specifics and also on Soviet and Western monographs that would provide a uniform approach to the problem of validating the use of liquid metal coolants for heat pipes and energetics **Periodico di mineralogia**, 1991 *Methods in the Determination of Partial Structure Factors* J. B. Suck, B. Maier, 1993 *Amorphous Metallic Alloys* F. E. Luborsky, 1983 Index of amorphous alloys

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