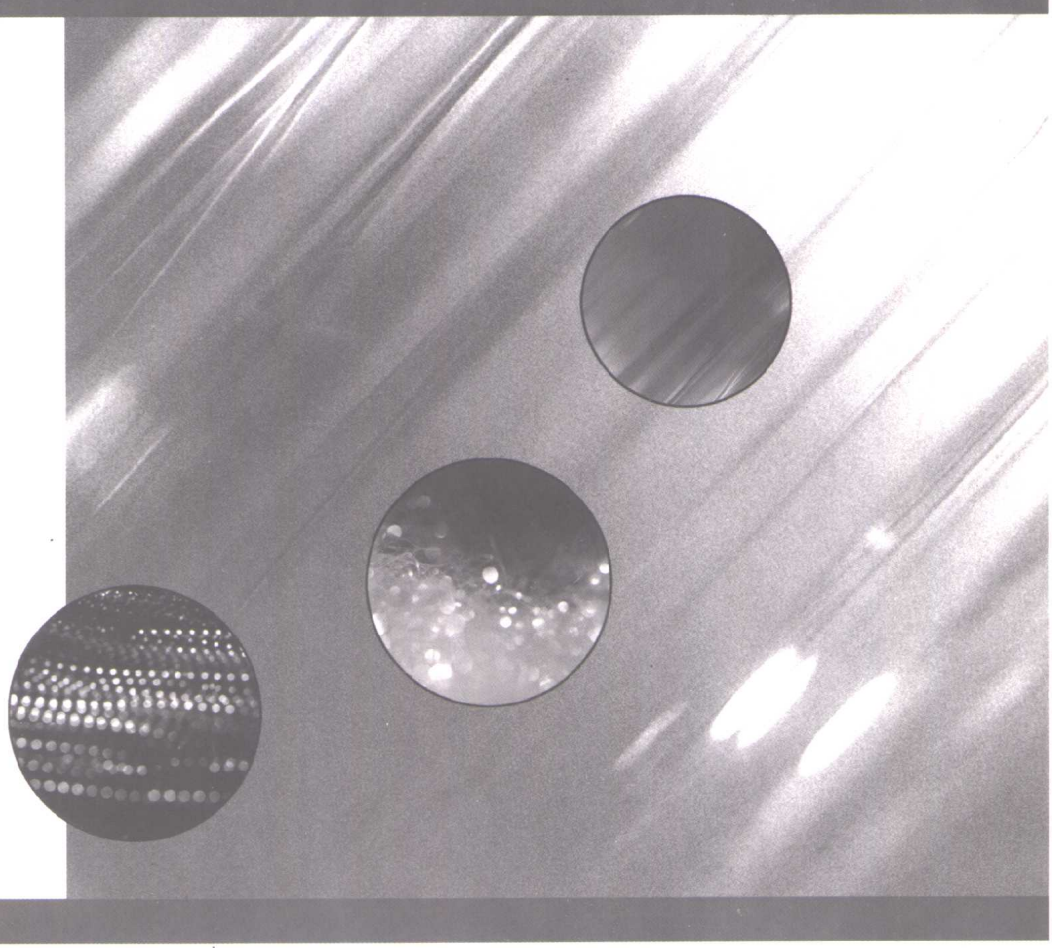
HEJINXIANG LILUN YU FEIJING TAI HEJIN CAILIAO

ZHANGBANGWEI LUNWENJI

张邦维论文集

合金相理论与非晶态合金材料



湖南大学出版社

合金相理论与非晶态合金材料
——张邦维论文集

Theory of Alloy Phases and Amorphous Alloy materials
—Selected papers for Zhang Bangwei

张邦维 著

湖南大学出版社

2001年·长沙

内 容 简 介

全书编选了作者已发表的论文50篇。包括四个方面的内容：一是合金相理论，包括非晶态合金形成理论、固溶体理论及合金形成热的热力学计算，二是原子尺度计算材料科学——分析型嵌入原子方法理论及其应用；三是非晶态合金及纳米固体粉末材料，包括液态淬火非晶态合金材料，化学镀非晶态合金镀层及合金和氧化物陶瓷纳米固体粉末材料；四是合金表面溅射与表面聚集以及热电转换材料等。

本书可供从事物理学、材料科学和工程、化学以及与材料紧密相关的工程学科等领域的高等院校师生和科研工作者参考。

图书在版编目(CIP)数据

合金相理论与非晶态合金材料：张邦维论文集/张邦维著 —长沙：湖南大学出版社，2001.12

ISBN 7-81053-432-7

Ⅰ合… Ⅱ张… Ⅲ.①合金相—论文集②非晶态合金材料—研究—论文集 Ⅳ TG14-53

中国版本图书馆CIP数据核字(2001)第083164号

合金相理论与非晶态合金材料
——张邦维论文集

Hejinxiang Lilun Yu Feijingtai Hejin Cailiao
——Zhang Bangwei Lunwenji

张邦维 著

□责任编辑 卢 宇 张高明
□装帧设计 吴颖辉
□出版发行 湖南大学出版社
社址 长沙市岳麓山 邮码 410082
电话 0731-8821691 0731-8821315
□经 销 湖南省新华书店
□印 装 核工业中南306印刷厂

□开本 787×1092 16开 □印张 25 □字数 640千
□版次 2001年12月第1版 □2001年12月第1次印刷
□书号 ISBN 7-81053-432-7/TG·4
□定价 60.00元

前　言

本论文集是我迄今为止在国内外学术刊物上所发表科研论文的选编。共选入 50 篇，其中用中文发表的 4 篇，英文的 46 篇；国内学术刊物发表的 13 篇，国际的 37 篇；SCI 和/或 EI 收录的 42 篇，未收录的 8 篇。其内容与我所从事的科研领域相同，属于材料物理，包括在材料科学与工程之内。细分一下，包括四个方面。一是合金相理论，包括非晶态合金形成理论、固溶体理论以及合金形成热的热力学计算。二是原子尺度计算材料科学——分析型嵌入原子方法理论及其应用。三是非晶态合金及纳米固体粉末材料，包括液态淬火非晶态合金材料，化学镀非晶态合金镀层以及合金和氧化物陶瓷纳米固体粉末材料。四是合金表面溅射与表面聚集以及热电转换材料等。

在合金相理论研究中，提出了非晶态合金形成理论(纯 Miedema 坐标理论以及化学坐标理论)，能够对液态淬火(LQ)方法、离子束混合(IBM)方法、离子注入(II)方法以及机械合金(MA)方法等多种制备方法所形成的非晶态合金进行理论描述，而且都有定量的描述方程式，使之在同类型理论中具有了自己的特色。所提出的键参数函数和尺寸因素方法固溶体理论对 56 种基体金属的近 4 000 种二元合金的固溶度进行了系统研究，这是自 20 世纪 30 年代英国科学家 Hume-Rothery 对固溶度进行开创性研究，60 年代美国科学家 Waber 和 Gschneidner 运用 Darken 和 Gurry 的 D-G 图形方法研究了近 1 500 种合金固溶度以来更为全面、系统和有成效的研究，所得定量方程式的物理意义进一步深化，与实验结果符合的程度进一步提高。

计算材料科学的出现和兴起，将以往基本上是实验的材料研究推入了更为深刻、更加快速的研究轨道，确立了自己的学科地位并正在欣欣向荣地发展着。介于宏观热力学和第一原理电子层次计算材料科学之间的原子尺度计算材料科学的代表理论是 20 世纪 80 年代中期在美国最先提出的嵌入原子方法（EAM）模型。考虑到它的原型计算复杂性，难于系统化和推广应用，美国弗吉尼亚大学材料科学系的 Johnson 教授自 20 世纪 80 年代末开始提出分析型嵌入原子方法（AEAM）理论。当时我正在该系合作研究，有幸结识了 Johnson 教授和他的 AEAM 理论。回国后的这些年，针对 AEAM 理论存在的问题，我和合作者提出了改进分析型嵌入原子方法（MAEAM）理论。该理论能够统一地对各种结构的金属及其合金进行描述，现在已对各种典型晶体结构金属的一些性质，比如缺陷性能，特别是对它们合金的热力学性质，进行了首次系统有成效的计算。目前该理论正在深入研究和完善中，有望在原子尺度计算材料方面建立起应用广泛的理论。

非晶态合金及纳米固体粉末材料，是我科研工作的另一个重头戏。主要是针对材料科研前沿某些先进材料进行较系统的基础性研究，以期为新材料的发展提供新的科学数据和

新概念。比如，液态淬火非晶态材料研究主要集中于 Cu-P 基二元、三元及四元非晶合金态焊料的基础性能，包括系统地研究结构和非晶形成区、热稳定性、晶化、润湿性能和力学性能以及稀土元素的影响等，所得到的不少新结果丰富了这方面的科学数据。化学镀非晶态合金镀层方面，我主要集中于新型合金镀层的制备和基础研究。在 Ni 基合金镀层研究中，我先后首次制备研究了 Ni-Sn-P，Ni-Sn-Cu-P 和 Ni-Cu-B 非晶态合金镀层。我找到了制备 Fe-B 基合金镀层的方法，制备和系统研究了二元 Fe-B，三元 Fe-W-B 和 Fe-Mo-B 以及四元 Fe-W-Mo-B 合金镀层，为化学镀合金镀层开拓了新生面。纳米固体粉末方面，我进行了化学还原方法和机械合金化制备合金纳米粉末，以及溶胶-凝胶方法制备氧化物陶瓷纳米粉末的研究。包括 Fe-Cr-B 和 Fe-Ni-P-B 合金粉末、Zr 基合金粉末、Cu-Sn-P 合金粉末以及 $MgO\text{-}Al_2O_3$ 和 $MgO\text{-}Y_2O_3\text{-}Al_2O_3$ 氧化物陶瓷纳米粉末的制备、结构和性能研究。这些合金或氧化物系统纳米粉末是我们首先制备的。它们的研究结果为科学数据库增添了新的内容。

合金表面溅射和表面聚集是我作为客座教授在德国等离子体物理研究所合作科研时所进行的课题。不论是两相合金 AgNi 系的研究，还是非晶态 CuTi 合金系，特别是它从非晶态转变为晶态的表面溅射和表面聚集研究，都是文献上所没有进行过的。它们的研究和所得到的结果为合金表面聚集的研究增添了新内容。我受聘于美国弗吉尼亚大学材料科学系作为高级科学家时所从事的合作科研课题是热电转换材料 Si-Ge 和 Si-Ge-GaP 合金，所找到的双层 W 接触材料就是高温下也具有低的接触电阻，为热电转换材料提高输出效率提供了支持。

早在远古的石器、青铜器和铁器时代，我们的祖先就受益于他们自己在材料方面的新发现和发明，创造了辉煌的历史和灿烂的文明。今天，在新的 21 世纪，新材料仍然是人类文明再进一步高度发展不可或缺的重点科学技术之一。作为一个献身于教育和科学的人，几十年来，奋斗于材料科学领域之中，已感到很荣幸，如果我的研究为材料科学贡献了一点什么的话，那就更是心热了，因为我的劳动与人类密不可分的科学技术相联系。

科学要求为其奋斗和献身者必须老老实实，兢兢业业，严肃认真，一丝不苟。我在自己的科研活动中之所以能一贯如此，与我过去的老师，特别是多年来一直保持着联系的老师和前辈对我的教育和影响紧密相关，是他们的引导使我培养起一个科学工作者必备的素养。在我的研究中，特别是实验研究，由于实验设备的不足和经费的短缺，经常求援于同行、朋友和以前的同学，而他们总是有求必应，或减价或只收取成本费或干脆无偿相助进行我们无力进行的有关测试和实验。借此机会向他们表示衷心感谢。我在国家自然科学基金委员会，原国家机械部以及湖南省科委申请获准了多项科研课题，没有这些课题经费的支持，这些研究成果是难以取得的。我先后两次到美国弗吉尼亚大学材料科学系和德国等离子体物理研究所进行合作科研，他们都提供了资助，因而才使合作研究得以顺利进行并取得成果，在此表示感谢。我的大部分研究课题是我的研究生们及研究组中的同事共同进

行的，对本论文集中论文的选定，他们提出了很好的意见，并对所选定的部分论文进行了内容和文字上的再审定，使得原发表论文中尚存在的个别错误能得以改正。感谢他们的劳动、支持和帮助。

我出身于长满青苔的湘西南偏僻秀美的山村，是父母的养育，兄弟姐妹的支持和帮助，才使我得以成长，是他们的伟大亲情才使我成了在众兄弟姐妹中惟一有机会迈进神圣科学殿堂的人，这种伟大的亲情令我永世不忘。此刻，我要特别感谢与我朝夕相处的夫人，同时非常怀念我那过早仙逝的发妻，她们的帮助、支持、关怀和鼓励是我能够取得科研成果的重要保证和必要条件，她们功不可灭！

最后，我要感谢湖南大学出版社，是他们的劳动才使本论文集得以出版和面世。

限于水平，本论文集中难免有差错和不妥之处，敬请专家同行和广大读者不吝赐教。

张　邦　维

于岳麓山下

2001 年 4 月 6 日

Foreword

The papers in this selected works are selected from the author's published scientific papers in the national and international academic magazines. Only 50 papers are selected because of limited space. 4 papers are published in Chinese and 46 papers are published in English; 13 papers are published in the national and 37 ones in the international magazines; and 42 papers are but 8 papers are not cited by SCI and/or EI. The content of these papers is consisted with my research fields, which belongs to the materials physics that is involved in the materials science and engineering. They can divide into four classes. The first is the theory of alloy phases, which consists of the formation theory of amorphous alloys, the theory of solid solution and calculations of the enthalpies of alloys with thermodynamic theory. The second is the calculated materials science at the atomic level, which is the modified analytic embedded atomic method model and its applications. The third is the amorphous alloy and nano-size solid powder materials, which consist of the amorphous alloy materials prepared by melt quenching, amorphous alloy electroless deposits, and nano-size solid powder materials of alloys and oxides. The last one is the surface segregation and sputtering of alloys, thermal-electron transition materials and etc.

The formation theory of amorphous alloys (pure Miedema coordinate and chemical coordinate theories) is proposed in the theory of alloy phases, which can describe theoretically the amorphous alloys prepared by various methods such as liquid quenching (LQ), ion beam mixing (IBM), ion implantation (II) and mechanical alloying (MA). There are quantitative equations in the theories, which indicates its special features compared to the similar theories. As for the theory of solid solution cooperated with the bond-parameters and size factor developed by the author is concerned, near 4000 solid solubilties of binary alloys based on the 56 metals have been studied systematically. This is a more complete, systematical and successful study on the theory of solid solubility since Hume-Rothery studied originally the solid solubilitites of alloys in the 30 years of twenty century, and Waber and Gschenidner studied near 1500 solid solubilities of binary alloys with the so-called D-G graph by Darken and Gurry in 60 years of twenty century. The obtained quantitative equation for describing the solid solubilities by the author has more distinct physical meaning, and the agreement compared to the experimental data is improved further.

Since the calculated materials science is established and developed, the study of materials has changed its researching method from the original basically experimental study to theoretical calculation and experimental studies together. Therefore, its research is more deep and fast. Today, the calculated materials science is developed prosperous. The representative theory of calculated materials science at the atomic level, which is between the calculated materials sciences at the macroscopic thermodynamic theory and at the first principle i. e. electron level, is the embedded atomic method (EAM) theory proposed by American scientists in the middle of 80 years of twenty century. Considering its calculation of original EAM theory is rather complicated and it is rather difficult to systematize and apply for, Professor Johnson in the Department of Materials Science, Virginia University of America developed the analytic EAM

model (AEAM) from the last years of 80 years of twenty century. I just worked in the Department at that time, so I had the honor of making the acquaintance of him and his AEAM theory. Because the AEAM is still having its problems and shortcomings, so I and my students proposed and developed the modified analytic EAM (MAEAM) theory based on the original EAM and AEAM in the passed years after I returned to China. The MAEAM can describe analytically and systematically the various typical structure metals and their alloys. Up to date, we have calculated some properties of the metals and their alloys, such as the defect nature, thermodynamic properties etc. successfully and systematically first time. This theory is developing deeply and completely, and a theory of calculated materials science at the atomic level with wide applications would be developed and expected.

Another important research field of mine is the amorphous and nano-size solid powder materials. The main contents in the field investigate the fundamental research systematically for some advanced materials in the frontier research of materials science in order to provide the scientific data and new idea for the development of novel materials. For example, the research in the amorphous materials prepared by liquid quenching concentrates on the basic properties, including studying the structures and amorphous formation range, thermal stability, crystallization, wettable and mechanical properties, and effect of rare-earth elements on the properties for the binary, ternary and quaternary Cu-P based alloys of amorphous brazing. The new results obtained by us in this aspect enhance the scientific data for the amorphous materials by LQ. As for the amorphous electroless deposits of alloys, we concentrate on the study of preparation and basic properties for new alloy deposits. We first prepared and studied Ni-Sn-P, Ni-Sn-Cu-P and Ni-Cu-B amorphous alloy deposits in the Ni based alloy deposits. We found how to prepare the Fe-B based alloy deposits by electroless, and studied the binary Fe-B, ternary Fe-W-B, Fe-Mo-B and quaternary Fe-W-Mo-B deposits, thereby a new field of electroless plating has been created and developed. In the nano-size powders, we studied the preparation, structure and properties of the nano-size solid powders of alloys by chemical reduction and mechanical alloying, and the nano-size solid powders of oxides by sol-gel method. The content consists of Fe-Cr-B and Fe-Ni-P-B alloy powders, Zr based alloy powders, Cu-Sn-P alloy powders, and MgO-Al_2O_3 and MgO-Y_2O_3 – Al_2O_3 nano-size powders of oxides. All of these nano-size solid powders are prepared first time by us. The results gained from the studying these powders therefore enrich new content for the scientific data in such aspect.

Surface segregation and sputtering of alloys were the content of the collaboration project when I worked at the Max-Planck-Institut für Plasmaphysik, West Germany as a visiting professor from 1987 to 1989. Not only the study of surface segregation and sputtering for the two-phase Ag-Ni alloy system, but also for the amorphous Cu-Ti alloy system, especially for the transition from the amorphous state to crystallization of the amorphous alloys, all were not studied in the literature before. These researches and the gained results enhance the new content for studying surface segregation of alloys. The research project is the thermal-electron transition materials of Si-Ge and Si-Ge-GaP alloys when I was engaged as a senior scientist in the Department of Materials Science and Engineering, University of Virginia of America in 1989. The contact material of the double W-W layer we studied has low resistance even at high temperature up to 1000 K, supporting the improvement and enhancement of out-put efficiency for the thermal-electron transition materials.

Early in the ancient Stone Age, the Bronze Age and the Iron Age, our ancestry were benefited by their new discovery and development in the materials, thereby created the brilliant history and bright civilization over all the world. Today, in the new twenty-one century, the new and advanced materials are still one of the key and important sciences and technologies for highly developing the further civilization for the mankind. As a devoted person for the education and science, I have worked and strived in the field of the materials science for several decades. I am so proud and so honored for that. I would be burst with joy if I have really supplied something for the field because my work is connected with the science and technology that is closely and tightly related to the mankind.

Science and technology require the person who devotes and strives for them must be honestly, conscientiously, seriously, and meticulously. I can do my research according to these requirements persistently just because the advice and help from my teachers in the schools and my seniors benefit me, especially who are still connected with me today. Their guidance and influence helped and promoted me having such characters that a scientist must have. I resorted my former schoolmates, friends and people of the same occupation usually in my research because of lacking of experimental equipment and/or my limited research funds. And they always helped me to do the experiments that we could not perform them ourselves with a reduced price, or just the cost price, or even free. I appreciate them very well. I have applied for and performed several research projects from the National Nature Science Foundation, the former Ministry of Machine and from the Committee of Science and Technology of the Hunan Province. The research fruits of mine were very difficult to obtain if no such funds to support me. I am indebted to them. I went to the Department of Materials Science and Engineering, University of Virginia of America and the Max-Planck-Institut für Plasmaphysik, West Germany for the collboration projects two times, and they supported me, therefore the projects could be carried out smoothly and successfully. Thanks for them. My major projects were carried out with my students and colleagues in my group. Some of them provided good idea how to select the papers for the collection, and reviewed and checked the selected papers carefully and thoroughly, therefore one or two mistakes of content and/or characters existed in the published papers could be recorrected. Thanks for their work, support and help.

I was born in a very beautiful village, which is grown and covered with moss in the southwest of the Hunan Province. My parents brought up me. And my brothers and sisters helped and supported me. Thus I could grow up. Just because of their gereat love and sentiment, I am only the person in my brothers and sisters who could have opportunity to stride forward the brilliant and bright scientific palace. Therefore, I can not forget such great love and sentiment from them for ever and ever. This moment, I appreciate particularly to my wife who lives with me day and night, where and there. At the same time, I cherish the memory of my old first wife who has passed too early very much. Their love, help, support and encourage for me are the important guarantee and the necessary conditions for the research fruits I gained, so their contribution and meritorious service cannot be neglected and should be remembered forever.

Lastly I want to thank the Press of the Hunan University. Their labor ensures the collec-

tion published and met to the readers.

It is difficult to avoid smoe mistakes or shortcomings in the collection, I would be appreciated to receive the criticism and opinion from the specialists worked in the same occupation and the reading public.

Zhang Bangwei
Yuelu Mountain, Changsha
April 6, 2001

目　次

尺寸因素在非晶态合金形成中的作用*

张邦维

(湖南大学)

【摘要】 本文提出在非晶态合金的形成中,元素的原子半径采用实测的原子间距之半来衡量 在总结归纳大量实验资料的基础上发现二元或多元非晶态合金,其组成元素的尺寸因素($\Delta R/R_1$)都大于9%(个别例外).分析了影响形成二元非晶态合金的因素,得到了形成二元非晶态合金的必要条件为

$$\left|\left(\frac{Z}{r_k}\right)_B(\delta x_P)_A(x_{PA}-x_{PB})\frac{\Delta R}{R_1}\right|\geqslant 0\ 09$$

对于用液态淬火法形成的非晶态合金,其准确度达到90%

一、引 言

对于非晶态合金的形成规律,Mader等[1]提出:1 两组元在平衡相图中的溶解度有限;2.组分原子的大小差需大于10% Chen等人[2]在自己的实验基础上将影响非晶态合金形成的因素归结为:1 组分原子间的化学键合;2 原子大小;3 晶体对称性 他们的工作,未能取得定量的判据 最近,施天生等[3]运用键参数图研究二元非晶态合金的形成条件,得到了用液态急冷法获得二元系非晶态合金的必要条件.

我们在分析大量实验资料的基础上,发现原子尺寸因素$\left(\Delta R/R_1=\dfrac{R_1-R_2}{R_1}\right)$在决定非晶态合金的形成中具有重要作用.提出非晶态合金的形成中用实测的元素原子间距之半作为元素的原子半径之值.同时提出用陈念贻的键参数和尺寸因素联合作图来探求二元非晶态合金的形成条件.

二、尺寸因素的作用

我们以实测的元素的原子间距之半作为原子半径的量度,分析和归纳已有的二元非晶态合金的实验资料,探求尺寸因素在形成非晶态合金中的作用 在计算合金系统的尺寸因素时,含量多的元素的原子半径作为R_1,含量少的作为R_2.结果发现表1所列举的能生成非晶态的70种二元合金除了4种合金(AuSn7.6%,FeSi6%,MgBi3.1%,PtSb5 1%)其尺寸因素小于9%外,其他的皆大于9% 说明尺寸因素在非晶态合金的形成中确实具有不可忽视的作用.为了说明问题,在表1中亦列出各元素的Goldschmidt原子半径之值以及由此计算的合金系统的尺寸因素.显然看不出尺寸因素的重要作用.尤其是对于类金属作为一个组元的非晶态合金,在所研究的26种系统中,竟有16种的尺寸因素小于9%(达60%),完全看不出尺寸因素的作用了,而有些作者[3,5,6]就是据此作出结论的.

对于由金属元素和非金属元素组成的多元系非晶态合金系统,我们取成分大者的金属元素的原子半径和成分大者的非金属元素的原子半径来计算尺寸因素,而把其他含量少的金属元素视为添加剂,略去其对尺寸因素的影响.如$Pd_{70}Cr_{10}Si_{20}$以Pd-Si计

* [原发表在《金属学报》,1981,17(3):285~292]

表 1 非晶态合金的尺寸因素

Table 1 Size factor of amorphous alloy

Alloy system	Composition range x, at%	At. radius[4] Å	Size factor $\left\|\frac{\Delta R}{R_1}\right\|$, %	At. radius[4] Goldschmidt Å	Size factor $\left\|\frac{\Delta R}{R_1}\right\|$, %
$Au_{100-x}Si_x$	18.6～30	1.44～1.17	18.8	1.44～1.32	8.3
$Au_{73}Ge_{27}$		1.44～1.22	15.3	1.44～1.37	4.9
$Ag_{100-x}Si_x$	17～30	1.44～1.17	18.8	1.44～1.32	8.3
$Fe_{84}C_{16}$		1.24～0.77	37.9	1.28～0.77	39.8
$Mn_{100-x}Si_x$	25～28	1.3～1.17	10	1.3～1.32	1.5
$Pd_{100-x}Ge_x$	18～20	1.37～1.22	11	1.37～1.37	0
$Pd_{100-x}Si_x$	15～23	1.37～1.17	14.6	1.37～1.32	3.6
$Pt_{100-x}Ge_x$	17～30	1.38～1.22	11.6	1.38～1.37	0.7
$Pt_{100-x}Si_x$	23,25,68	1.38～1.17	15.2	1.38～1.32	4.3
RhGe	?	1.34～1.22	9	1.34～1.37	2.2
$Rh_{78}Si_{22}$		1.34～1.17	12.7	1.34～1.32	1.5
$Al_{100-x}Ge_x$	30～80	1.43～1.22	14.7	1.43～1.37	4.2
$Co_{100-x}Px$	18～25	1.25～1.09	12.8	1.25～1.28	2.4
$Fe_{100-x}Si_x$	0～75	1.24～1.17	6	1.28～1.32	3.1
$Fe_{80}B_{20}$		1.24～0.97	21.8	1.28～0.97	24.2
$La_{80}Ga_{20}$		1.87～1.22	34.8	1.87～1.35	27.8
$Mg_{81.27}Ga_{18.73}$		1.6～1.22	23.8	1.6～1.35	15.6
$Ni_{100-x}P_x$	8.6～26.2	1.25～1.09	12.8	1.25～1.28	2.4
$Ni_{80}S_{20}$		1.25～1.04	16.8	1.25～1.04	16.8
$Ni_{81.5}B_{18.5}$		1.25～0.97	22.4	1.25～0.97	22.4
$Te_{100-x}Ga_x$	10～30	1.43～1.22	14.7	1.6～1.35	15.6
$Te_{100-x}Ge_x$	10～25	1.43～1.22	14.7	1.6～1.37	14.4
$Te_{100-x}In_x$	10～30	1.43～1.62	13.3	1.6～1.57	1.9
$Te_{100-x}Pb_x$	14.5,20,22.5,30	1.43～1.75	22.4	1.6～1.75	9.4
$Tl_{100-x}Te_x$	15～60	1.71～1.43	16.4	1.71～1.6	6.4
$Ti_{80}Si_{20}$		1.47～1.17	20.4	1.47～1.32	10.2
$Au_{75}Pb_{25}$		1.44～1.75	21.5	1.44～1.75	21.5
$Au_{100-x}Snx$	29～31	1.44～1.55	7.6	1.44～1.58	9.7
$Al_{82.7}Cu_{17.3}$		1.43～1.28	10.5	1.43～1.28	10.5
$Pb_{52}Sb_{48}$		1.75～1.45	17.1	1.75～1.61	8
$Pt_{100-x}Sb_x$	33～37	1.38～1.45	5.1	1.38～1.61	16.7
$Sn_{90}Cu_{10}$		1.55～1.28	17.4	1.58～1.28	19
$Tl_{100-x}Au_x$	25～60	1.71～1.44	15.8	1.71～1.44	15.8
CuBi	?	1.28～1.55	21.1	1.28～1.82	42.2
$Gd_{81}Al_{19}$		1.8～1.43	20.6	1.8～1.43	20.6
$Mg_{65}Cu_{35}$		1.6～1.28	20	1.6～1.28	20
MgBi	?	1.6～1.55	3.1	1.6～1.82	13.8
$Mg_{60}Sb_{40}$		1.6～1.45	9.4	1.6～1.61	0.6
$Cu_{100-x}Ti_x$	30～35	1.28～1.47	14.8	1.28～1.47	14.8
CuLa	?	1.28～1.87	46.1	1.28～1.87	46.1
$Gd_{100-x}Co_x$	39～96	1.8～1.25	30.6	1.8～1.25	30.6
$Gd_{100-x}Fe_x$	15～94	1.8～1.24	31.1	1.8～1.28	28.9

续表 1

Alloy system	Composition range x, at%	At. radius[4] Å	Size factor $\left\|\frac{\Delta R}{R_1}\right\|$, %	At. radius[4] Goldschmidt Å	Size factor $\left\|\frac{\Delta R}{R_1}\right\|$, %
$La_{100-x}Au_x$	0～40	1.87～1.44	23	1.87～1.44	23
$Nb_{100-x}Ni_x$	25～60	1.43～1.25	12.6	1.47～1.25	15
NiLa	?	1.25～1.87	49.6	1.25～1.87	49.6
$Ta_{100-x}Ni_x$	25～70	1.43～1.25	12.6	1.47～1.25	15
YFe_2		1.81～1.24	46	1.81～1.28	41.4
$Zr_{72}Co_{28}$		1.6～1.25	21.9	1.6～1.25	21.9
$Zr_{100-x}Cu_x$	40～75	1.6～1.28	20	1.6～1.28	20
$Zr_{100-x}Ni_x$	20～40	1.6～1.25	21.9	1.6～1.25	21.9
$Zr_{100-x}Pd_x$	20～35	1.6～1.37	14.4	1.6～1.37	14.4
$Zr_{100-x}Rh_x$	18～26	1.6～1.34	16.3	1.6～1.34	16.3
Ag_xCu_y	$x=35-65$ $y=35-60$	1.44～1.28	11.1	1.44～1.28	11.1
$Ag_{100-x}Mn_x$	4～13	1.44～1.3	9.7	1.44～1.3	9.7
$Au_{100-x}Fe_x$	45－97	1.44～1.24	13.9	1.44～1.28	11.1
$Co_{100-x}Au_x$	23～65	1.25～1.44	15.2	1.25～1.44	15.2
$DyFe_2$		1.77～1.24	42.7	1.77～1.28	38.3
$Er_{64}Fe_{36}$		1.75～1.24	29.1	1.75～1.28	26.9
$Gd_{100-x}Ag_x$	12～14	1.8～1.44	20	1.8～1.44	20
$HoFe_2$		1.76～1.24	42	1.76～1.28	37.5
$PrCo_5$		1.83～1.25	46.4	1.83～1.25	46.4
$PrFe_2$		1.83～1.24	47.6	1.83～1.28	43
$SmCo_5$		1.794～1.25	43.5	1.794～1.25	43.5
$SmFe_2$		1.794～1.24	44.7	1.794～1.28	40.2
$TbFe_2$		1.77～1.24	42.7	1.77～1.28	38.3
$TmFe_2$		1.74～1.24	40	1.74～1.28	35.9
$Ti_{100-x}Be_x$	37～41	1.47～1.13	23.1	1.47～1.13	23.1
YCo_5		1.81～1.25	44.8	1.81～1.25	44.8
$YbFe_2$		1.93～1.24	55.6	1.93～1.28	50.8
$Zr_{100-x}Be_x$	30～50	1.6～1.13	29.4	1.6～1.13	29.4

算，$Co_{72}P_{16}B_{12}$ 以 Co-P 计算，$Fe_{70-x}Cr_{10}Ni_xP_{13}C_7$（$x=5-20$）以 Fe-P 计算．这样做不免带来些误差，但不会影响问题的本质，这种近似是合理的．结果发现在所计算的 62 种非晶态合金中（只含 1 种非金属元素的合金为 38 种，含有 2 种以上非金属元素的合金为 24 种）只有 1 种合金（$Fe_{100-x}Co_x)_{75}Si_{15}B_{10}$（$x=0-100$）的尺寸因素小于 9%，其余的 61 种皆大于 9%．这也说明了尺寸因素在形成非晶态合金中的作用．

如果计算不能生成非晶态合金系统的尺寸因素，则对下一节所列的 57 种不能生