Abschlussbericht (Sachbericht)

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<td>Projekttitel</td>
<td>Investigation of Metallic Glasses under Stress by Synchrotron Radiation Techniques</td>
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<tr>
<td>Federführende/r Wissenschaftler/in</td>
<td>Dr. Hermann Franz</td>
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<td>Helmholtz-Zentrum</td>
<td>DESY</td>
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1) Fortschritt des im Antrag beschriebenen Arbeitsprogramms

This report summarized the results of the very successful cooperation between Zhejiang University, Hangzhou, PR China, and DESY, Hamburg, Germany, on the topic of “Investigation of Metallic Glasses under Stress by Synchrotron Radiation Techniques”. In five years, from 2007 to 2012, more than 90 papers in reviewed journals have been published. Some of the results are still under evaluation, so that the project will continue to produce contributions to the research field even after the end of the funding period. Based on the exceptional success we are currently investigating pathways to continue this well-established cooperation.

Besides scientists and post-docs several students have been involved, both at Zhejiang University and at DESY. Scientists from Zhejiang University have been trained in the use of Synchrotron Radiation based experimental techniques during long term visits at DESY. In addition every year several mutual short term visits have been arranged. Results have been presented on various national and international conferences and seminars.

Most important achievements have been the development of several new and innovative alloys with optimized glass forming abilities, the unraveling of structure – property relations, correlation of microscopic and macroscopic deformation mechanism, and the development of advanced data collection and evaluation procedures.

In the following a short description on the most important achievements will be presented.

I. Atomic structures of metallic glasses

Atomic structures of a wide range of metallic glasses (La-based, CuZr, CuZrAl, ZrNi, NiNbZr, ZrCuPd, FeCoNbB, and many more) have been investigated by a combination of advanced experimental techniques (synchrotron radiation-based x-ray diffraction (XRD) and extended x-ray absorption fine structure (EXAFS)) with computational methods (reverse Monte Carlo (RMC) and \textit{ab initio} molecular dynamics (VASP) simulation) [3-5,14,15]. Three-dimensional atomic configurations of the studied metallic glasses have been established. Icosahedron-like clusters have been detected in many of the studied metallic glasses. The question about the nature of the amorphous-to-amorphous phase transition induced by pressure, a very active field in materials science and condensed matter physics, has been tackled. We discovered that LaCe-based bulk metallic glass exhibits a sudden change in compressibility, which might originate from the Kondo coupling between 4f spin and conductive electrons due to the addition of cerium [1]. Such an effect has never been reported in any bulk metallic glasses before. This seems to be the first observation of an amorphous-to-amorphous phase transition in bulk metallic glassy systems. The origin for the crossover was detected to be delocalization of f
electrons under pressure. One new Ca-Al metallic glass system with non-f electron also demonstrates an amorphous-to-amorphous crossover due to a charge transfer from s or p electrons to d orbital. Based on atomistic structural data the group at Zhejiang University developed the largest Zr-based bulk metallic glass prepared by copper mold casting with 73 mm diameter[64]; the largest rare-earth based BMG rods prepared by copper mold casting with a critical diameter of 35 mm [2] and a novel ZrCu-based bulk metallic glass with at least 20 mm diameter[12].

II. Structural evolution of BMGs under stress

We discovered an intrinsic plastic CuZrAlTi bulk metallic glass with high strength and superior compressive plastic strain of up to 32.5 %. The correlation of mechanical properties with atomic structure of that alloy was investigated by using Synchrotron Radiation techniques. The superior compressive plastic strain is attributed to a large amount of randomly distributed free volume, induced by Ti minor alloying, which results in extensive shear band formation, branching, interaction and self-healing of minor cracks. In order to confirm the idea of free-volume effect on mechanical behavior of BMGs proposed, we further carried out a study on CuZrAl BMG and indeed revealed that the plasticity of the BMG can be tailored by introducing different amounts of free volume in BMGs[16]. These results demonstrate that introducing free volume to BMGs could be one promising way to improve plasticity of BMGs. In addition, we explored various possibilities to overcome the restriction of limited plastic deformation and lack of work-hardening of BMGs. We successfully achieved large macroscopic compressive plastic deformation (over 15%) and work-hardening-like behavior in a monolithic BMG through tailoring loading stress distribution experimentally [13]. We explored a new method to study tension behavior by in situ XRD under tension to quantitatively determine elastic properties and a new method to characterize residual stress in BMGs was developed [14]. These new tools for structural characterization were successfully applied to four BMGs [27]. It is found that the local strain is basically homogeneously distributed at low stress. However, heterogeneity appears obviously when the stress is close to the fracture strength. The amplitude of fluctuation in local strain for several BMGs could relate to the distribution of excess free volume within the medium range order. This might be a precursor for the formation of shear bands. Conclusions drawn for structure data could be supported by molecular dynamics simulations of stress-strain behavior [94].

Publications related to the project

2007

Anomalous compression behavior in Lanthanum/curium-based metallic glass under high pressure
Proceedings of the National Academy of Sciences (PNAS) 104, 13565 (2007)

La-based bulk metallic glasses with critical diameter up to 30 mm

3. X.D. Wang, J. Bednarcik, K. Saksll, H. Franz, Q.P. Cao, J.Z. Jiang
Tensile behaviour of bulk metallic glasses by in-situ high energy X-ray diffraction

4. L. Yang, S. Yin, X.D. Wang, Q.P. Cao, J.Z. Jiang, K. Saksll, H. Franz
Atomic structure in Zr70Ni30 metallic glass
5. L. Yang, J.Z. Jiang, K. Saksl, H. Franz
Origin of pre-peak in Zr70Cu25Pd5 metallic glass

Enhancement of plasticity in Zr-based bulk metallic glasses

Tension and stress relaxation behavior of a La-based bulk metallic glass

Catching the Ni-based ternary metallic glasses with critical diameter up to 3 mm in Ni-Nb-Zr system

Ultrahigh-strength binary Ni-Nb bulk glassy alloy composite with good ductility

Microstructure and crystallization in Cu56Zr43Al5 metallic glass
Journal of Alloys and Compounds 441, 185 (2007)

2008

New class of plastic bulk metallic glass
Physical Review Letters 100, 075501 (2008)

Zr-(Cu,Ag)-Al bulk metallic glasses

Achieving large macroscopic compressive plastic deformation and work-hardening-like behavior in a monolithic bulk metallic glass by tailoring stress distribution

14. X.D. Wang, S. Yi, Q.P. Cao, J.Z. Jiang, H. Franz, Z.H. Jin
Atomic structure of binary Cu54.5Zr45.5 bulk metallic glass

15. X.D. Wang, Q.K. Jiang, Q.P. Cao, J. Bednarcik, H. Franz, J.Z. Jiang
Atomic structure and glass forming ability of Cu48Zr46Al8 bulk metallic glass

Free-volume induced superior ductility in a bulk metallic glass at room temperature
Scripta Materialia 59, 75 (2008)

17. L.Y. Chen, Q. Ge, S. Qu, J.Z. Jiang
Stress induced softening and hardening in a bulk metallic glass
Scripta Materialia 59, 1210 (2008)

Formation of Ni-Nb-Zr-X (X=Ti, Ta, Fe, Cu, Co) bulk metallic glasses

Bulk ferromagnetic glasses in the Fe-M-Y-B (M=transition metals) system

In situ energy dispersive X-ray diffraction analysis of the temperature pressure stability of Co-Fe-(Ta,W)-B alloys

Strain distribution in Zr64.13Cu15.75Ni10.12Al10 bulk metallic glass investigated by in situ tensile tests under synchrotron radiation

22. E. Komova, M. Varga, R. Varga, P. Vojtanik, J. Bednarcik, J. Kovac, M. Provencio, M. Vazquez
Nanocrystalline glass-coated FeNiMoB microwires

Microstructural changes induced by thermal treatment in Cu47Ti33Zr11Ni8Si1 metallic glass
Materials Science and Engineering A 498, 335 (2008)

Influence of cryomilling on structure of CoFeZrB alloy

The soft magnetic properties and temperature stability of Co-Fe-Zr-B metallic glasses

2009

Novel alloy of incompatible elements
Proceedings of the National Academy of Sciences (PNAS) 106, 2515 (2009)

27. X.D. Wang, J. Bednarcik, H. Franz, H.B. Lou, Z.H. He, Q.P. Cao, J.Z. Jiang
Local strain behavior of bulk metallic glasses under tension studied by in situ high energy x-ray diffraction

28. X.M. Huang, X.D. Wang, Y. He, Q.P. Cao, J.Z. Jiang
Are there two glass transitions in Fe-M (M=Mo, W, Nb)-Y-B bulk metallic glasses?
Scripta Materialia 60, 152 (2009)

Catching Fe-based bulk metallic glass with combination of high glass forming ability, ultrahigh strength and good plasticity in Fe-Co-Nb-B system
Materials Science and Engineering A 517, 246 (2009)

Effect of microalloying of Nb on corrosion resistance and thermal stability of ZrCu-based bulk metallic glasses

31. Y. Xu, J.Z. Jiang, X.M. Ge
Preparation and Growth Behavior of Amorphous Pd$_{60}$Ni$_{40}$P$_{20}$ Film by electrodeposition

Synthesis, Thermal Stability and Properties of ZnO$_2$ Nanoparticles

33. S. Pauly, J. Das, J. Bednarcik, N. Mattern, K. B. Kim, D. H. Kim, J. Eckert
Deformation-induced martensitic transformation in Cu-Zr-(Al,Ti) bulk metallic glass composites Scripta Materialia 60, 431 (2009)

34. S. Michalk, P. Sovak, J. Bednarcik, P. Kollar, V. Girman
Structure and Magnetic Properties of Fe(Mn)-Si-B-Nb-Cu Alloys

35. G. Wang, N. Mattern, S. Pauly, J. Bednarcik, J. Eckert
Atomic structure evolution in bulk metallic glass under compressive stress

Structural evolution of Cu-Zr metallic glasses under tension
Acta Materialia 57, 4133 (2009)

Initiation and evolution of shear bands in bulk metallic glass under tension - an in-situ SEM observation

Homogeneity of Zr$_{64.13}$Cu$_{15.75}$Ni$_{10.12}$Al$_{10}$ bulk metallic glass

39. X.D. Wang, J.Z. Jiang, H. Franz
Mechanical properties of monolithic Zr$_{62}$Al$_{6}$Ni$_{13}$Cu$_{13}$ bulk metallic glass

40. X.M. Huang, X.D. Wang, J.Z. Jiang
Origin of high glass forming ability of Y-containing FeB-based alloys

41. M. Stefan, K. Saksl, P. Svovic, J.Z. Jiang
Crystallization of Zr$_{50}$Fe$_{20}$Cu$_{20}$ amorphous alloy
Journal of Alloys and Compounds 478, 441 (2009)

42. J. Bednarcik, H. Franz
Deformation of metallic glasses: Insight from in-situ high-energy x-ray diffraction
Journal of Physics, Conference Series 144, 0120581 (2009)
43. I. Kaban, W. Hoyer, P. Jóvári, T. Petkova, A. Stoi-lova, A. Schöps, J. Bednarcik, B. Beuneu
Atomic structure of As₃₄Se₃₅Ag₁₅ and As₃₄Te₃₅Ag₁₅ glasses studied with XRD, ND and EXAFS and modeled with RMC

44. S. Michalik, P. Sovak, J. Bednarcik, P. Kollar, V. Girman
Structure and Magnetic Properties of Fe(Mn)-Si-B-Nb-Cu Alloys

45. X.P. Nie, X.H. Yang, and J.Z. Jiang
Ti microalloying effect on corrosion resistance and thermal stability of CuZr-based bulk metallic glasses

2010

Phase separation in Ni-Nb-Y metallic glasses.

Thermal expansion of La-based BMG studied by in-situ high-energy X-ray diffraction

48. J. Bednarcik, M. Miglierine, C. Curfs, H. Franz
Thermal expansion of NANOPERM-type alloys from in-situ X-ray diffraction

Modeling the atomic structure of Al₃₂U₈ metallic glass.

Changes in short-range order of Zr₅₅Cu₃₀Al₁₀Ni₅ and Zr₅₅Cu₂₀Al₁₀Ni₁₅Ti₅ BMGs upon annealing

Tensile behavior of orthorhombic β’ Titanium alloy studied by in situ X-ray diffraction
Materials Science and Engineering A 527, 6596 (2010)

52. S. Pauly, J. Bednarcik, U. Kühn, J. Eckert
Plastically deformable Cu-Zr intermetallics
Scripta Materialia 63, 336 (2010)

53. S. Michalik, J. Bednarcik, K. Brzozka, P. Sovak, B. Gorka,
Microstructural Study of Fe-Si(Ge)-Nb-Cu-B Finemet Alloys

54. J. Bednarcik, S. Michalik, P. Kollar, S. Roth
Influence of Ball Milling on the Local Atomic Structure of an Amorphous CoFeSiB Alloy

Mechanical Response of Metallic Glasses: Insights from In-situ High Energy X-ray Diffraction
JOM 62, 76 (2010)

56. Qiao-shi Zeng, Yang Ding, Wendy L. Mao, Wenge Yang, Stas.V. Sinogeikin, Jinfu Shu, Ho-kwang Mao
and J.Z. Jiang
Origin of Pressure-Induced Polyamorphism in Ce\textsubscript{75}Al\textsubscript{25} Metallic Glass

Effect of pre-existing shear bands on the tensile mechanical properties of a bulk metallic glass

Shear band evolution and hardness change in cold-rolled bulk metallic glasses

Properties of Polyamorphous Ce\textsubscript{75}Al\textsubscript{25} Metallic Glasses

60. L. Yang, G.Q. Guo, L.Y. Chen, S.H. Wei, J.Z. Jiang, X.D. Wang
Atomic structure in Al-doped multicomponent bulk metallic glass
Scripta Materialia \textbf{63}, 879 (2010)

“Soft” atoms in \textit{Zr}\textsubscript{70}Pd\textsubscript{30} metal-metal amorphous alloy

\textbf{2011}

A plastic Zr-based bulk metallic glass
Acta Materialia \textbf{59}, 1037 (2011)

63. X.D. Wang, H.B. Lou, S.G. Wang, J. Xu, J.Z. Jiang
Atomic packing in Mg\textsubscript{61}Cu\textsubscript{28}Gd\textsubscript{11} bulk metallic glass

64. H.B. Lou, X.D. Wang, F. Xu, S.Q. Ding, Q.P. Cao, K. Hono, J.Z. Jiang
73 mm-diameter Bulk Metallic Glass Rod by Copper Mould Casting

65. X.P. Nie, X.H. Yang, Y. Ma, L.Y. Chen, K.B. Yeap, K.Y. Zeng, D. Li, J.S. Pan, X.D. Wang, Q.P. Cao, S.Q. Ding, J.Z. Jiang
The effect of oxidation on the corrosion resistance and mechanical property of a Zr-based metallic glass
Corrosion Science \textbf{53}, 3557 (2011)

Atomic level structural modifications induced by severe plastic shear deformation in bulk metallic glasses
Scripta Materialia \textbf{64}, 81 (2011)

Heterogeneities in CuZr-based bulk metallic glasses studied by X-ray scattering

Isochronal crystallization kinetics of Cu$_{60}$Zr$_{20}$Ti$_{20}$ bulk metallic glass
Journal of Non-Crystalline Solids 357, 1182 (2011)

69. F. Xu, H.B. Lou, X.D. Wang, S.Q. Ding, Q.P. Cao, J.Z. Jiang
Glass forming ability and crystallization of Zr-Cu-Ag-Al-Be bulk metallic glasses
Journal of Alloys and Compounds 509, 9034 (2011)

Low temperature transport properties of Ce-Al metallic glasses
Journal of Applied Physics 109, 113716 (2011)

71. C. Hostert, D. Music, J. Bednarcik, J. Keckes, V. Kapakis, B. Hjoervarsson, J. M. Schneider
Ab initio molecular dynamics model for density, elastic properties and short range order of Co-Fe-Ta-B metallic glass thin films

Thermal expansion of a La-based bulk metallic glass: insight from in situ high-energy x-ray diffraction

73. J. Bednarcik, S. Michalik, H. Franz
In situ tensile deformation of Fe-rich metallic glass at elevated temperatures using hard X-ray diffraction
Journal of Alloys and Compounds 509, S92 (2011)

74. Stoica, V. Kolesar, J. Bednarcik, S. Roth, H. Franz, J. Eckert
Thermal stability and magnetic properties of partially Co-substituted (Fe$_{71.2}$B$_{24}$Y$_{4.8}$)$_{96}$Nb$_{4}$ bulk metallic glasses
Journal of Applied Physics 109, 054901 (2011)

75. S. Michalik, J. Gamcova, J. Bednarcik, R. Varga
In situ structural investigation of amorphous and nanocrystalline Fe$_{40}$Co$_{38}$Mo$_{4}$B$_{18}$ microwires
Journal of Alloys and Compounds 509, 3409 (2011)

2012

Pressure-induced amorphous-to-amorphous configuration change in Ca-Al metallic glasses
Scientific Reports 2, 376 (2012)

77. Q.K. Jiang, P. Liu, Y. Ma, Q. P. Cao, X. D. Wang, D.X. Zhang, X. D. Han, Z. Zhang, J.Z. Jiang
Super elastic strain limit in metallic glass films
Scientific Reports 2, 852 (2012)

78. Min Wu, Yunfeng Liang, Jian-Zhong Jiang, John S. Tse
Structure and Properties of Dense Silica Glass
Scientific Reports 2, 398 (2012)

Atomic-scale mechanisms of the glass-forming ability in metallic glasses

80. Y. Ma, Q.P. Cao, S.X. Qu, X.D. Wang, J.Z. Jiang
Effect of structural relaxation on plastic flow in Ni-Nb metallic glassy film

2) **Finanz-/Zeitplan**

*Können Sie Finanz- und Zeitplan einhalten oder sind Anpassungen notwendig?*

Finanz- und Zeitplan wurden eingehalten.

3) **Strategischer Mehrwert**

*Welchen strategischen Mehrwert für die Helmholtz-Gemeinschaft hat das Vorhaben bisher erreicht oder inwieweit ist er absehbar?*


4) **Drittmittel**

*Wurden Drittmittel eingeworben? Wenn ja, von wem und in welcher Höhe?*

Es wurden keine weiteren Drittmittel eingeworben.

---

2013


*Structural evolution in bulk metallic glass under high-temperature tension*

Impuls- und Vernetzungsfonds
Federführendes Zentrum:
Deutsches Elektronen-Synchrotron,
DESY
Notkestr. 85
D-22607 Hamburg

Partner Institut:
Zhejiang University

Einfacher Verwendungsnachweis

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Zwischennachweis
Verwendungsnachweis (Schlussnachweis)
für den Zeitraum 01.03.2007 bis 31.08.2012

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Zutreffendes bitte ankreuzen:

- Wir bestätigen, dass die Partner die Verwendung der an sie weitergeleiteten Mittel aus dem Zuwendungsvertrag nachgewiesen haben.


... Hamburg, den 27.12.2012
Ort, Datum

Unterschrift(en) U. Wolfram, Leiter Finanzabteilung

Sachlich richtig | rechnerisch richtig

(mit Euro)

... den ...

Intervention:

1 Bei mehreren Partnern bitte auf separatem Blatt einzeln ausweisen.
Usage List

Helmholtz Research Centre:
Deutsches Elektronen-Synchrotron, DESY
Notkestr. 85
D-22607 Hamburg

Partner Institut:
Zhejiang University,
310027 Hangzhou,
P.R. China

Name of the Helmholtz Project: Investigation of Metallic Glasses under Stress by Synchrotron Radiation Techniques

Funding No: VH- IK-Ch-002

Received funds from DESY: 357,500 €

Costs appeared in the time period: 2007-2012

Personal costs: 82,135 €
Travel costs: 39,068 €
Costs for workshops, conferences, etc: 6,307 €
Other direct costs: 242,348 €

Total costs: 369,858 €

2012-11-10, hangzhou

Date, Place

Signature of the Funding Office

Signature of Leading Scientist
Impuls- und Vernetzungsfonds
Federführendes Zentrum:
Deutsches Elektronen-Synchrotron (DESY)
Notkestr. 85
D-22607 Hamburg

Partner Institut:
Zhejiang University

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Zutreffendes bitte ankreuzen:

☐ Wir bestätigen, dass die Partner die Verwendung der an sie weitergeleiteten Mittel aus dem Zuwendungsvertrag nachgewiesen haben.


Ort/Datum

Unterschriften

Deutsches Elektronen-Synchrotron DESY
in der Helmholtz-Gemeinschaft
Notkestr. 85 - 22607 Hamburg - Tel. 040 / 89 98-0

1 Bei mehreren Partnern bitte auf separatem Blatt einzeln ausweisen.
Usage List of Funds

Name of the project: Investigation of Metallic Glasses under Stress by Synchrotron Radiation Techniques

Costs of the project partner(s) Zhejiang University in the fiscal year 2007:

- Personal costs __13,558__ €
- Travel costs __8,634__ €
- Costs for workshops, conferences, etc __1,057__ €
- Other direct costs __58,329__ €
- Total costs __81,578__ €

Total funds sent by DESY to the partner(s) or received by the partner __81,475__ €

Brief description of the activities (achieved goals, time schedule and perspectives):

In the year 2007, the group, Laboratory of New-Structured Materials, Zhejiang University, has been pursuing all research activities planned in the Zhejiang University-Helmholtz Research Collaboration Program with a project entitled “Investigation of Metallic Glasses under Stress by Synchrotron Radiation Techniques”. The summary of all activities are expressed as follows:

1. **Research activities**

1.1 Atomic structures of Zr_{20}Ni_{50} and Zr_{50}Cu_{50}Pd_{x} (x = 0, 1, 5, 10, 20 and 30 at.%) metallic glasses were investigated by reverse Monte Carlo simulation combining with x-ray diffraction, Ni and Zr K-edge extended x-ray absorption fine structure measurements [1,2]. We performed in situ room-temperature high-pressure x-ray diffraction (XRD) using synchrotron radiation up to 40 GPa for a LaCo-based bulk metallic glass [3], which might be the first observation of amorphous-to-amorphous phase transition in bulk metallic glass systems.

1.2 Tensile behaviors of two Zr_{62}Al_{8}Ni_{13}Cu_{17} and La_{62}Al_{14}(Cu_{56}Ag_{44})_{14}Co_{5}Ni_{5} bulk metallic glasses (BMGs) were studied [4]. The tensile elastic modulus and Poisson’s ratio have been accurately evaluated. Such experiments confirm that the XRD technique is suitable to study tension behavior of bulk metallic glasses. We also studied compression behavior of monolithic Zr-based bulk metallic glasses [5] and found that a minor adjustment in Zr/Ni concentration ratio can dramatically enhance the plasticity of monolithic Zr-based bulk metallic glasses, from only about 2.2% for Zr_{62}Al_{8}Ni_{10}Cu_{17} BMG to 14% for Zr_{62}Al_{8}Ni_{13}Cu_{17} BMG. Tension and stress relaxation behaviors of a La_{62}Al_{14}Cu_{11}Ag_{23}Ni_{5}Co_{5} bulk metallic glass (BMG) as a function of isothermal annealing time have been investigated [6]. We found that annealing at 373 K below the glass transition temperature (423 K) of the BMG alloy, causes an increase of special heat difference at glass transition and density of the alloy, indicating a reduction of free volume in the BMG alloy with annealing time.

1.3 We developed the second largest bulk metallic glass: 35 mm La_{65}Al_{14}(Cu_{56}Ag_{44})_{14}(Ni_{13}Co_{17}) BMG rod by copper mold casting [7]. The origin of the high GFA enhanced by the Ag and Ni-Co substitution were investigated from the kinetic, structural and thermodynamic points of view. It is found that high GFA is attributed to the smaller difference in Gibbs free energy between amorphous and crystalline phases in the pseudo quaternary alloy system. The developed La-based BMG alloys with high GFA, low glass-transition temperatures and relatively
wide supercooled liquid regions should be useful for both scientific and engineering applications. We also
developed the Ni-based ternary bulk metallic glasses with critical diameter up to 3 mm in Ni-Nb-Zr system using a
strategy for catching the best glass former based on relative glass forming ability of alloys [8].

2. Manpower
Zhejiang University has put 1 staff member, 1 postdoc, 2 ph.d. and 3 master students to work on the present
research project. They worked hard and obtained many interesting results, which have been published in the
international recognized journals.

3. Meeting and exchange visiting
In the year 2007, Prof. Jianzhong Jiang visited Hasylab, Hamburg for two weeks and Dr. Xiaodong Wang
worked at Hasylab, Hamburg for 8 months. Dr. H. Franz visited Zhejiang University for one week. Both sides
exchanged their research results often via visiting and e-mail.
Four people from Zhejiang university also performed synchrotron radiation experiments at KEK in Japan.
Two workshops were held at Zhejiang University. They are

4. Time schedule and perspectives
In the year 2008, we will continue our effort to study the correlation of mechanical properties with atomic
structure of bulk metallic glasses using Synchrotron Radiation techniques. Simple systems, e.g., CuZr BMG, will
be studied by using a combination of state-of-the-art experimental techniques (synchrotron radiation-based XRD,
XAFS and neutron diffraction) and computational techniques (reverse Monte Carlo (RMC) and ab initio molecular
dynamics simulation) to resolve the atomic-level structure of metallic gasses. We expect to deduce three-
dimensional atomic configuration of the CuZr BMG, which will link with mechanical behaviour of the BMG.
Based on results obtained in the year 2008, new mechanism for mechanical behaviour of BMG will be proposed.
We expect that about 8 research articles will be published in the international recognised journals.
In the year 2008, we will put 2 staff members, 2 postdocs and 3 ph.d. and 3 master students to work on the
present research project. Exchange visiting will be arranged between both sides. One workshop will be held at
Zhejiang University.

5. References
(2007).
Mater. 55, 4409 (2007)

Date

Signature of funding office

Signature of leading scientist
**Impuls- und Vernetzungsfonds**

Federführendes Zentrum:

Deutsches Elektronen-Synchrotron, DESY
Notkestr. 85
D-22607 Hamburg

Partner Institut:

Zhejiang University

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## Einfacher Verwendungsnachweis

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**Zutreffendes bitte ankreuzen:**

\(\checkmark\) Wir bestätigen, dass die Partner die Verwendung der an sie weitergeleiteten Mittel aus dem Zuwendungsvertrag nachgewiesen haben.


---

Hamburg, den 27.08.2009

Ort, Datum

Unterschriften

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\(^1\) Bei mehreren Partnern bitte auf separatem Blatt einzeln ausweisen.
Usage List of Funds

Name of the project: *Investigation of Metallic Glasses under Stress by Synchrotron Radiation Techniques*

Costs of the project partner(s) Zhejiang University in the fiscal year 2008:

- Personal costs: 17,906 €
- Travel costs: 9,477 €
- Costs for workshops, conferences, etc: 1,000 €
- Other direct costs: 43,972 €
- **Total costs**: 72,355 €

Total funds sent by DESY to the partner(s) or received by the partner: 72,000 €

Brief description of the activities (achieved goals, time schedule and perspectives):

In the year 2008, the group, Laboratory of New-Structured Materials, Zhejiang University, has been pursuing all research activities planned in the Zhejiang University-Helmholtz Research Collaboration Program with a project entitled "Investigation of Metallic Glasses under Stress by Synchrotron Radiation Techniques". The summary of all activities are expressed as follows:

1. **Research activities**

   1.1 **Deformation of bulk metallic glasses**

   We discovered an intrinsic plastic Cu$_4$Zr$_{66}$Al$_{14}$Ti$_2$ BMG with high strength and superior compressive plastic strain of up to 32.5 %, which was successfully fabricated by copper mold casting [1]. The correlation of mechanical properties with atomic structure of the BMG was investigated by using Synchrotron Radiation techniques. It is found that the superior compressive plastic strain is attributed to large amount of randomly distributed free volume induced by Ti minor alloying, which results in extensive shear band formation, branching, interaction and self-healing of minor cracks. The mechanism of plasticity presented here suggests that the creation of large amount of free volume in BMGs by minor alloying or other methods might be a new promising way to enhance plasticity of BMGs. In order to confirm the idea of free-volume effect on mechanical behavior of BMGs, we further report the improvement of plasticity in a ternary monolithic CuZrAl BMG caused by large amount of randomly-distributed free volume induced during solidification using high cooling rate [2]. It reveals that the plasticity of BMGs can be indeed tailored by introducing different amounts of free volume in BMGs. These results demonstrate that introducing free volume to BMGs could be one promising way to improve plasticity of BMGs. We also successfully achieved large macroscopic compressive plastic deformation (over 15%) and work-hardening-like behavior in a monolithic BMG through tailoring loading stress distribution experimentally [3]. To uncover the influence of the preexisting/residual stress on mechanical behavior of BMGs, we performed microvickers indentation studies of a stressed BMG [4]. The preexisting stress was introduced by bending. The results show that the nominal hardness decreases with preexisting tensile stress and increases with preexisting compressive stress. The real hardness decreases with preexisting tensile stress, but does not increase obviously with preexisting compressive stress. The finite element analysis indicates that the strong hardness dependence on stress results from the large elastic limit of BMGs. The compressive stress induced the formation of high density...
shear bands, which results in softening, reducing the enhancement of hardness induced by applied compressive stress. The results obtained in this work are helpful to understand the mechanical behavior of BMGs. The relationship of hardness difference vs. applied stress reported here indicates that indentation technique might be a promising method to characterize residual stress in BMGs.

1.2 Development of novel bulk metallic glasses

Our group at Laboratory of New-Structured Materials, Zhejiang University, developed the a novel ZrCu-based bulk metallic glass at least 20 mm [5] together with the formation of about 25 gram amorphous metallic ingots in a wide Zr-(Cu,Ag)-Al composition range using conventional arc-melting machine. The effect of Ag addition on glass forming ability of the quaternary alloy has been systematically investigated from the structural, thermodynamic and kinetic points of view. The origin of high glass forming ability in the studied system is attributed to denser local atomic packing and the smaller difference in Gibbs free energy between amorphous and crystalline phases of Zr-(Cu,Ag)-Al BMGs (for Zr₆₄Cu₂₀₅₅Al₁₅, ΔG* = 1.5 kJ/mol). The alloy shows good thermal and mechanical properties: glass-transition temperature T_g = 703 K, relatively wide supercooled liquid region ΔT_L = 72 K, high activation energy for crystallization E_a = 3.0 eV, fragility parameter m = 49, yield strength 1822 MPa, fracture strength 2163 GPa, Vicker’s hardness 533±3, Young’s modulus 92 GPa, shear modulus 33.8 GPa, and Poisson ratio 0.367. It also exhibits high corrosion resistance in H₂SO₄ solution. The combination of high glass forming ability (critical sizes for BMG more than 20 mm), relatively wide supercooled liquid region ΔT_L = 72 K, excellent mechanical properties (up to 2100 MPa fracture strength and about 28 % compressive plasticity), high corrosion resistance (in H₂SO₄ solution), with cheap and environment-friend raw materials enables to make the newly-developed Ni-free Zr-(Cu,Ag)-Al BMG alloys as promising engineering materials.

We studied the effect of the fourth element on glass forming ability (GFA) in Ni-Nb-Zr-X (X = Ti, Ta, Fe, Cu, Co, V, Y, Mo, Sn, Al, Si) BMG system [6]. Among these elements, Co addition can increase GFA of the Ni-Nb-Zr BMG system. The best glass former is Ni₅₂Nb₅Zr₁₂Co₅ alloy with critical diameter of 3.5 mm. The corrosion rate of this alloy is approximately one order of magnitude less than that of the stainless steel in aggressive 6 M HCl open to air at room temperature. This alloy exhibits high T_g of 866 K, supercooled liquid region ΔT_L of 45 K, compressive fracture strength of 2.9 GPa, 1 % compressive plasticity, and excellent corrosion resistance as compared to stainless steel. Furthermore, we studied quaternary Fe₇₋₂₋₅₋₂₋₂₋₂₋₂ (M = Ni, Co, and Mo) BMGs [7]. It is found that a fully amorphous Fe₇₋₂₋₅₋₂₋₂₋₂ cylinder rod with 6.5 mm in diameter can be prepared by copper mold injection. These alloys have a high glass transition temperature of about 900 K with high fracture strengths up to about 3 GPa although they are still brittle. Magnetic measurements reveal that they are ferromagnetic at ambient temperature with low coercive force of about 2 A/m, saturation magnetization of about 0.7 T and effective permeability of about 7000 at 100 kHz. The newly-developed Fe-based quaternary alloys exhibit excellent combination properties: superior glass forming ability (GFA), high glass transition temperature, and soft magnetic properties, which could have potential applications in electronic industries.

1.3 Atomic structures of metallic glasses

Recently, binary Cu-Zr BMGs have been synthesized. It was found that the glass forming ability in the system strongly depends on compositions, even narrow down to 1 at.%. Thus, to determine the atomic structure of binary Cu-Zr BMG becomes very important. In this work [8], atomic structures of Cu₄₄Zr₅₅ BMG, together with eutectic composition Cu₄₄Zr₃₂ MG ribbon for a comparison, have been investigated by a combination of state-of-the-art experimental techniques (synchrotron radiation-based x-ray diffraction (XRD) and extended x-ray absorption fine structure (EXAFS)) with computational methods (reverse Monte Carlo (RMC) and ab initio molecular dynamics (VASP) simulation). Three-dimensional (3D) atomic configuration of the binary Cu₄₄Zr₅₅ BMG is established. It is found thaticosahedron-like clusters are dominant in both MGs. However, icosahedron-like clusters centered by Cu atoms are slightly denser packing and less distorted in Cu₄₄Zr₅₅, which can enhance the glass forming ability by suppressing atomic movements and increasing the structural incompatibility with competing crystalline phases. The atomic arrangements from short to medium range order are envisaged and compared between both glasses. The significant increase in critical size of BMGs from binary Cu-Zr (2 mm) to ternary Cu-Zr-Al (over 5 mm) provides a suitable prototype of BMGs to study the correlation of structure with GFA by using available experimental and computational methods. In this work [9], atomic structures of Cu₄₄Zr₄₆Al₁₈ BMG, together with binary Cu₅₀Zr₅₀ MG ribbon for comparison, have been investigated. Based on the atomic configuration of the ternary Cu₄₄Zr₄₆Al₁₈ BMG, we explain high GFA of ternary Cu₄₄Zr₄₆Al₁₈ alloy from three aspects of atomic structure: (1) rather homogeneous distribution of Al atoms around Cu and Zr atoms, (2) modifying the environment around Cu and Zr atoms away from the local structures of the competing crystalline phase, (3) increasing the amount of icosahedron-like clusters and making their distribution more homogeneous.
among different polyhedra in three dimensional space. The atomic arrangements from short to medium range order are explored and a favorable configuration is also mapped for Cu_{62}Zr_{16}Al_{12} BMG with high GFA. We believe that the results obtained here will trigger more atomic structure studies to uncover the nature of GFA for various systems.

2. Manpower
Zhejiang University has put 1 postdoc, 5 ph.d. and 4 master students to work on the present research project. They worked hard and obtained many interesting results, which have been published in the international recognized journals.

3. Meeting and exchange visiting
In the year 2008, Prof. Jianzhong Jiang visited Hamburg and attended the RQ13 meeting and Dr. Xiaodong Wang worked at Hasylab, Hamburg for about 3 months (October-December 2009). Dr. H. Franz visited Zhejiang University for one week. Dr. J. Bendnarcik attended the RQ13 meeting. Both sides exchanged their research results often via visiting and e-mail. One joint workshop: International Symposium of Amorphous Alloys, was held at Zhejiang University in the time period 19-22 November. About 100 participants attended the meeting and Dr. H. Franz and Prof. J.Z. Jiang both gave one invited talk at the meeting.

4. Time schedule and perspectives
In the year 2009, we will continue our effort to study atomic structure, phase transformation and mechanical properties of metallic glasses using Synchrotron Radiation techniques. More systems will be studied by using a combination of state-of-the-art experimental techniques to resolve the atomic-level structure of metallic glasses. We expect to uncover atomic configuration of some metallic glasses. Based on results obtained in the year 2009, new mechanism for mechanical behavior of BMGs will be proposed. We expect that about 8 research articles will be published in the international recognised journals.

In the year 2009, we will put 2 staff members, 1 postdoc and 3 ph.d. and 4 master students to work on the present research project. Exchange visiting will be arranged between both sides. One workshop will be held at Zhejiang University.

5. References
A list of cost

1. Personal costs
   1 postdoc: 7,622 €
   2 ph.d.: 7,108 €
   3 master students: 3,176 €
   Zhejiang university puts the 26930 € for one staff, one ph.d. and one master student.

   17,906 €

2. Travel costs
   The cost for Prof. Jianzhong Jiang’s visit to Germany: 2,554 €
   The flight ticket for Dr. Xiaodong Wang’s visit to Hamburg: 1,012 €
   The cost for four persons to perform SR experiments at KEK: 5,911 €

   9,477 €

3. Costs for workshop, conferences, etc
   The cost for one workshop held in Zhejiang University: 1,000 €

   1,000 €

4. Other direct costs
   The cost for some parts for the DSC: 1,761 €
   The cost for some parts for the compression machine: 1,921 €
   The cost for raw materials: 30,756 €
   The cost for gas, quartz tube, polishing materials, copper mold etc.: 9,534 €

   43,972 €

Total costs

   72,355 €

Total funds sent by DESY to the partner(s)
or received by the partner

   72,000 €
**Impuls- und Vernetzungsfonds**

Federführendes Zentrum:

Deutsches Elektronen-Synchrotron, DESY  
Notkestr. 85  
D-22607 Hamburg

Partner Institut:  
Zhejiang University

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**Einfacher Verwendungsnachweis**

Förder-Nr.: IK-CH-002

- ☑ Zwischennachweis
- □ Verwendungsnachweis (Schlussnachweis)
  für den Zeitraum 01.01.2009 bis 31.12.2009

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Zutreffendes bitte ankreuzen:

- ☑ Wir bestätigen, dass die Partner die Verwendung der an sie weitergeleiteten Mittel aus dem Zuwendungsvertrag nachgewiesen haben.

Hamburg, den 22.04.2010  
Ort, Datum

Unterschrift(en)

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Sachlich richtig | rechnerisch richtig
(mit Euro)

... , den ...  
Unterschrift(en)

Intervention:

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¹ Bei mehreren Partnern bitte auf separatem Blatt einzeln ausweisen.
**Usage List of Funds**

Name of the project: **Investigation of Metallic Glasses under Stress by Synchrotron Radiation Techniques**

Costs of the project partner(s) _Zhejiang University_ in the fiscal year _2009_:

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Total funds sent by DESY to the partner(s) or received by the partner: 

- _55,000_ €

Brief description of the activities (achieved goals, time schedule and perspectives):

In the year 2009, the group, Laboratory of New-Structured Materials, Zhejiang University, has been pursuing all research activities planned in the Zhejiang University-Helmholtz Research Collaboration Program with a project entitled "Investigation of Metallic Glasses under Stress by Synchrotron Radiation Techniques". The summary of all activities are expressed as follows:

1. **Research activities**
   1.1 **Metallic glasses under tension**
   
   Mechanical properties of bulk metallic glasses (BMGs) are currently of great interest. One key issue is the failure mechanism of BMGs upon loading, which still remains unclear. Under uniaxial compression or bending conditions, some BMGs exhibit pronounced plasticity. More recently, pronounced tensile ductility for BMG composites was also reported. However, no tensile plasticity has been found so far for monolithic BMGs at ambient temperature and by uniaxial tension. To further understand the evaluation of STZ or the distribution of free volume upon loading, the deformation at the stress close to the fracture strength is greatly concerned. Usually the plastic deformation of BMGs is regarded to be similar to that of most crystalline counterparts, linearly and reversibly. However, some reports show that preloading below the fracture strength of BMGs can enhance excess free volume and produce extended plasticity upon reloading, indicating that some irreversible effect happens in the elastic deformation. We carried out the uniaxial tensile behavior of Zr_{52}Al_{18}Ni_{23}Cu_{15}, Cu_{46}Zr_{44}Al_{8}, Zr_{56}Cu_{25}Al_{15}Ag_{2} and La_{0.5}Al_{15}Cu_{46}Ag_{20}Co_{10}Ni_{5} bulk metallic glasses (BMGs). Different local atomic responses to tensile stress for four BMGs were investigated by in situ high energy x-ray diffraction (HEXRD). It is found that the local strain is basically homogeneously distributed at low stress. However, heterogeneity appears obviously when the stress is close to the fracture strength. The largest fluctuation happens in the range of 10 - 14 Å that seems the boundary between superclusters, where excess open volume may accumulate. The amplitude of fluctuation in local strain for these four BMGs could relate to the distribution of excess free volume within the medium range order. This might be a precursor for the formation of shear bands. The results obtained in this work suggest that relatively homogeneous atomic packing within the medium range order may promote plasticity of monolithic BMGs, which shed light to design novel BMGs with tensile plasticity.

1.2 **Metallic glasses under compression**
Combining one metal with another leads to a range of alloys with properties superior to each individual end member. Since the Bronze and Iron Ages, the quest for new metallic alloys through various chemical and metastable quenching paths has played a crucial role in the advancement of civilizations. The most common type of alloy is a substitutional crystalline solid solution in which atoms of one element randomly substitute for atoms of another element in a crystal structure. The possibilities for substitution, however, are restricted by the classic empirical Hume-Rothery (HR) Rules (1) which require the components have atomic size within 15%, and electronegativity within 0.4 of each other. For instance, the archetypal 4f metal Ce alloys with similar rare-earth metals to form “miscellaneous” which has unusual pyrophoric properties and strength for a broad range of chemical and physical applications, and the sp-bonded light metal Al alloys with similar atoms to form a family of aluminum alloys that have enormous technological importance and application in everyday life, but no known binary substitutional crystalline alloy exists between Ce and Al because their differences of 28% in atomic radii and 0.45 in electronegativity far exceed the HR limit. They can only form stoichiometric compounds in which Ce and Al are chemically ordered and occupy separate crystallographic sites, or metallic glass synthesized by rapidly quenched from melt in which Ce and Al are disordered both chemically and structurally. We carried out compression behavior of Ce3Al metallic glass. Using high-pressure at 298 K, we synthesized a face-centered cubic (fcc) disordered alloy of highly dissimilar elements — large Ce and small Al atoms — by compressing the Ce3Al metallic glass above 25 GPa. Synchrotron x-ray diffraction, Ce L3-edge absorption spectroscopy, and ab-initio calculations revealed that the pressure-induced Kondo volume collapse and 4f electron delocalization of Ce reduced the differences between Ce and Al and brought them within the Hume-Rothery limit for substitutional alloying. The novel alloy remained after complete release of pressure which was also accompanied by the transformation of Ce back to its ambient 4f electron localized state and reversal of the Kondo volume collapse, resulting in a non-Hume-Rothery alloy at ambient conditions. The present discovery opens a new route for making novel alloys including Ce-Al alloys of ratios other than 3:1, Ce alloys with other incompatible elements, and other f-electron alloys. Such alloys may display a range of unusual and useful mechanical, electronic and magnetic properties and greatly increase the choice of materials for a variety of applications.

1.3 Development of Fe-based bulk metallic glasses

In the year 2009 our group at Laboratory of New-Structured Materials, Zhejiang University, focuses our efforts on the development of Fe-based BMGs. This is one of the most important BMG systems because of the low cost and abundance of Fe element in earth. However, the Fe-based BMGs with combination of all the merits (high glass forming ability, high mechanical strength and good plasticity) were rarely reported. In fact, the combination of all the merits is essential/desirable (even imperative) for the wide application of Fe-based BMGs as engineering materials. In this work, we developed a Fe-Co-Nb-B system BMG with enhanced glass forming ability (critical diameter up to 2.5 mm), high glass transition temperature of 821 K, large supercooled region of 58 K, ultrahigh compressive strength of about 4.5 GPa, ultrahigh Vickers hardness of about 13 GPa, and good compressive plastic strain of about 0.6%, which was searched using a strategy for catching the best glass former based on relative glass forming ability of alloys. The combination of high glass forming ability, high thermal stability, ultrahigh strength and good plasticity makes this alloy of potential applications as a structural material. We further investigated glass forming ability (GFA), mechanical and magnetic properties of Fe77W13B6 (x=0, 1, 2 and 3 at. %) and Fe75.5W7.5Y5B22 (x=1, 2, 3, 4, 5 and 6 at.%) alloys. It is found that fully amorphous Fe50W7.5Y9B22 and Fe80W4Y6B22 cylindrical rods with 4 mm in diameter can be prepared by using copper mold casting. The newly-developed Fe-based quaternary alloys exhibit excellent combination properties: good GFA, high onset crystallization temperature of 970 K, high fracture strength of about 4 GPa, Vickers hardness of about 1000 kg/mm², and good soft magnetic properties at ambient temperature (saturation magnetization of about 0.8 T and coercive force of below 2 A/m), which show potential applications in electronic industries. The effect of W addition on GFA in the Fe-Y-B alloy system is also discussed.

Minor addition of several particular elements, such as Co, Mo, Nb and Y, was found to be an effective way to enhance glass forming ability (GFA) of Fe-based BMGs, while its origin still remains an open question. Recently, a remarkable enhancement of GFA (from about 0.025 to 2 mm) was reported in simple Fe-RE-B (RE=Y, Sc, Dy, Ho, and Er) ternary system by just adding tiny RE (about 4-6 at.%). The result raises an interesting question: what are the roles of RE atoms for the enhancement of GFA in the Fe-B system? In this work, we select Fe-Y-B system, as a prototype, to investigate the correlation of GFA with its atomic structure by using extended X-ray absorption fine structure (EXAFS), together with differential scanning calorimetry (DSC) and X-ray diffraction (XRD). Two questions are addressed: (1) why can tiny Y addition enhance GFA and (2) why does more
Y addition (> 7 at.%) deteriorate GFA. It is confirmed that the incorporation of minor large-sized Y atoms promotes the formation of complex B_{6}(Fe,Y)_{22} phase, compared with Fe_{2}B phase in the Fe-B binary alloy. With further addition of Y (up to 6 at.%), excessive internal strain leads to the distortion of B_{6}(Fe,Y)_{22}-like phase and eventually favors the formation of amorphous state during solidification. Consequently, GFA increases from 0.025 mm Fe_{70}B_{30} thin ribbon to 2 mm Fe_{82}Y_{2}B_{8} rod.

2. Manpower
Zhejiang University has put 2 postdoc, 3 ph.d. and 4 master students to work on the present research project. They worked hard and obtained many interesting results, which have been published in the international recognized journals.

3. Meeting and exchange visiting
In the year 2009, Prof. Jianzhong Jiang visited Hasylab, Hamburg and Prof. Fang Yunzhuang, Dr. Xiaodong Wang, Mr. Luo Hongbo worked at Hasylab, Hamburg for about 2 months (July-August 2009). Dr. H. Franz visited Zhejiang University for one week. Prof. Jianzhong Jiang attended three international conferences giving invited talks. Both sides exchanged their research results often via visiting and e-mail.

4. Time schedule and perspectives
In the year 2010, we will continue our effort to study atomic structure, phase transformation and mechanical properties of bulk metallic glasses using Synchrotron Radiation techniques. More systems will be studied by using a combination of state-of-the-art experimental techniques (synchrotron radiation-based XRD, XAFS and neutron diffraction) and computational techniques (reverse Monte Carlo (RMC) and ab initio molecular dynamics simulation) to resolve the atomic-level structure of metallic glasses. We expect to uncover atomic configuration of some metallic glasses. Based on results obtained in the year 2010, new mechanism for mechanical behavior of BMG will be proposed. We expect that about 8 research articles will be published in the international recognized journals.

In the year 2010, we will put 2 staff members, 2 postdoc and 4 ph.d. and 4 master students to work on the present research project. Exchange visiting will be arranged between both sides. One joint workshop: International Conference for Mechanical Properties of Materials, will be planned to be held at Zhejiang University in the time period 24-28 May, 2010.

5. References
1 X.D. Wang, J. Bednarick, H. Franz, H.B. Lou, Z.H. He, Q.P. Cao, and J.Z. Jiang
   Local strain behavior of bulk metallic glasses under tension studied by in situ high energy x-ray diffraction, Appl. Phys. Lett. 94, 011911 (2009)
3 X.D. Wang, J.Z. Jiang, and H. Franz, Mechanical properties of monolithic Zr_{52}Al_{15}Ni_{15}Cu_{12} bulk metallic glass, J Alloys and Compounds 483, 132 (2009)
8 X.M. Huang, X.D. Wang, Y. He, Q.P. Cao and J.Z. Jiang, Are there two glass transitions in Fe-M (M=Mo, W, Nb)-Y-B bulk metallic glasses? Scripta Mater. 60, 152 (2009)
9 X.M. Huang, X.D. Wang, and J.Z. Jiang, Origin of high glass forming ability of Y-containing FeB-based alloys.


_2010,4,24__
Date

___________________________
Signature of funding office

___________________________
Signature of leading scientist
A list of cost

1. Personal costs \(13,676\) €
   - 1 postdoc (partial): 5,823 €
   - 2 ph.d. (partial): 5,430 €
   - 3 master students (partial): 2,423 €
   Zhejiang university puts the 26930 € for one staff, two ph.d. and three master students.

2. Travel costs \(7,240\) €
   - The cost for Jianzhong Jiang’s visit to Germany, France and Japan for meetings: 3,980 €
   - The flight tickets for Fang Yunzhuang visit to Hamburg: 1,236 €
   - The flight tickets for Xiaodong Wang visit to Hamburg: 1,012 €
   - The flight tickets for Luo hongbo visit to Hamburg: 1,012 €

3. Costs for workshop, conferences, etc \(760\) €
   - The cost for one workshop held in Zhejiang University: 760 €

4. Other direct costs \(33,594\) €
   - The cost for raw materials: 32,549 €
   - The cost for gas, quatz tube, polishing materials etc.: 1,045 €

Total costs \(55,270\) €

Total funds sent by DESY to the partner(s)
or received by the partner \(55,000\) €
Impuls- und Vernetzungsfonds
Federführendes Zentrum:
Deutsches Elektronen-Synchrotron,
DESY
Notkestr. 85
D-22607 Hamburg

Partner Institut:
Zhejiang University

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| 4 | Abgerechnet insgesamt (Summe von Spalte 2) | **145.311,48** | Anerkannt |
| 5 | Eigenmittel | 0,00 |
| 6 | Erhaltene Zahlungen aus dem Impulsfonds | -162.500,00 |
| 7 | Kassenbestand aus Vorjahr (Guthaben) | -45.932,20 |
| 8 | Kassenbestand (Guthaben) zum 31.12.2010 | -63.120,72 |

Zutreffendes bitte ankreuzen:

- [ ] Wir bestätigen, dass die Partner die Verwendung der an sie weitergeleiteten Mittel aus dem Zuwendungsvertrag nachgewiesen haben.

... Hamburg, den 03.05.2011,.................. Ort, Datum

Unterschrift(en) U. Wolf, Vorsitzender Finanzabteilung

Sachlich richtig | rechnerisch richtig
(mit Euro)

Unterschrift(en) U. Wolf, Vorsitzender Finanzabteilung

Intervention:

1 Bei mehreren Partnern bitte auf separatem Blatt einzeln ausweisen.
Usage List of Funds

Name of the project: Investigation of Metallic Glasses under Stress by Synchrotron Radiation Techniques

Costs of the project partner(s) Zhejiang University in the fiscal year 2010:

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<th>Personal costs</th>
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Total funds sent by DESY to the partner(s) or received by the partner: €70,000

Brief description of the activities (achieved goals, time schedule and perspectives):

In the year 2010, the group, Laboratory of New-Structured Materials, Zhejiang University, has been pursuing all research activities planned in the Zhejiang University-Helmholtz Research Collaboration Program with a project entitled “Investigation of Metallic Glasses under Stress by Synchrotron Radiation Techniques”. The summary of all activities are expressed as follows:

1. Research activities

1.1 Atomic structures of Zr_70Ni_30-Pd_x (x-0-30 at.%) and Zr_45Cu_55Al_15 metallic glasses were investigated by reverse Monte Carlo simulation combining with x-ray diffraction, Cu, Ni, Zr, and Pd K-edge extended x-ray absorption of fine structure measurements [1,2]. Minor Al addition increases closer atomic packing and strong bonding effect, which enhance the glass forming ability in Zr-Cu system. A series of features in S(Q)s and G(r)s for Zr_70Ni_30-Pd_x (x=0-30 at.%) metallic glasses suggest that Zr_70Pd_30 has even higher atomic packing efficiency than Zr_70Ni_30. Structural information obtained by reverse Monte Carlo simulation upon experimental data is compared with those calculated according to hard sphere dense packing principle and corresponding crystal phase. Strong bonding effect is determined to be intrinsic character in Zr_70Pd_30 metallic glass. Electronic structure calculations also confirm the strong bonding.

1.2 Local atomic structures at glassy, supercooled liquid and liquid states for La_80Al_10Cu_10Ag_3Ni_5Co_5, La_80Al_10Cu_10Ag_3 and La_80Al_15Cu_15Ag_5 bulk metallic glasses have been investigated by in situ high temperature X-ray diffraction [3]. We found that the coordination number to be about 15.1±0.1 for the alloy does not depend on temperature up to liquid temperature, while it decreases slightly with temperature for the La_80Al_15Cu_15 and La_80Al_15Cu_15Ag_5 alloys. The S(q) data recorded at supercooled liquid region can be well described by the Debye theory. For the three alloys, volume expansion coefficient and the slopes of radial variation for the first to third nearest neighboring coordination shells show differences at glassy-to-supercooled liquid transition while no obvious changes were detected at supercooled liquid-to-liquid transition for them. The linear expansion coefficient value (1.6±0.1×10^-5 K^-1) below glass transition temperature deduced from S(q) data is consistent with that detected by dilatometer (1.25±10^-5 K^-1) for the La_80Al_15Cu_15Ag_3Ni_5Co_5 bulk metallic glass.

1.3 Using high-pressure synchrotron x-ray absorption spectroscopy [4], we observed the Ce 4f electron in Ce_75Al_25
metallic glass transform from its ambient localized state to an itinerant state above 5 GPa. A parallel x-ray diffraction study revealed a volume collapse of about 8.6%, coinciding with 4f delocalization. The transition started from a low-density state below 1.5 GPa, went through continuous-densification ending with a high-density state above 5 GPa. This new type of electronic polymorphism in densely-packed metallic glass is dictated by the Ce constituent, and is fundamentally distinct from the well-established structural polymorphism in which densification is caused by coordination change and atomic rearrangement.

2. Manpower
Zhejiang University has put 2 staff member, 2 postdoc, 2 ph.d. and 3 master students to work on the present research project. They worked hard and obtained many interesting results, which have been published in the international recognized journals.

3. Meeting and exchange visiting
In the year 2010, Dr. Xiaodong Wang worked at Hasylab, Hamburg for 2 months. Mr. Lou Hongbo worked at Hasylab, Hamburg for 2 months. Dr. H. Franz visited Zhejiang University for one week. Both sides exchanged their research results often via visiting and e-mail. Seven people from Zhejiang university also performed synchrotron radiation experiments at APS in USA and SSRF in Shanghai. One conference: The First International Conference on Mechanical Properties of Materials (ICMPM) was held at Zhejiang University in the time period of 24-28 May, 2010. About 150 people from about 12 countries attend the conference. Dr. H. Franz gave us an invited talk at the meeting. We received very positive response from all participants. Thus, in 2011, we will hold the second International Conference on Mechanical Properties of Materials (ICMPM) at Zhejiang University in the time period of 12-15 June, 2011. About the same size will be expected.

4. Time schedule and perspectives
In the year 2011, we will continue our effort to study the correlation of mechanical properties with atomic structure of bulk metallic glasses using Synchrotron Radiation techniques. Simple systems, e.g., CeAl, NiNb, CuZr metallic glasses, will be studied by using a combination of state-of-the-art experimental techniques (synchrotron radiation-based XRD, and XAFS) and computational techniques (reverse Monte Carlo (RMC) and ab initio molecular dynamics simulation) to resolve the atomic-level structure of metallic glasses. We expect to deduce three-dimensional atomic configuration of the CeAl, NiNb and CuZr metallic glasses, which will link with mechanical behaviour of the metallic glasses. Based on results obtained in the year 2010, new mechanism for mechanical behaviour of metallic glasses will be proposed. We expect that about 5 research articles will be published in the international recognised journals.

In the year 2011, we will put 2 staff members, 2 postdocs and 3 ph.d. and 3 master students to work on the present research project. Exchange visiting will be arranged between both sides. One workshop: “The Second International Conference on Mechanical Properties of Materials (ICMPM)” will be held at Zhejiang University in the time period of 12-15 June, 2011. About 150 participants will be expected.

5. References

2011,5,6
Date

Signature of funding office

Signature of leading scientist
A list of cost

1. Personal costs

   1 postdoc: 8,978 €
   1 ph.d.: 5,672 €
   3 master students: 3,163 €

   Zhejiang university puts the 33,209 € for one staff and one ph.d. student.

2. Travel costs

   6,917 €

   The flight ticket for Dr. Xiaodong Wang's visit to Hamburg: 1,058 €
   The flight ticket for Mr. Lou Hongbo's visit to Hamburg: 1,058 €
   The cost for seven persons to perform SR experiments at APS and SSRF: 4,801 €

3. Costs for workshops, conferences, etc

   1,123 €

   The cost for one conference held in Zhejiang University:

4. Other direct costs

   44,218 €

   The cost for raw materials: 35,149 €
   The cost for crucibles: 4,178 €
   The cost for gas, quartz tube, copper mold etc.: 4,891 €

Total costs

   70,071 €

   Total funds sent by DESY to the partner(s) or received by the partner

   70,000 €
**Impuls- und Vernetzungs fonds**

**Förderner Nr.:** IK-CH-002

- **Zwischennachweis**
- **Verwendungsnachweis (Schlussnachweis)** für den Zeitraum 01.01.2011 bis 31.12.2011

**Partner Institut:**
Zhejiang University

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|  | Nachgewiesen | Anerkannt |
| 62 | 156,742,99 | |
| 6 | Eigenmittel | 0,00 |
| 7 | Erhaltene Zahlungen aus dem Impulsfonds | -162,500,00 |
| 8 | Kassenbestand aus Vorjahr (Guthaben) | -63,120,72 |
| 9 | Kassenbestand zum 31.12.2011 | -68,877,73 |

Zutreffendes bitte ankreuzen:
- Wir bestätigen, dass die Partner die Verwendung der an sie weitergeleiteten Mittel aus dem Zuwendungsvertrag nachgewiesen haben.


... Hamburg, den 30.04.2012

Ort, Datum

Unterschrift(en): [Unterschrift]

Deutsches Elektronen-Synchrotron,
Forschungszentrum der Helmholtz-Gemeinschaft
Notkestr. 85 | 22607 Hamburg | Tel. 040-89925-0

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1 Bei mehreren Partnern bitte auf separatem Blatt einzeln ausweisen.
Usage List of Funds

Name of the project: Investigation of Metallic Glasses under Stress by Synchrotron Radiation Techniques

Costs of the project partner(s) Zhejiang University in the fiscal year 2011:

- Personal costs: 17,813 €
- Travel costs: 5,980 €
- Costs for workshops, conferences, etc: 1,367 €
- Other direct costs: 56,414 €

[In the year 2011, raw materials and others get expense]

Total costs: 81,574 €

Total funds sent by DESY to the partner(s) or received by the partner: 70,000 €

Brief description of the activities (achieved goals, time schedule and perspectives):

In the year 2011, the group, Laboratory of New-Structured Materials, Zhejiang University, has been pursuing all research activities planned in the Zhejiang University-Helmholtz Research Collaboration Program with a project entitled “Investigation of Metallic Glasses under Stress by Synchrotron Radiation Techniques”. The summary of all activities are expressed as follows:

1. Research activities

1.1 Structural evolution of an Au-based bulk metallic glass (BMG) after severe plastic deformation (SPD) was investigated. The newly-formed glass contains high-density shear bands, a reduced ordering and a concomitant excess free volume determined by SR techniques. Moreover, it exhibits a temperature-independent local structure even in the supercooled liquid region, but a reduced thermal stability reflected in an accelerated crystal nucleation and growth process. These results suggest that SPD modifies the atomic structure of BMGs by localized shear band formation and thus, producing so-called nanoglasses. Constant-rate heating experiments using a fast x-ray camera (time resolution of 2s) reveals detailed information about the thermal stability of the L62Al60(G32Ag18)5Cu5Ni5Co5 (at.%) bulk metallic glass (BMG). Analyzing diffraction patterns in a reciprocal space yields thermal expansion of amorphous alloy providing insight about the thermally activated relaxation effects and kinetics of glass transition. The glass transition appears as a brake in the value of the coefficient of the volume thermal expansion αV. Furthermore, real space analysis based on reduced pair distribution function G(r) allows tracing the changes in the local atomic structure of amorphous material during constant-rate heating.

1.2 To be new structural materials, the critical size is always the bottleneck of bulk metallic glasses (BMGs) due to the cooling rate restriction. In the year 2011, we successfully develop a new alloy of Zr46Cu30.14Ag36Al8Be7.5, which can be cast into amorphous rods in 73 mm diameter by copper mould casting. This finding is linked with our understanding of atomic structure of metallic glasses. The strong glass forming ability of this alloy is closely related to the Be addition, which not only suppresses the phase separation happening in the as-cast Be-free BMG but also sustains low Gibbs free energy difference for crystallization. This finding will stimulate more interests in developing BMGs and their industrial applications. Furthermore, we successfully fabricate an intrinsic plastic Zr53.5Cu31.6Ag7.6Al7.5 bulk metallic glass (BMG) with excellent bending and compressive properties in contrast to the poor plasticity that is usually observed in bulk metallic glasses. No inhomogeneous distribution can be observed. We suggest that the superior compressive and bending plastic strain was attributed to a large amount of randomly distributed free volume after a serial of comparison. The thermal, corrosion and thermal expansion properties, as well as elastic constants for the newly developed ZrCuAgAl BMG, are also presented.
1.3 Glass lacks the long-range periodic order that characterizes a crystal. In the Ce₇₅Al₂₅ metallic glass (MG), however, we discovered a long-range topological order corresponding to a single crystal of indefinite length. Structural examinations confirm that the MG is truly amorphous, isotropic, and unstrained, yet under 25 GPa hydrostatic pressures, every segment of a cm-length MG ribbon devitrifies independently into a face-centered cubic (fcc) crystal with the identical orientation. Using molecular dynamics simulations and synchrotron x-ray techniques, we elucidate that the mismatch between the large Ce and small Al atoms frustrates the crystallization and causes amorphization, but a long-range fcc topological order still exists. Pressure induces electronic transition in Ce which eliminates the mismatch and manifests the topological order by the formation of a single crystal.

2. Manpower
Zhejiang University has put 2 staff members, 2 postdocs, 2 ph.d. and 3 master students to work on the present research project. They worked hard and obtained many interesting results, which have been published in the international recognized journals.

3. Meeting and exchange visiting
In the year 2011, Prof. Jianzhong Jiang visited Hasylab for one week and Mr. Lou Hongbo worked at Hasylab, Hamburg for 2 months. Dr. H. Franz visited Zhejiang University for one week. Both sides exchanged their research results often via visiting and e-mail. Fifteen people from Zhejiang university also performed synchrotron radiation experiments at SSRF in Shanghai.

One conference: "The Second International Conference on Mechanical Properties of Materials (ICMPM)" was held at Zhejiang University in the time period of 12-15 June, 2011. About 120 people from about 10 countries attend the conference. Dr. H. Franz gave us an invited talk at the meeting. We received very positive response from all participants. Thus, in 2012, we will hold "The Third International Conference on Mechanical Properties of Materials (ICMPM)" at Zhejiang University in the time period of 12-15 November, 2012.

4. Time schedule and perspectives
In the year 2012, we will continue our effort to study the correlation of mechanical properties with atomic structure of bulk metallic glasses and liquid melts using Synchrotron Radiation techniques. Simple systems, e.g., CaAl, NiNb, ZrCuAl metallic glasses, will be studied by using a combination of state-of-the-art experimental techniques (synchrotron radiation-based XRD, and XAFS) and computational techniques (reverse Monte Carlo (RMC) and ab initio molecular dynamics simulation) to resolve the atomic-level structure of metallic glasses. We expect to deduce three-dimensional atomic configuration of metallic glasses, which will link with mechanical behaviour of the metallic glasses. Based on results obtained in the year 2011, new mechanism for mechanical behaviour of metallic glasses will be proposed. We expect that about 5 research articles will be published in the international recognized journals.

In the year 2012, we will put 2 staff members, 2 postdocs and 3 ph.d. and 3 master students to work on the project. The Third International Conference on Mechanical Properties of Materials (ICMPM) will be held at Zhejiang University in the time period of 12-15 November, 2012. About 120 participants will be expected.

5. References

Date

Signature of leading scientist
A list of cost

1. Personal costs _17,813________€
   1 postdoc: 8,978 €
   1 ph.d. 5,672 €
   3 master students. 3,163 €
   [Zhejiang university puts the 41,762 € for one staff and one ph.d. student]

2. Travel costs _5,980________€
   The flight ticket for Mr Lou Hongbo’s visit to Hamburg: 1,179 €
   The cost for fifteen persons to perform SR experiments at SSRF: 4,801 €

3. Costs for workshops, conferences, etc _1,367________€
   The cost for one conference held in Zhejiang University: 1,367 €

4. Other direct costs _56,414________€
   The cost for raw materials: 45,149 €
   The cost for crucibles: 5,351 €
   The cost for gas, quartz tube, copper mold etc.: 5,914 €
   [In the year 2011, raw materials and others get expense]

Total costs _81,574________€

Total funds sent by DESY to the partner(s)
or received by the partner _70,000________€
### Impuls- und Vernetzungsfonds

Federführendes Zentrum:

Deutsches Elektronen-Synchrotron, DESY
Notkestr. 85
D-22607 Hamburg

Partner Institut:
Zhejiang University

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### Einfacher Verwendungsnachweis

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- [x] Zwischennachweis
- [ ] Verwendungsnachweis (Schlussnachweis) für den Zeitraum 01.01.2012 bis 31.08.2012

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#### Nachgewiesen | Anerkannt

| 4 Abgerechnet insgesamt (Summe von Spalte 2) | 99.907,85 |
| 5 Eigenmittel                                 | 0,00      |
| 6 Erhaltene Zahlungen aus dem Impulsfonds    | -27.083,00|
| 7 Kassenbestand aus Vorjahr (Guthaben)       | -68.877,73|
| 8 Kassenbestand zum 31.08.2012 (Mehrbedarf)  | 3.947,12  |

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Zutreffendes bitte ankreuzen:

- [x] Wir bestätigen, dass die Partner die Verwendung der an sie weitergeleiteten Mittel aus dem Zuwendungsvertrag nachgewiesen haben.


... Hamburg, den 27.12.2012...

Ort, Datum

Unterschrift(en): U. Wolfram, Leiter Finanzabteilung

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Sachlich richtig | rechnerisch richtig

(unterschrift)

... , den ...

Unterschrift(en)

Intervention:
Usage List of Funds

Name of the project: Investigation of Metallic Glasses under Stress by Synchrotron Radiation Techniques

Costs of the project partner(s) Zhejiang University in the fiscal year 2012:

- Personal costs: 1,369 €
- Travel costs: 0,820 €
- Costs for workshops, conferences, etc: 1,000 €
- Other direct costs: 5,821 €

Total costs: 9,010 €

Total funds sent by DESY to the partner(s) or received by the partner: 9,000 €

Brief description of the activities (achieved goals, time schedule and perspectives):

In the year 2012, the group, Laboratory of New-Structured Materials, Zhejiang University, has been pursuing all research activities planned in the Zhejiang University-Helmholtz Research Collaboration Program with a project entitled “Investigation of Metallic Glasses under Stress by Synchrotron Radiation Techniques”. The summary of all activities are expressed as follows:

1. Research activities

1.1 Pressure-induced amorphous-to-amorphous configuration changes in Ca-Al metallic glasses (MGs) were studied by performing in-situ room-temperature high-pressure x-ray diffraction up to about 40 GPa. Changes in compressibility at about 18 GPa, 15.5 GPa and 7.5 GPa during compression are detected in Ca₆₉Al₀₂₀, Ca₇₂Al₀₂₇, and Ca₆₆₄Al₃₃₆ MGs, respectively, whereas no clear change has been detected in the Ca₅₀Al₅₀ MG. The transfer of s electrons into d orbitals under pressure, reported for the pressure-induced phase transformations in pure polycrystalline Ca, is suggested to explain the observation of an amorphous-to-amorphous configuration change in this Ca-Al MG system. Results presented here show that the pressure induced amorphous-to-amorphous configuration is not limited to f electron-containing MGs.

1.2 The issue, composition dependence of glass-forming ability (GFA) in metallic glasses (MG), has been investigated by by systematic synchrotron radiation-based experimental measurements (XRD and XAFS) coupled with theoretical calculations in Cu-Zr and Ni-Nb alloy systems. It is found that the atomic-level packing efficiency strongly relates to their GFA. The best GFA was located at the largest difference in the packing efficiency of the solute-centered clusters between the glassy and crystal alloys in both MG systems. This work provides an understanding of GFA from atomic level and will shed light on the development of new MGs with larger critical sizes.

1.3 On monolithic Ni-Nb metallic glass films, we experimentally revealed 6.6% elastic strain limit by in-situ transmission electron microscopy observations. The origin of high elastic strain limit may link with high free volume in the film, causing the rearrangement of loosely bonded atomic clusters
(or atoms) upon elastic deformation. This high elastic limit of metallic glass films will shed light on new application fields for metallic glasses, and also trigger more studies for deformation mechanism of amorphous materials in general.

2. Manpower
Zhejiang University has put 2 staff members, 2 postdocs, 2 ph.d. and 3 master students to work on the present research project. They worked hard and obtained many interesting results, which have been published in the international recognized journals.

3. Meeting and exchange visiting
In the year 2012, both sides exchanged their research results often via e-mail. Fifteen people from Zhejiang university also performed synchrotron radiation experiments at SSRF in Shanghai.
One conference: "Workshop on Disordered Alloys" will be held at Zhejiang University in the time period of 13-14 November, 2012. About 60 people will attend the conference. Dr. H. Franz was invited to give an invited talk at the meeting.

4. We strongly wish to continue this joint research project.

5. References

_2012,11,10_

Date

Signature of funding office

Signature of leading scientist
A list of cost

1. Personal costs
   1 master student. 1,369 €
   [Zhejiang university puts another 58,762 € for one staff, two postdocs, two ph.d. and two master students.]

2. Travel costs
   The cost for 3 persons to perform SR experiments at SSRF: 0,820 €
   [Zhejiang university puts another 6,145 € for travelling cost]

3. Costs for workshops, conferences, etc
   The cost for one workshop held in Zhejiang University: 1,000 €
   [Zhejiang university puts another 4,000 € for the workshop]

4. Other direct costs
   The cost for raw materials: 5,821 €
   [Zhejiang university puts another 68,762 € for direct costs]

**Total costs**

9,010 €

Total funds sent by DESY to the partner(s) or received by the partner 9,000 €