

**Zwischenbericht**

Förderprogramm:	Sondermaßnahmen
Impulsfonds-Projektnummer:	IK-Ch-002
Projekttitle:	Investigation of Metallic Glasses under Stress by Synchrotron Radiation Techniques
Federführende/r Wissenschaftler/in	Dr. H. Franz
Berichtszeitraum	1.1.2010 bis 31.12.2010

**Hinweis:**

Sondermaßnahmen sind Einzelprojekte außerhalb von Ausschreibungen zur Förderung herausragender Exzellenz. Ziele, Arbeitsprogramm, Finanzplan etc. sind individuell im jeweiligen Antrag beschrieben.

**Sachbericht**

- a) Fortschritt des im Antrag beschriebenen Arbeitsprogramms  
siehe Anhang
- b) Erreichte Meilensteine
- c) Bisher erreichter oder erkennbarer Mehrwert der Förderung, strategischer Nutzen für die Helmholtz-Gemeinschaft  
Durch das Forschungsprojekt wird die Zusammenarbeit mit der Volksrepublik China, einem der strategische Partner der Helmholtzgemeinschaft, gestärkt. Durch den regelmässigen Austausch werden Beziehungen zu den Kollegen und der Zhejiang Universität gepflegt, aber auch Kontakte zu anderen Universitäten z.B. in Nanjing geknüpft. Längerfristige Besuche chinesischer Kollegen am DESY tragen zur erfolgreichen Druchführung von Forschungsprojekten bei. Das wird auch durch eine Anzahl von gemeinsamen Publikationen und die erfolgreiche Zwischenbegutachtung dokumentiert. Durch das gemeinsame Projekt haben wir Zugang zu den Präparationslabors an der Universität Zhejiang, und können deren Expertise in der Entwicklung von massiven metallischen Gläsern nutzen. Langfristig trägt diese Kollaboration mit chinesischen Wissenschaftlern zu einer Intensivierung der wissenschaftlichen Zusammenarbeit bei, die vor allem im Hinblick auf die leider immer noch nicht stabile Beteiligung Chinas am Europäischen XFEL von großer strategischer Bedeutung ist.
- d) Einhaltung des Finanzierungs- und Zeitplans  
Der Finanzplan wurde im Wesentlichen eingehalten, einige Mittel mussten von 2010 auf 2011 übertragen werden um eine größere Anschaffung tätigen zu können. Der Zeitplan ist eingehalten.
- e) Publikationen, Vorträge, Preise etc. bitte gegebenenfalls als Anhang beifügen

Siehe Anhang

## Activity report for IK-Ch-002 2010

We continued the study of phenomena associated with mechanical and thermal treatment of BMGs. In this field extensive tests of a new detector system (borrowed from the PETRA III team) have been performed. It turned out that using advanced flat panel detectors the efficiency of experiments can be increased significantly. Moreover, the structural response of sample treatments can now be followed with atomic resolution on the time-scales relevant for applications.

In 2010 we focused on thermally activated plasticity in BMGs. Using our test rig equipped with a heater we could demonstrate that increasing the temperature significantly enhances plastic deformation in various metallic glasses. We investigated Fe-based thin ribbons and Pd-Si and Cu-Zr systems. Moreover, ZrNiPd and ZrCuAl metallic glasses were investigated by reverse Monte Carlo simulation combining with x-ray diffraction, and EXAFS. A series of features in the structure of ZrNiPd metallic glasses suggest that Zr<sub>70</sub>Pd<sub>30</sub> has even higher atomic packing efficiency than Zr<sub>70</sub>Ni<sub>30</sub>. Structural information obtained by reverse Monte Carlo simulations was compared with those calculated according to hard sphere dense packing and corresponding crystal phases. Strong bonding effects are determined to be intrinsic in character in the Zr<sub>70</sub>Pd<sub>30</sub> metallic glass. Electronic structure calculations also confirm the strong bonding.

Local atomic structures at glassy, supercooled liquid and liquid states for La-based bulk metallic glasses have been investigated by *in situ* high temperature X-ray diffraction. We found the coordination number to be around 15 for the alloys. The temperature dependence shows no general features up to the liquid phase, but depends on the detailed composition. The scattering data recorded in the supercooled liquid region can be well described by the Debye theory. For three alloys, volume expansion coefficients and the variations of the radii of 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. The linear expansion coefficient below the glass transition temperature deduced from S(q) data is consistent with that detected by a dilatometer.

Using high-pressure synchrotron x-ray absorption spectroscopy we observed the Ce 4f electron to transform from its ambient localized state to an itinerant state above 5 GPa in Ce<sub>75</sub>Al<sub>25</sub> metallic glass. A parallel x-ray diffraction study revealed a parallel volume collapse of about 8.6%. The transition starts from a low-density state below 1.5 GPa, goes through continuous-densification ending with a high-density state above 5 GPa. This new type of electronic polyamorphism in densely-packed metallic glass is dictated by Ce, and is fundamentally distinct from the well-established structural polyamorphism in which densification is caused by coordination change and atomic rearrangement.

## PUBLICATIONS in 2010

- 1 N. Mattern, T. Gemming, J. Thomas, G. Goerigk, H. Franz, J. Eckert  
*Phase separation in Ni-Nb-Y metallic glasses.*  
Journal of Alloys and Compounds **495**, 299 (2010)
- 2 J. Bednarcik, C. Curfs, M. Sikorski, H. Franz, J.Z. Jiang  
*Thermal expansion of La-based BMG studied by in-situ high-energy X-ray diffraction.*  
Journal of Alloys and Compounds **504**, 155 (2010)
- 3 J. Bednarcik, M. Miglierine, C. Curfs, H. Franz  
*Thermal expansion of NANOPERM-type alloys from in-situ X-ray diffraction.*  
AIP Conference Proceedings **1258**, 1 (2010)
- 4 S. Michalik, J. Bednarcik, P. Jiovári, V. Honkimäki, A. Webb, H. Franz, E. Fazakas, L.K. Varga  
*Modeling the atomic structure of Al<sub>92</sub>U<sub>8</sub> metallic glass.*  
Journal of Physics: Condensed Matter **22**, 404209 (2010)
- 5 M. Stoica, N. Van Steenberge, J. Bednarcik, N. Mattern, H. Franz, J. Eckert  
*Changes in short-range order of Zr<sub>55</sub>Cu<sub>30</sub>Al<sub>10</sub>Ni<sub>5</sub> and Zr<sub>55</sub>Cu<sub>20</sub>Al<sub>10</sub>Ni<sub>10</sub>Ti<sub>5</sub> BMGs upon annealing.*  
Journal of Alloys and Compounds **506**, 85 (2010)
- 6 X.D. Wang, H.B. Lou, K. Ståhl, J. Bednarcik, H. Franz, J.Z.Jiang  
*Tensile behavior of orthorhombic  $\alpha''$ -Titanium alloy studied by in situ X-ray diffraction.*  
Materials Science and Engineering A **527**, 6596 (2010)
- 7 S. Pauly, J. Bednarcik, U. Kühn, J. Eckert  
*Plastically deformable Cu-Zr intermetallics*  
Scripta Materialia **63**, 336 (2010)
- 8 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, In Press, Corrected Proof:–, 2010,
- 9 K. Pawlik, J. Bednarcik, P. Pawlik, J.J. Wysocki, W. Kaszuwara, B. Michalski, P. Gebara  
*Phase structure and crystallization of the bulk glassy FeCoZrWB alloys*  
Phys. Status Solidi C **7**, 1336 (2010)
- 10 M. Stoica, J. Das, J. Bednarcik, G. Wang, G. Vaughan, W.H. Wang, J. Eckert  
*Mechanical Response of Metallic Glasses: Insights from In-situ High Energy X-ray Diffraction*  
J. Miner. Met. Mat. Soc. **62**, 76 (2010)

- 11 J. Bednarcik, S. Michalik, P. Kollar, S. Roth  
*Influence of Ball Milling on the Local Atomic Structure of an Amorphous CoFeSiB Alloy*  
Acta Phys. Pol. A **118**, 825 (2010)
- 12 S. Michalik, J. Bednarcik, K. Brzozka, P. Sovak, B. Gorka  
*Microstructural Study of FeSi(Ge)NbCuB Finemet Alloys*  
Acta Phys. Pol. A **118**, 818 (2010)
- 13 D. Olekšáková, P. Kollár, J. Füzer, J. Bednarcik, S. Roth  
*Magnetic Properties of Crystalline NiFe Alloy Prepared by High-Energy Ball Milling and Compacting*  
Acta Phys. Pol. A **118**, 797 (2010)

---

## Conferences and workshops in 2010

In 2010 we organized two workshops were results of the collaboration were discussed: "ICMPM2010" in Hangzhou and "High Energy X-Ray Beamlines at the PETRA III Extension" in Hamburg.

## Talks on conferences in 2010

- [1] **Hard X-ray scattering: powerful tool for investigation of disordered materials**  
J. Bednarcik  
Condensed Matter Physics Seminar at the P.J. Safarik Uni. in Kosice, Kosice, Slovakia (February 8 2010)
- [2] **In situ tensile deformation of Fe-rich metallic glass at elevated temperatures using hard X-ray diffraction**  
J. Bednarcik  
17th International Symposium on Metastable, Amorphous and Nanostructured Materials (ISMANAM 2010), Zurich, Switzerland (July 4-9 2010)
- [3] **Thermal expansion of Nanoperm-type alloys from in-situ x-ray diffraction**  
J. Bednarcik  
Mössbauer Spectroscopy in Materials Science (MSMS2010), Liptovsky Jan, Slovakia (January 1-February 5 2010)
- [4] **Metallic glass in the light of X-rays**  
H. Franz  
International Conference on Mechanical Properties of Materials (ICMPM2010), Hangzhou, PRP China, (May 24-27 2010)
- [5] **Tensile behavior of Cu<sub>46</sub>Zr<sub>46</sub>Al<sub>8</sub> metallic glass with necking**  
X.D. Wang  
International Conference on Mechanical Properties of Materials (ICMPM2010), Hangzhou, PRP China, (May 24-27 2010)

[6] **Applications of Hard X-Ray to Metallic Glasses**

J. Jiang

"High Energy X-Ray Beamlines at the PETRA III Extension", Hamburg, Germany,  
(September 8-9 2010)

## Posters on conferences in 2010

[1] **Influence of ball milling on the local atomic structure of an amorphous CoFeSiB alloy**

J. Bednarcik, S. Michalik, P. Kollár, S. Roth

14th Czech and Slovak Conference on Magnetism (CSMAG 2010), Kosice,  
Slovakia (July 6-9 2010)

[2] **Magnetic behavior and thermal stability of Fe-Pt-B-Nb alloy ribbons**

A.D. Crisan, N. Randrianantoandro, H. Chiriac, N. Lupu, I. Skorvanek, J.  
Bednarcik, S. Michalik, O. Crisan

4th Seeheim Conference on Magnetism, Frankfurt, Germany (March 28-April 1  
2010)

[3] **Microstructural study of Fe-Si(Ge)-Nb-Cu-B Finemet alloys**

S. Michalik, J. Bednarcik, K. Brzózka, P. Sovák, B. Górká

14th Czech and Slovak Conference on Magnetism (CSMAG 2010), Kosice,  
Slovakia (July 6-9 2010)

[4] **Magnetic Properties of Crystalline NiFe Alloy Prepared by High-Energy Ball Milling and Compacting**

D. Olekšáková, P. Kollár, J. Füzer, J. Bednarcik and S. Roth

14th Czech and Slovak Conference on Magnetism (CSMAG 2010), Kosice,  
Slovakia (July 6-9 2010)

---

