MM 47: Liquid and Amorphous Metals III

Time: Friday 10:15-12:00

MM 47.1 Fri 10:15 IFW A

On physical properties and the atomic structure of Al-Pd alloys — •NAN JIANG, JAN RAUCHHAUPT, and PETER HÄUSSLER — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz

In recent years we reported on an electronic influence on phase stability of Al-3d-TM alloys (TM: Sc, ..., Cu). The electronic influence is based on an internal exchange of momentum between global subsystems, namely the electronic system and the forming static structure. Both systems come into resonance to each other. The resonance is enhanced by a hybridization effect between the Al-p- and the empty TM-d-states causing a reduced effective electron density of the total system. Structure formation, phase stability and the evolution of electronic transport properties were found to be strongly related. In the present contribution we start to replace systematically the 3d-TM elements by the 4d-TM.

For thin films of amorphous Al-Pd alloys, deposited in situ at about 4 K, the resistivity and the thermopower are measured from 4 K to 350 K, the atomic structure after annealing to 350 K. By comparing the strongest diffraction ring at $K_{\rm Pe}$ with $2k_{\rm F}$, the Fermi-sphere diameter, stabilizing resonances are detected, indicating two stable regions, one at around Al_{66.7}Pd_{33.3}, where a hybridization effect seems to be most prominent, and another one around Al₄₀Pd₆₀ without hybridization.

 $\begin{array}{cccc} {\rm MM} \ 47.2 & {\rm Fri} \ 10:30 & {\rm IFW} \ {\rm A} \\ {\rm Strukturelle} \ {\rm und} \ {\rm elektronische} \ {\rm Charakterisierung} \ {\rm binärer} \\ {\rm amorpher} \ {\rm Al-Sc-Legierungen} \ - \ {\rm \bullet MARTIN} \ {\rm STIEHLER}^1, \ {\rm DANNY} \\ {\rm M\"{U}LLER}^2 \ {\rm und} \ {\rm PETER} \ {\rm H\"{A}USSLER}^1 \ - \ {}^1{\rm TU} \ {\rm Chemnitz}, \ 09107 \ {\rm Chemnitz} \\ - \ {}^2{\rm Roth} \ \& \ {\rm Rau} \ {\rm AG}, \ 09337 \ {\rm Hohenstein-Ernstthal} \end{array}$

Untersuchungen an binären amorphen Übergangsmetall-Aluminiden haben in der Vergangenheit gezeigt, dass Hybridisierungseffekte zwischen Al-p- und ÜM-d-Zuständen einen optimierenden Einfluss auf die Phasenstabilität besitzen. Dies wurde in einem HUME-ROTHERYähnlichen Bild, dem Besonanzmodell, erklärt, bei dem der Durchmesser der FERMI-Kugel mit dem Durchmesser der Pseudo-BRILLOUIN-Zone übereinstimmt und so zu einem stabilisierenden Pseudogap führt. Mit Al-Sc konnten wir die Untersuchung der Legierungsreihe der 3d-ÜM mit Al bezüglich der statischen Struktur und des elektrischen Widerstandes nun abschließen. Durch das daraus folgende Vorliegen von Daten für Systeme sowohl mit frühen als auch mit späten Übergangsmetallen konnten interessante Ergebnisse bezüglich des Einflusses der Elektronegativitätsdifferenz der Legierungsbestandteile gewonnen werden. Es zeigt sich, dass die Unterscheidung in frühe und späte Übergangsmetalle zumindest für diese Legierungen überdacht und durch eine neue Interpretation ersetzt werden muss. Ob sich die gefundene Systematik auch in anderen Eigenschaften widerspiegelt, müssen ergänzende Untersuchungen zeigen.

MM 47.3 Fri 10:45 IFW A

Thermal stability of Fe-Co-B-Si-Nb glassy alloy — •TRISHA KARAN^{1,2}, SHANKER RAM², MIHAI STOICA¹, and JÜRGEN ECKERT^{1,3} — ¹IFW Dresden, Institute for Complex Materials, P.O. Box 270116, D-01171 Dresden, Germany — ²Materials Science Centre, Indian Institute of Technology, Kharagpur 721302, India — ³TU Dresden, Institute of Materials Science, D-01062 Dresden, Germany

The thermal stability of Fe-Co-B-Si-Nb glassy alloy is studied by using high temperature differential scanning calorimetery. When the ribbons/rods made from this alloy are heated with a constant heating rate, the glass transition appears as a change in heat capacity and it is followed by one exothermic peak which corresponds to the crystallization process. The glass transition temperature T_g and the crystallization temperature T_x were measured as the onsets of the respective events. Higher the value of T_q and T_x higher is the thermal stability. It was found that in case of continuous heating with a constant rate of 10 K/min the value of T_g and T_x are 808 K and 844 K, respectively. Moreover, a small difference in thermal stability between the rods and the ribbons was observed, which may be due to the different degree of relaxation as a result of different cooling rates reached during solidification. The enthalpy of crystallization, which indicates the stability of super cooled liquid, was found to be -29.72 J/g. Thus, the alloy has good thermal stability and can be used for industrial applications. Additionally, the crystallization behaviour will be discussed.

Location: IFW A

MM 47.4 Fri 11:00 IFW A

Localization and delocalization of free volume and stress field during structural relaxation of metallic glasses — JIXIANG FANG, HORST HAHN, and •HERBERT GLEITER — Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Karlsruhe 76021, Germany

Molecualr dynamics (MD) simulation indicated that a delocalization phenomenon can be happened in the nanoglasses. The atomic structures as well as the density (and hence all structure/density-dependent properties) of nanoglasses may be tuned by controlling the degree of delocalization (by modifying the annealing time and/or annealing temperature). Here, we show another system to quantitively characterize the localization and delocalization (i.e, its generation and annihilation) of the additional free volume which may be introduced by a stress field of crystal/glass interface formed via embedding crystals into metallic glasses. In this model, W/CuZrAl and W/PdNiP crystal/glass system were selected to obtain a maximum thermal residual stress for the samples prepared from the melt spinning process. Finite element analysis (FEA) was used to optimize the volume faction of tungsten into glass and to study the stress field distribution. Differential scanning calorimetry (DSC) was adopted to quantitively calculate the average free volume in glass and its variation as annealing under different conditions. The thermal residual stresses for the samples as-quenched and annealed under various conditions were measured by the in situ heating X-rays diffraction (XRD) techniques. Above structural relaxation processes was studied in atomic scale by MD simulation.

MM 47.5 Fri 11:15 IFW A

Structural Change of Zr-Ti-Cu-Ni-Al Metallic Glass with Hydrogen Absorption Treatment — •JEROME PAILLIER, ANNETT GEBERT, CHRISTINE MICKEL, MARGITTA UHLEMANN, and LUDWIG SCHULTZ — Leibniz-IFW Dresden, Helmholtzstr. 20, Dresden

The use of metallic glasses for mechanical properties-based application is expected because of high yield strength and hardness. Nevertheless, a lack of ability to be strained plastically leading to brittle-fracture behaviour in both tension and compression experiments hinder their development as structural materials. Many routes are contemplated to enhance the toughness of the metallic glasses ; a possibility is to prepare a material with structural/chemical fluctuations on the nanometre scale.

Zr-Ti-Cu-Ni-Al metallic glass alloys have been studied since they exhibit a high-glass forming ability, a wide undercooled liquid region and a high thermal stability. Copper clusters formation within the amorphous matrix is expected to widen the plastic domain of the alloy. For that purpose, hydrogen has been absorbed electrochemically within the alloys. The interaction between hydrogen and the amorphous matrix is complex and dependent on the charging conditions and on the amount hydrogen absorbed. Among others, Cu-rich clusters of 10-15 nm can be formed under certain conditions. The aim is to understand/establish the relationship between the amount of hydrogen absorbed and the evolution of material characteristics. The microstructure changes have been notably characterized by XRD and TEM and also in an indirect way by the change of the thermal properties.

MM 47.6 Fri 11:30 IFW A Enthalpy relaxation study of Zr45.0Cu39.3Al7Ag8.7 bulk metallic glass and quantification of its free volume by freevolume theory — •YUE ZHANG, HORST HAHN, and HERBERT GLEITER — Institute of Nanotechnology, Forschungszentrum Karlsruhe, Germany

Enthalpy relaxation study of Zr45.0Cu39.3Al7Ag8.7 bulk metallic glass (BMG) is performed at 648, 658, 668, 678 and 684 respectively. It is found that the recovered enthalpy follows the VFT relationship, the fragility parameter D and characteristic temperature T0 are 15.9 and 475K respectively. The activation energy Ea of the glass transition is derived from a modified Kissinger method. Finally, the free volume in the samples is calculated using free-volume theory with D, T0 and Ea as parameters.

 $\begin{array}{cccc} MM \ 47.7 & Fri \ 11:45 & IFW \ A \\ \textbf{Corrosion behaviour of the (Fe_{44.3}Cr_5Co_5Mo_{12.8}Mn_{11.2}C_{15.8}\\ \textbf{B}_{5.9})_{98.5}\textbf{Y}_{1.5} & \textbf{bulk metallic glass and its crystalline counterpart — \bullet PETRE GOSTIN, UWE SIEGEL, ANNETT GEBERT, UTA KÜHN, \end{array}$

JÜRGEN ECKERT, and LUDWIG SCHULTZ — IFW, Dresden, Germany The corrosion behaviour of the bulk glassy (Fe_{44.3}Cr₅Co₅Mo_{12.8}Mn_{11.2} C_{15.8}B_{5.9})_{98.5}Y_{1.5} alloy and its crystalline counterpart was assessed by employing anodic polarization tests in combination with microscopy techniques: transmission and scanning electron microscopy and atomic force microscopy. The crystalline counterpart is composed mainly of simple and complex carbides surrounded by an iron based solid solution phase which is preferentially dissoluted in most of the electrolytes used in the tests. The passivation ability was studied in electrolytes with various pH values ranging from 0 to 14. When compared with the bulk glassy alloy, the crystalline counterpart is less noble in all the electrolytes, but exhibits no significant difference in the anodic polarization behaviour. Both of them exhibit low corrosion current densities in the whole pH value range (<3 μ A/cm²). The passivation ability is very poor in strongly acidic solutions and improves with increasing pH, being the best at pH 11. Passive films on the glassy sample were characterized by Auger electron spectroscopy. They are composed mainly of Fe and Cr oxides. Passivity greatly depends on the electrolyte composition: sulphates, as well as chlorides worsen the passive film protective character. Still, at room temperature, chloride concentrations up to 1 M do not bring about pitting. The influence of the alloy composition on passivity is discussed.