MM 31: Liquid and Amorphous Metals IV: Structure and Electronic Properties of Glasses

Time: Wednesday 10:15–11:30 Location: H 0107

MM 31.1 Wed 10:15 H 0107

Computer simulations of glasses: the potential energy landscape — •Zamaan Raza, Björn Alling, and Igor Abrikosov — Department of Physics, Chemistry and Biology (IFM), Linköping University, Linköping 581 83 SWEDEN

Interest in amorphous materials and glasses is increasing with the advent of physical vapour deposition techniques that are capable of creating ultrastable metallic glasses with properties that can only otherwise be be achieved by aging a glass formed from a supercooled liquid by thousands of years. However, our understanding of the microscopic structure of glasses is poor, and our ability to model them using *ab initio* techniques is limited. We discuss the potential energy landscape paradigm to account for the phenomenology of structural glasses, and the way in which it can be applied in simulations and the interpretation of their results. Our aims include determining a parameter that describes glass-forming ability from first principles, and developing methods for generating high quality structural models of glasses and amorphous solids.

We consider amorphous boron carbide as an example. With a worldwide shortage of ^{3}He, an affordable neutron detecting material is required for projects such as the European Spallation Source (ESS). In spite of its unique properties, including a high neutron-capture cross section, self healing and high mechanical strength, its structure is still poorly understood; for example, it is unknown whether it has an intrinsic length scale.

MM 31.2 Wed 10:30 H 0107

On the process of structure formation and emergence of properties in AlMnCu — •Syed Sajid Ali Gillani, Steffen Schulze, and Peter Häussler — Chemnitz University of Technology, Physics Institute, 09107 Chemnitz

Most AlTM-alloys (TM : transition metal), which become amorphous for less than 60 at%TM, whereas AlMn stays amorphous up to much higher Mn-contents. The different influence of Mn may depend on its unique properties compared to the other 3*d*-TMs. It has outstanding structural and magnetic properties and hence is claimed to be one of the most complex elements. In its pure state it has three different crystalline phases which causes strong disorder, seen e.g. by its very high resistivity, as high as the surrounding elements in the Periodic Table have in their liquid state. To get a deeper insight we replace partially Mn by Cu along two different cuts through the corresponding ternary AlMnCu. Here we report on the emerging structural and physical transport properties and discuss the particular role of the TM.

Our analysis is based on self-organizing global *spherical-periodic* resonance effects between the Fermi gas and the forming static structure. The global resonances are self-organizing by their exchange of characteristic momenta. They trigger particle-density anomalies, hybridization effects as well as phase separation. The corresponding structure factors $S(K)$ shows the resonance peak at $K_{\mathrm{pe}}=2k_{\mathrm{F}}$, indicating a *spherical-periodic* atomic order in r-space. The self-organizing processes are limited since e.g. hybridization needs minimal as well as maximal contents of TMs and depends on the chosen TM.

MM 31.3 Wed 10:45 H 0107

Structure and electronic properties of amorphous In-Mn-alloys — •Benny Böhm, Syed Sajid Ali Gillani, Martin Stiehler, Steffen Schulze, and Peter Häussler — Technische Universität Chemnitz, D-09107 Chemnitz

Basic principles during structure formation have been reported in former contributions for binary amorphous Al-transition metal-alloys (*a*-Al-TM). Presently, Al in those alloys has been replaced by other elements of the boron group and the focus hence has shifted to *a*-Ga-Mn and *a*-In-Mn. Here we report on the latter. Structure and properties emerge from the coupling of two global subsystems, the Fermi gas and the structure-forming ions. Along several degrees of freedom and via an exchange of momentum they come into resonance and form a new equilibrium. Under resonance the electronic dispersion forms a pseudogap at E_{F} with consequences on structure, its thermal stability, and electronic transport.

Thin films of In-Mn with different compositions from 40 - 70 at%Mn were deposited at low-T. The electrical resistivity up to several hundred Kelvin was measured and electron diffraction performed on a TEM at T=350 K. Close to this temperature *a*-In-Mn-alloys, unfortunately, seem to segregate into two phases, shows two main structural peaks in its structure factor S(K). One seems to be related to pure In, the other one to a phase which is still amorphous at T=350 K. Due to the two peaks in real space structural beats in the pair-distribution function g(r) occur. Transport properties support these indications.

MM 31.4 Wed 11:00 H 0107

Structure and electronic transport of amorphous Ga-Mn alloys — •Leopold Koch[1], Hans Weber[2], Martin Stiehler[1], Steffen Schulze[1], and Peter Häussler[1] — [1]Technische Universität Chemnitz, 09107 Chemnitz — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung, Helmholtzstraße 20, 01069 Dresden

The last years we reported on structure formation in binary amorphous Al-transition metal alloys (*a*-Al-TM). The formation of structure is the result of global resonance effects between the Fermi gas and the forming static structure. The resonance causes a pseudogap at $\mathrm{E_F}$ and defines the observed transport properties. During structure formation the resonance gets optimized by hybridization effects between the TM-d- and Al-p-bands at E_{F}. While this behavior proved to be nearly independent on the particular TMs, the necessity of Al as the second element was unclear. Accordingly, Al has been replaced by other elements from the boron group, e.g. Ga or In. In the present contribution we report on structural and electronic properties of a-Ga-Mn alloys.

Thin films ($d \approx 50$ nm) were deposited in high-vacuum at low T. The electrical resistivity was measured during annealing to several hundred K, the static atomic structure at around 300 K. Pure Ga itself becomes amorphous at very low T, but crystallizes already around T=14 K. By adding Mn the stability rises tremendously and amorphicity could be achieved in a wide concentration range. The overall structural as well as the electric transport properties of a-Ga-Mn are very close to a-Al-Mn. The magnetic behavior still has to be measured.

MM 31.5 Wed 11:15 H 0107

Structure and electronic properties of Al-Pd-Alloys — •Pierre Pudwell, Martin Stiehler, Steffen Schulze, and Peter Häussler — Technische Universität Chemnitz, Institut für Physik, 09107 Chemnitz

During the last years we reported on the influence of resonance-like effects during structure formation in condensed matter physics. These are based on an internal exchange of momentum between global subsystems, namely the valence electrons and the forming static structure. Hereby both subsystems are able to adjust their internal properties along different degrees of freedom. Amorphous (a) alloys proved to be perfectly suited to explore the evolution of this mutual adjustment in detail. Structure formation, phase stability and electronic transport properties were found to be strongly related. Especially in a-Al-transition metal (TM) alloys, due to the TM-d-states at E_{F}, a high flexibility of the electronic subsystem was observed.

In the present contribution we report on binary a-Al-Pd alloys in the form of thin films (≈ 50 nm). For different concentrations in the range from 20 to 75 at.% Pd, we measured the resistivity from 4K to several hundred K. The static atomic structure and the plasma resonance were obtained after annealing to 350K in a transmission electron microscope, the latter using electron energy loss spectroscopy (EELS). Although the overall behaviour of Al-Pd is comparable with other Al-TM systems distinctive deviations become obvious.