Experimental report

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Proposal: 6-05-1048 **Council:** 4/2021

Title: Chemical short range order in S-bearing metallic glass forming liquids

Research area: Physics

This proposal is a continuation of 6-05-1011

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Samples: Ti75Ni17S8
Ti75Ni14S11
(Nb38Ni62)S3
(Nb38Ni62)S5
Ti75Ni20S5

Instrument	Requested days	Allocated days	From	To
D20	5	3	08/10/2021	12/10/2021

Abstract:

We intend to study the chemical short-range order in the sulfur containing glass forming liquid TiNiS and NiNbS as function of temperature and sulfur content. Taking advantage of the isotope sensitivity of the neutron diffraction technique, we propose experiments with "zero scattering" alloys and that varying scattering contrast of sulfur, in order to directly access chemical short-range order of the melt and the sulfur related partial structure factors. With this, the local sulfur environment in the melt and its relation with the more sluggish dynamics upon sulfur addition can be revealed. An in-depth analysis of the correlation between the local atomic structure and the atomic mobility of metallic liquids will allow a comprehensive understanding of the impact of sulfur on the glass forming ability, where vitrification is possibly facilitated by geometrical frustration.

Chemical short range order in S-bearing metallic glass forming liquids

The current experiment intends to study the impact of S and P addition on the melt structure and crystallization behavior in Ni-Nb-based glass forming melts, in order to reveal the mechanisms behind the improved glass forming ability. It is also aimed to understand the general glass forming phenomena upon “minor alloying”.

The binary Ni-Nb alloy was chosen due to its ability to form bulk metallic glasses without the addition of S and P. Therefore, this system provides the capability to study the influence of subsequent S and P addition in a ternary system. For this, an electrostatic levitation facility was set up at the D20 instrument to process the samples without a container, which allows both to access the undercooled melts and to avoid artefacts due to sample-container reactions.

For this experiment we took also advantage of the possibility to vary the scattering contrast in a neutron diffraction experiment by using different Ni isotopes. Particularly, we measured several “zero-scattering alloys”, where the scattering contrast was constructed such that the chemical-chemical partial structure factor (S_{cc}) can be directly measured. As an example, the result for a $Ni_{58}Nb_{39}P_3$ melt is shown in Fig. 1.

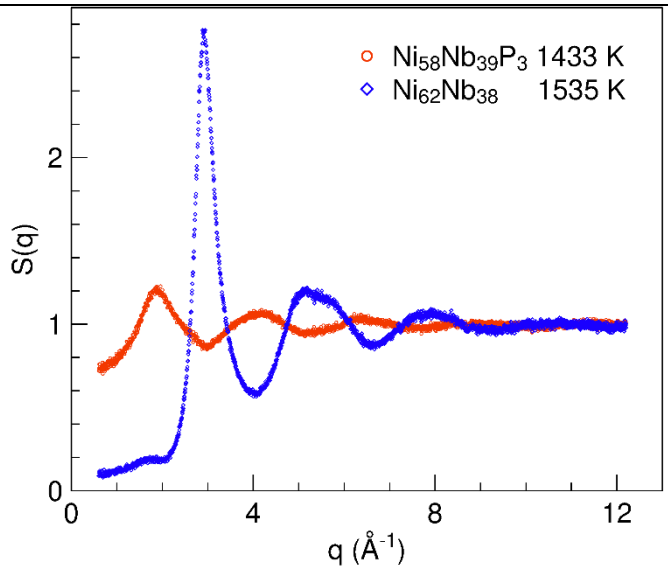

Fig.1 Liquid structure factor S(q) measured for binary $Ni_{62}Nb_{38}$ melts and for ternary $Ni_{58}Nb_{39}P_3$ melts. The $Ni_{58}Nb_{39}P_3$ alloy was enriched in ^{62}Ni to construct a “zero-scattering” alloy. Thus, the chemical-chemical partial structure factor (S_{cc}) is directly accessible.

We were able to measure the binary $Ni_{62}Nb_{38}$ alloy, and the ternary Ni-Nb-S and Ni-Nb-P alloys with different S and P concentrations. Fig. 1 shows the first analysis results of the liquid structure factor in binary $Ni_{62}Nb_{38}$ and in ternary $Ni_{58}Nb_{39}P_3$. Compared to the available partial structure factors for binary $Ni_{59.5}Nb_{40.5}$ melts [1], it seems that the addition of P reduced the chemical order of the liquid. More detailed analysis, including the S and P concentration dependence is currently being conducted.

Reference:

[1] Holland-Moritz et al. (2014). Structural aspects of glass-formation in Ni-Nb melts. *Journal of Applied Physics*, *115*(20), 203509.