



**Experiment title:**  
Short-Range Order and Phase Selection in Binary  
Glass-Forming Metallic Melts

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Report:

In the current experiment X-ray diffraction measurements on electrostatically levitated Zr-, Ti, and Hf-based alloy melts were studied. The primary aim is to investigate the temperature dependence of the total structure factor  $S(q)$  down to deep undercoolings, and the corresponding crystalline phases solidified as a function of degrees of undercooling. Particularly, we focused on the comparison between binary alloys with different early- and later-transition metals. During the experiment, we measured the  $Zr_{50}Ni_{50}$ ,  $Hf_{50}Ni_{50}$ ,  $Zr_{35}Ni_{65}$ ,  $Hf_{35}Ni_{65}$ , as well as as the  $La_{60}Ni_{40}$ ,  $La_{60}Co_{40}$ ,  $La_{60}Cu_{40}$  alloy compositions. Moreover,  $Ti_{59}Cu_{41}$  and  $Ti_{66.7}Cu_{33.3}$  were also studied in order to be compared with our previous results on Zr-Cu melts [Holland-Moritz et al, Europhys. Lett., **100**, 56002 (2012)].

**\*\* Short range order \*\***

One interesting feature observed in the measured total structure factors is that for La-based alloys, as shown in Fig. 1, the total structure factors of the  $La_{60}Ni_{40}$  and  $La_{60}Co_{40}$  liquids are very similar, whereas the  $La_{60}Cu_{40}$  melt exhibits a considerably different structure. The second oscillation of the  $S(q)$  for  $La_{60}Cu_{40}$  is much broader and extends to higher  $q$  values. Note that Ni, Co, and Cu all exhibit similar atomic radii and X-ray scattering cross sections. Thus, the differences in the obtained

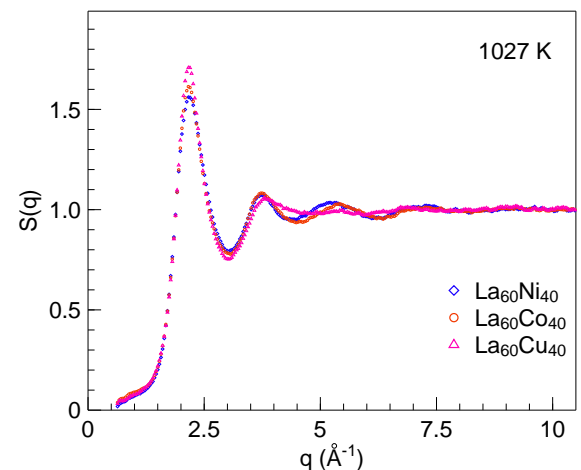


Fig. 1: Measured total structure factors of liquid  $La_{60}Ni_{40}$ ,  $La_{60}Co_{40}$ , and  $La_{60}Cu_{40}$ .

total structure factors indicate different melt structures. This is similar to our previous observations that Zr-Cu melt exhibits a different structure compared to Zr-Ni/Co melts. Here the changes observed in the total  $S(q)$  is mainly contributed from the La-related partial structure factors, since La exhibits a significantly higher atomic number compared to that of the early transition metals.

## \*\* Phase selection \*\*

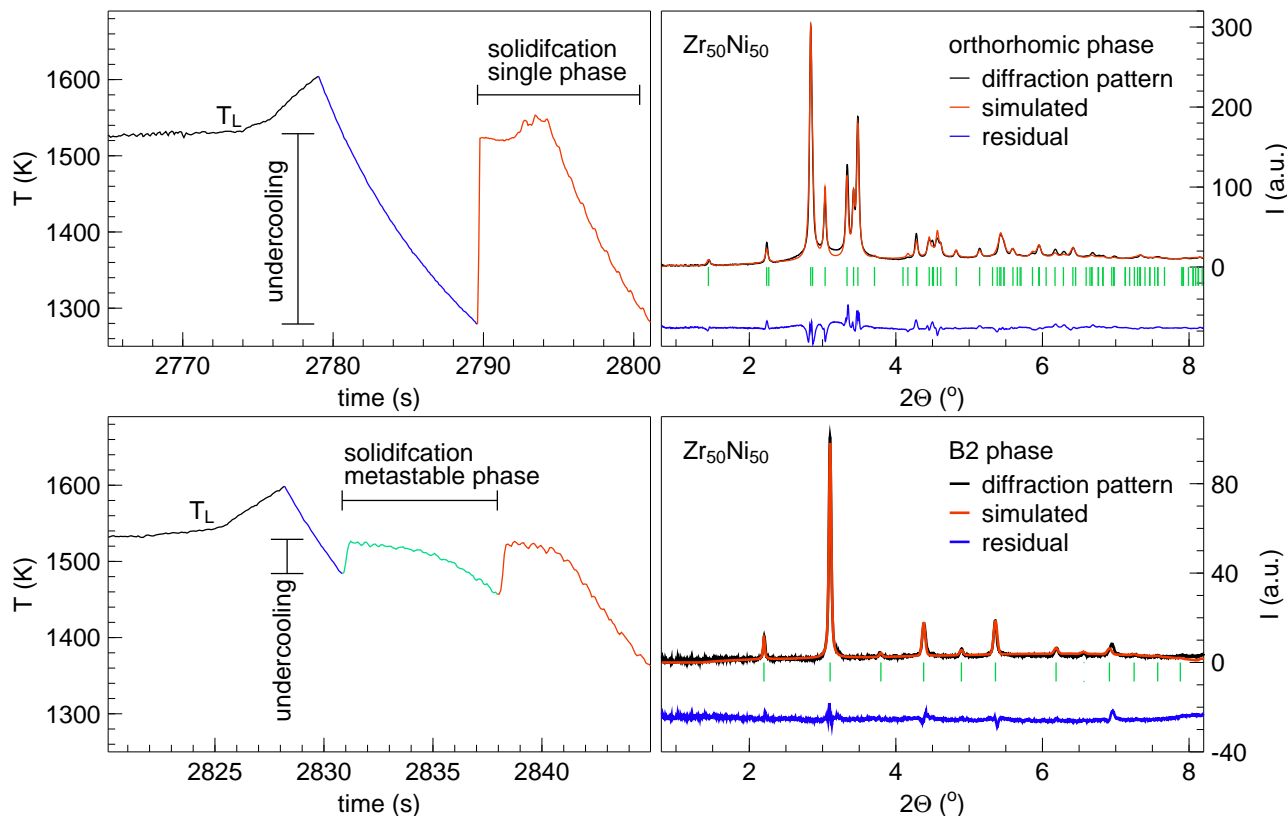


Fig. 2: Temperature profile and the corresponding diffraction diagram of the primary phases solidified from the undercooled Zr<sub>50</sub>Ni<sub>50</sub> melt.

The excellent time resolution provided by in-situ X-ray diffraction allows us to identify also metastable phases during the solidification. As shown in Fig. 2, the studied Zr<sub>50</sub>Ni<sub>50</sub> melt can be solidified in two different ways: either a single solidification event occurs, or the liquid solidifies in two steps. Via the Rietveld refinement analysis we further identified that in first case a stable orthorhombic phase (Fig. 2 upper row) is formed, whereas in the later case during the first solidification step a metastable, cubic B2 phase (Fig. 2 lower row) is formed, which transforms into the stable orthorhombic phase during the second step. The occurrence of both scenarios seems to be independent of the maximum temperature reached during heating. However, the metastable phase forms at considerable smaller undercoolings. Similar behaviour has been also observed for the Hf<sub>50</sub>Ni<sub>50</sub> melt. This may provide an explanation to the observed crystal growth velocities as a function of undercooling and the corresponding microstructure formed. Such behaviour is in contrast to the Zr<sub>50</sub>Cu<sub>50</sub> melt, where a single B2 phase is always formed, independent of the degree of undercooling [J. Gegner et al, J. Alloys Comp., **576**, 232 (2013)]. The correlation between the crystal structure and the growth velocity/glass forming ability is under further investigation with the other alloys systems studied in the current experiment.