



Contribution ID: 146

Type: **Talk**

Structure-dynamics relation in Zr-Ti melts

Thursday, 10 December 2020 15:30 (15 minutes)

The early transition metals Zirconium and Titanium show very similar chemical and structural properties. The binary Zr-Ti alloys compose a completely miscible system, which is also a boundary system for many bulk metallic glasses (BMGs) and stable quasicrystals. However, the detailed formation mechanisms of these special structures remain largely unknown and are often speculative, since for these chemically reactive, high melting temperature alloys accurate knowledge of melt properties is largely missing. Using containerless levitation techniques, we successfully investigated the microscopic structure and dynamics of the Zr-Ti melts over a large temperature range. Neutron and synchrotron diffraction experiments reveal a melt structure exhibiting barely any chemical short-range order. On the Zr-rich side, the Ti diffusivity obtained by quasi-elastic neutron scattering decreases with increasing Ti content. Such a concentration dependent atomic dynamics can be fully understood according to the prediction of the Mode-Coupling Theory (MCT) on a binary hard-sphere mixture with a small size disparity. Our results indicate the dominant impact of the topological structure on the atomic motion in the Zr-Ti melts.

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Session Classification: DN2020: Materials

Track Classification: DN: Materials