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Correlation of structure and dynamics in Cu-Ti melts

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Binary Cu-Ti alloys feature a large, undercooled liquid region and a high glass-forming ability (GFA). Thus, they provide the rare possibility to obtain two component bulk metallic glasses (BMGs), which is mainly addressed to special properties of the Cu-Ti system i.e., in the melt, it features a positive excess volume, whereas it still has a negative enthalpy of mixing.

Although, the scientific interest in Cu-Ti-based BMGs increased, the relevant atomic mechanisms responsible for such good GFA are still to be explored. In our study, we discuss the temperature-dependent dynamical and structural properties of Cu-Ti melts, within a compositional range of 24 to 69 at% Ti. Electrostatic levitation is used to process the Cu-Ti samples without any container, which enables to obtain data about viscosity, density, and atomic structure with high accuracy. We found a non-monotonous trend of the viscosity, with the highest values at intermediate Ti contents. The measurement of the (weighed) self-diffusion coefficient of the pure Cu and Ti melts and of the Cu₇Ti₂₄ alloy confirms the viscosity results. Notably, this dynamical trend is not reflected by the macroscopic packing fraction, meaning a high viscosity does not necessarily correlate with a dense packing. In contrast, on the atomic scale, diffraction measurements with x-rays and neutrons reveal a denser, local packing and a pronounced chemical short-range order, which is based on attractive interactions between Cu and Ti. These short-range interactions can explain the high viscosity, while the macroscopic packing fraction is rather governed by long-range interactions.

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