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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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