



Impact of S addition on the dynamics and on the structure of glass forming $\text{Ti}_{75}\text{Ni}_{25-x}\text{S}_x$ melts

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S addition enables bulk metallic glass formation in Ti-based systems. To understand the role of S on glass formation, we analyzed the melt dynamics and the melt structure in $\text{Ti}_{75}\text{Ni}_{25-x}\text{S}_x$ ($x = 0, 5, 8, 11$). To process these reactive Ti-based melts, we applied containerless methods as electromagnetic and electrostatic levitation. The microscopic melt dynamics (self-diffusion) were studied by quasielastic neutron scattering, whereas the macroscopic melt dynamics (viscosity) were studied by the oscillation drop method. In both cases, S addition reduces the melt dynamics.

However, the decrease in melt dynamics is accompanied by a decrease in melt packing, as derived from melt density measurements. Employing neutron diffraction experiments in combination with Ni isotope substitution, we were able to extract the full set of partial structure factors for $\text{Ti}_{75}\text{Ni}_{25}$ melts. Using this partial structure information, our analysis shows that the change in melt structure for $\text{Ti}_{75}\text{Ni}_{25}$ upon S addition cannot be simply explained by an isomorphous substitution of Ni by S. S atoms seem to occupy a larger space in melt structure than Ni atoms, which is in accordance with the previously reported decrease in melt packing. This indicates that the decrease in melt dynamics is associated with chemical interactions between the S atoms and the transition metal atoms (Ti and Ni), rather than with a denser packing of the melt.

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