Diffusion in Metallic Glasses

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Background

- Most of Al-based metallic glasses consist of Al, RE—rare earth elements, and TM—transition metals.
- Metallic glasses are often devitrificated in order to obtain nano-crystalline structure.
- Devitrification involves multi-component diffusion in glasses, and the diffusion of RE is the controlling factor due to their low diffusivity.
- New models are needed to describe temperature and composition dependence of the diffusivity in metallic glasses.



Modeling of Diffusivity

Classic relation: $D = D_o \exp(-Q/RT)$ Stokes-Einstein relation: D = kT/3pah *k*—Boltzmann's constant *a*—an ionic diameter η —viscosity $h = \Gamma \exp[\Theta/(T-T')]$ T'—temperature at which $\Delta S(\text{configuration})=0$ or $\Delta V=0$ New relation:

$$D = \frac{kT}{3pa} \frac{1}{\Gamma} \exp\left[\frac{-\Theta}{T-T'}\right] = D_o T \exp\left[\frac{-\Theta}{T-T'}\right]$$



Diffusivity in Different States



SLS—supercooled liquid state SS—solid state (glass)

The new model derived from the Stokes-Einstein relation can describe the diffusivity in liquid and SLS, but not in SS. Furthermore, diffusivity in glass depends on time due to relaxation.

