

Point defects and self-diffusion in temperature-stabilized bcc metals

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Point defects are responsible for self-diffusion processes in crystalline solids. According to the classical concepts, diffusion in normal metals mainly occurs due to the formation and migration of monovacancies. The diffusion coefficient D can be expressed by the Arrhenius equation, where the activation energy is correlated with the melting temperature. However, the characteristic values of correlation coefficient in some anomalous bcc metals (Ti, Zr, Hf, U, Ce, Gd, La, Pr, Pu, Yb) are 1.5–2 times smaller than in normal metals. The pre-exponential factors are several orders of magnitude too small. The strong non-Arrhenius dependence of the diffusion coefficient is additionally observed for bcc Ti and Zr, as the temperature range for their phase stability is quite large. One common feature for all anomalous metals is that the bcc phase exists only at high temperatures or pressures and is mechanically unstable at 0 K.

In this work, I obtain the temperature dependence of the self-diffusion coefficient in bcc titanium directly from molecular dynamics (MD) calculation. MD simulations indicate that both vacancies and self-interstitials contribute to diffusivity in bcc Ti. The resultant self-diffusion coefficient is non-Arrhenius, but shows less curvature than observed in most experiments [1]. I also show that the formation free energy of self-interstitials in bcc uranium is much smaller than for vacancies. [2].

[1] Smirnov G 2020 *Phys. Rev. B* **102** 184110

[2] Smirnov G S and Stegailov V V 2019 *J. Phys. Condens. Matter* **31** 235704