Entropic effects in concentrated solid solutions : the unexpected role of diffusion prefactors

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High-entropy alloys, *i.e.* alloys with multiple elements present in similar concentration, have attracted considerable attention since they were introduced 20 years ago. These materials present a number of unexpected properties, including a higher compromise between elongation to fracture and tensile strength and, of interest here, anomalous vacancy diffusion. Although this latter property remains debated, it has been the topic of a fair number of experimental and numerical works. We revisited this problem in the light of our recent work on the origin of the compensation law (or Meyer-Neldel rule) [1], separating the role of the energy barrier and the entropic attempt frequency prefactor in the diffusion of point defects. This study, on a FeNiCr concentrated solid solution, a simplified high-entropy alloy proxy, revealed unexpected behavior for the entropic prefactor, which shows up to six orders of magnitude variation for the same vacancy diffusion mechanism and similar energy barrier as function of local environment [2]. In this talk, I'll discuss these results and present extensive kinetic ART simulations that highlight the effect of prefactor variation on the diffusion properties in this complex materials.

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[1] S. Gelin, A. Champagne-Ruel, N. Mousseau, Enthalpy-entropy compensation of atomic diffusion originates from softening of low frequency phonons, Nature Communications 11, 3977 (2020).

[2] A. Sauvé-Lacoursière, S. Gelin, G. Adjanor, C. Domain, N. Mousseau, Unexpected role of prefactors in defects diffusion: the case of vacancies in the 55Fe-28Ni-17Cr concentrated solid-solution alloys, Acta Materialia 237, 118153 (2022).