From Hamiltonians to Industrial Alloys: the gaps, the achievements and some perspective.

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The energetic/thermodynamics route from theory to commercial alloys is not continuous. Phenomenological shortcuts, like computational thermodynamics (*e.g.* CALPHAD) can describe binaries, ternaries and higher order systems quite satisfactory but there is still a gap for linking these approaches to a real multicomponent multiphase, sometimes metastable, industrial material (*e.g* [00Hec]).

This route will be illustrated by cu-alloys, where ab-initio/finite (*e.g.* [01Mul]) and CALPHAD approaches exist (*e.g.* [98Lia]), but trivial industrial alloys problems are, however, not understood or even described. In many alloy development or processing true predictions are required. They do not need, however, to be quantitatively exact, qualitative theoretical trends [01But]are sometimes enough and can be plugged on the phenomenological databases delimiting the experimental investigation to be followed. We point out the studies that should be prioritized when supporting applied Cu-alloys processing and development.

References

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