Stability and metastability in computational thermodynamics- Challenges and opportunities in the development of novel metallic alloys

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The basis of computational thermodynamics or the CALPHAD approach have been established in the decade of 1970. The technique has achieved its maturity in the following decades, with the development of models and methods to properly describe the thermodynamic properties of elements and phases. Since the start of this development, the question of how to model and quantify the properties of metastable or unstable (experimentally inaccessible) phases has had a central role in the discussions and evolution of the method. However, important challenges remain, to this date.

In this work, the importance of the proper treatment of the properties of experimentally inaccessible (unstable or metastable) phases is discussed using examples relevant to the development of novel metallic alloys that explore metastability.

In special, the methods proposed to describe the properties of the undercooled liquid phase and to include the possibility of correctly describe glassy and amorphous phases is discussed, highlighting the important advances and the current barriers. The relevance of this problem to the extension of the CALPHAD approach to low temperatures is also briefly discussed. Finally, the potential of the method in the prediction of phase transformations, phase stability and alloy design is highlighted.