(CT)THE CALPHAD APPROACH TO COMPUTATIONAL THERMODYNAMICS

L. Kaufman

CALPHAD,Inc.Brookline,Massachusetts,USA

Recent papers (1,2) presented many applications of Computational Thermodynamics.CALPHAD 26(2002) No 2 described software available for applying these methods.In a recent review(3)Nb alloys,giant magnetoresistance(3,4)metallic glasses,Lithium Batteries. Zirconia Ceramic (5,6)and multicomponent rhenium alloys(7,8), were discussed to note current problems that require attention.These techniques have also been applied to plutonium(9) and corrosion resistant superalloys(10,11) to deal with current problems which can benefit from the application

CALPHAD THERMODYNAMICS (CT) to deal with all possible phases that can exist over wide ranges of conditions uncommon in classical thermodynamics.This feature grew naturally in (CT) from the realization that commercial processing always trys to increase the rate of production to become more profitable. By contrast,thermodynami measurements are performed under equilibrium conditions!Since (CT) applies the results of measurements and observations,made under conditions where equilibrium prevails, to commercial practice where non-equilibrium or quasi-equilibrium persists,(CT) must have a broader scope than classical thermodynamics.The

(CT) descriptions have also attempted to establish an interface with description of stable, metastable and unstable phases describes by *ab-intio* methods.Good agreement has been attained between these methods in many cases but some differences still exist (12).

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