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论文

基于微观偏析统一模型及Thermo--Calc的三元合金凝固路径耦合计算

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摘要:

将合金凝固微观偏析统一模型推广到三元合金凝固微观偏析的预测, 并提出了能够计算三元匀晶与共晶合金凝固路径的数值计算方法. 实现了在源代码层次上与热力学计算软件Thermo-Calc及其数据库的耦合, 以获取多元合金凝固路径计算所需的凝固热力学数据. 通过Fe-40V-40Cr, Al-4.5Cu-1.0Si, Al-10Cu-2.5Mg和Al-1.49Si-0.64Mg(质量分数, %)等多元/多相合金在不同冷速下凝固路径的实例计算, 以及与相应的凝固组织定量金相实验结果对比, 验证了本文多元/多相凝固模型和算法的正确性.

关键词: 多元/多相凝固路径 微观偏析 Thermo-Calc耦合计算 多元铝合金

THERMO–CALC LINKED COMPUTATIONS OF SOLIDIFICATION PATHS OF TERNARY ALLOYS USING AN EXTENDED UNIFIED MICROSEGREGATION MODEL

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Abstract:

A model for predicting the microsegregation of ternary alloys was developed via extending a previously proposed unified microsegregation model for binary alloys. The present multicomponent/multiphase model retains the advanced features of the previous binary microsegregation model, in which the unified microscale parameter Φ takes a general function form to account for more possible influential factors, including the partition coefficient, solid fraction, solid diffusion coefficient, dendrite geometrical morphologies and solidification rate, *etc*.

The algorithms fr cacuating the solidification paths of ternary isomorphous and eutectic alloys were proposed, which closely couples with a commercial software package/database of Thermo–Calcvia its TQ6–interface in order to directly access to thermodynamic data needed in the multicomponent/multiphase solidification path computations. In the solidification of primary phase and three phases eutectic, solid fraction f_s was selected to be a control variable when solving the equations of the microsegregation models, while in the solidification of two phases eutectic, temperature was selected to be a control variable as the relationship between the concentrations of solutes *B* and *C* was unknown. In each calculation iterative step, the names and number of the equilibrium phases were obtained from Thermo–Calc, and then saved and compared with the calculation results of the previous step. As the names and number of the equilibrium phases in each solidification stage of ternary eutectic alloys are different, the three solidification types were determined by comparing with the results in the computation process.

The availability and reliability of the proposed multicomponent/multiphase model and algorithms were demonstrated by sample computations for the solidification paths of Fe–40V–40Cr, Al–4.5Cu–1Si, Al–10Cu–2.5g and Al–1.49Si–0.64Mg (mass fraction, %) alloys under different solidification/cooling rates, and by comparisons with the experimental results of quantitative measurementof corresponding solidification microstructures.

Keywords: multicomponent/multiphase solidification path microsegregtion Thermo–Calc coupled calculation multicomponent Al alloys

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参考文献：

[1] Fujii T, Poirier D R, Flemings M C. Metall Trans, 1979; 10B: 331
[2] Mehrabian R, Flemings M C. Metall Trans, 1970; 1: 455
[3] Cornelissen M C M. Ironmaking Steelmaking, 1986; 13(4): 204
[4] Ro´osz A, Exner H E. Acta Matall Mater, 1990; 38: 375
[5] Xie F Y, Kraft T, Zuo Y, Moon C H, Chang Y A. Acta Mater, 1999; 47: 489
[6] Kraft T, Rettenmayr M, Exner H E. Modell Simul Mater Sci Eng, 1996; 4: 161
[7] Zhao G W, Xu D M, Fu H Z. Int J Mater Res, 2008; 128: 680
[8] Vu˘sanovi´c I, ˘ Sarler B, Krane M J M. Mater Sci Eng, 2005; A413–414: 217
[9] Jie W Q, Zhang R J, Zhi H. Mater Sci Eng, 2005; A413–414:497
[10] Larouche D. Calphad, 2007; 31: 490
[11] Du Q, Jacot A. Acta Mater, 2005; 53: 3479
[12] Xu D M. Metall Mater Trans, 2001; 32B: 1129
[13] Xu D M, Fu H Z, Guo J J, Jia J, Li Q C. J Harbin Inst Technol, 2003; 35: 1156
(徐达鸣, 傅恒志, 郭景杰, 贾 钧, 李庆春. 哈尔滨工业大学学报, 2003; 35: 1156)
[14] Xu D M, Guo J J, Fu H Z. in Jones ed., SP07–Proceedings of the 5th Decennial International Conference on Solidification Processing, Sheffield: University of Sheffield, 2007: 94
[15] Song M H, Master Disertation, Harbin Institute of technology, Harbin, 2008
(宋梦华. 哈尔滨工业大学硕士论文, 哈尔滨, 2008)
[16] Wu B Y, Wang M D, Ding X H, LI D H. Theory of Numerical Analysis. Beijing: Science Press, 2003: 11
(吴勃英, 王德明, 丁效华, 李道华. 数值分析原理. 北京: 科学出版社, 2003: 11)
[17] Xu D M. Metall Mater Trans, 2002; 33B: 451
[18] Ganesan M, Thuinet L, Dye D, Lee P D. Metall Mater Trans, 2007; 38B: 557
[19] Dor´e X, Combeau H, Rappaz M. Acta Mater, 2000; 48: 3951
[20] Mondolfo L F. Aluminum Alloys: Structure and Properities. London: Butterworths, 1976: 253
[21] Thermo–Calc Software A B. ThermoCalc Software User'Guid (Version R). Stockholm Technology Park, 2006

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