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论文

ZA62镁合金中AB_2型金属间化合物的结构稳定性与弹性性能的第一原理计算

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摘要：

采用基于密度泛函理论Castep和Dmol程序软件包, 计算了ZA62镁合金中AB_2型金属间化合物 $MgZn_2$, Mg_2Sn和$MgCu_2$的结构稳定性、弹性性能与电子结构. 合金形成热和结合能的计算结果显示: Mg_2Sn具有最强的合金化形成能力, 而$MgCu_2$结构最稳定; 体模量(*B*)、弹性各向异性系数(*A*)、Young's模量(*E*)、剪切模量(*G*)和Poisson比(*v*)的计算结果表明: $MgZn_2$和$MgCu_2$为延性相, 而Mg_2Sn为脆性相, $MgZn_2$的塑性最好; 采用弹性常数、体模量和结合能的经验公式计算金属间化合物的熔点, 实验值均在采用弹性常数(±300 K)和体模量(±500 K)计算熔点预测的范围内, 采用弹性常数比采用体模量和结合能预测熔点的平均相对误差小, 其中采用弹性常数计算Mg_2Sn的熔点与对应的实验值十分接近, 相对误差仅为0.31%. 不同温度下热力学性质的计算结果表明, 在298-573 K温度范围内, $MgCu_2$的Gibbs自由能始终最小, 其结构热稳定性最好, 结构稳定性的强弱顺序并不随温度的升高而消失; 而对$MgZn_2$和Mg_2Sn, 以475 K为临界, 结构稳定性的强弱顺序随温度的升高发生了变化; 态密度和Mulliken电子占据数的计算结果表明: $MgCu_2$ 结构最稳定的原因主要在于体系在Fermi能级以下区域成键电子存在强烈的离子键作用.

关键词： 镁合金 金属间化合物 电子结构 结构稳定性 弹性性能

FIRST-PRINCIPLES CALCULATIONS OF STRUCTURAL STABILITIES AND ELASTIC PROPERTIES OF AB_2 TYPE INTERMETALLICS IN ZA62 MAGNESIUM ALLOY

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Abstract:

Structural stabilities, elastic properties and electronic structures of Mg_2Sn, $MgZn_2$ and $MgCu_2$ in ZA62 magnesium alloy have been determined from first-principles calculations by using Castep and Dmol program based on the density functional theory. The calculated heats of formation and cohesive energies showed that Mg_2Sn has the strongest alloying ability and $MgCu_2$ the highest structural stability. The calculated bulk moduli (*B*), anisotropy values (*A*), Young's moduli (*E*), shear moduli (*G*) and Poisson ratio (*v*) showed that $MgZn_2$ and $MgCu_2$ both are ductile, on the contrary, Mg_2Sn is brittle, and among the three phases $MgZn_2$ is a phase with the best plasticity. Their tested melting temperatures are within the ranges calculated from elastic constants (±300 K) and bulk moduli (±500 K), the estimated values from elastic constant have the smallest average relative error, the calculated melting temperature of Mg_2Sn phase is in well agreement with the experimental one and the error relative to the experiment result is about 0.31%. $MgCu_2$ has higher melting temperature, *i.e.* better structural stability among the three compounds. The calculations of thermodynamic properties show that the Gibbs free energy of $MgCu_2$ is also the smallest within 298-573 K range, indicating the structural stability of $MgCu_2$ does not change with the elevated temperature. The calculations of the density of states (DOS) and Mulliken electronic populations showed that the reason of $MgCu_2$ having highest structural stability in ZA62 magnesium alloy attributes to $MgCu_2$ phase having more ionic bonds below Fermi level compared with those of Mg_2Sn and $MgZn_2$ phases.

Keywords: magnesium alloy intermetallics electronic structure structural stability elastic property

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参考文献：

[1] Li Z J, Gu X N, Lou S Q, Zheng Y F. Biomaterials, 2008; 29: 1329
[2] Sun Y S,Wen K Z, Yuan G Y. Chin Nonferrous Met, 1999; 9: 55
(孙扬善, 翁坤忠, 袁广银. 中国有色金属学报, 1999; 9: 55)
[3] Au–Yang M Y, Cohen M L. Phys Rev, 1969; 178: 1358
[4] Arunsingh, Dayal B. J Phys, 1970; 3C: 2037
[5] Imai Y, Watanabe A. Intermetallics, 2002; 10: 333
[6] Grosch G H, Range K J. J Alloys Compd, 1996; 235: 250
[7] Ghosh G, Vaynman S, Asta M, Fine M E. Intermetallics, 2007; 15: 44
[8] Fast L, Wills J M, Johansson B, Eriksson O. Phys Rev, 1995; 51B: 17431
[9] Segall M D, Lindan P L D, Probert M J, Pickard C J, Hasnip P J, Clark S J, Payne M C. J Phys: Condens Matter, 2002; 14: 2717
[10] Marlo M, Milman V. Phys Rev, 2000; 62B: 2899
[11] Vanderbilt D. Phys Rev, 1990; 41B: 7892
[12] Hammer B, Hansen L B, Norkov J K. Phys Rev, 1999; 59B: 7413
[13] Franscis G P, Payne M C. J Phys: Condens Matter, 1990; 2: 4395
[14] Monkhorst H J, Pack J D. Phys Rev, 1976; 13B: 5188
[15] Huang K. Solid State Physics. Beijing: High Education Press, 1985: 68
(黄昆. 固体物理学. 北京: 高等教育出版社, 1985: 68)
[16] Zhang H, Shang S L, Saal J E, Saengdeejing A, Wang Y, Chen L Q, Liu Z K. Intermetallics, 2009; 17: 878
[17] Ganeshan S, Shang S L, Wang Y, Mantina M, Liu Z K. Intermetallics, 2009; 17: 313
[18] Corkill J L, Cohen M L. Phys Rev, 1993; 48B: 17138
[19] Medvedeva M I, Gornostyrev Y N , Novikov D L, Mryasov V, Freeman A J. Acta Mater, 1998; 46: 3433
[20] Sahu B R. Mater Sci Eng, 1997; B49: 74
[21] Li C H, Hoe J L, Wu P. Phys Chem Solids, 2003; 64: 201
[22] Ansara I, Dinsdale A T, Rand M H. Thermodynamic Database for Light Metal Alloys. Brussels: European Commission, 1998: 368
[23] Zubov V I, Tretiakov N P, Teixeira R J N, Sanchez O J F. Phys Lett, 1995; 198A: 470
[24] Ishii Y, Fujiwara T. Non–Cryst Solids, 2002; 312–314: 494
[25] Davis L C, Whitten W B, Danielson G C. J Phys Chem Solids, 1967; 28: 439
[26] Cheng C H. J Phys Chem Solids, 1967; 28: 413
[27] YuWY, Wang N, Xiao X B, Tang B Y, Peng L M, Ding W J. Solid State Sci, 2009; 11: 1400
[28] Hong S Y, Fu C L. Intermetallics, 1999; 7: 5
[29] Mehl M J, Osburn J E, Papaconstantopoulos D A, Klein B M. Phys Rev, 1990; 41B: 10311
[30] Mattesini M, Ahuja R, Johansson B. Phys Rev, 2003; 68B: 184108
[31] Fine M E, Brown H L M. Scr Metall Mater, 1984; 18: 951
[32] Zhang X D. Intermetallics, 1995; 3: 137

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1．李萧 杨平 孟利 崔凤娥.AZ31镁合金中拉伸孪晶静态再结晶的分析[J]. 金属学报, 2010,46(02): 147-154

2．胡逾.关于金属材料断裂试验的缺口敏感性[J]. 金属学报, 1988,24(1): 30-33

3．张康侯;陈黎莉.化合物SmPd_5和EuPd_5的晶体结构[J]. 金属学报, 1988,24(1): 135-137

4．朱凯;王崇愚.含Mg,W高温合金γ′相的电子结构[J]. 金属学报, 1988,24(6): 410-414

5．李辉;刘祥;郭建亭;胡壮麒.硼对快凝Ni_3Al组织结构及力学性能的影响[J]. 金属学报, 1989,25(1): 25-30

6．刘森英;高哲;李铿;李俊清;王崇愚.掺Cu的RECo_5型金属间化合物电子结构[J]. 金属学报, 1989,25(2): 15-21

7．周班;金石鸣;邵俊;陈念贻.IMEC——金属间化合物检索和预报的专家系统[J]. 金属学报, 1989,25(3): 137-142

8．郭建亭;孙超;李辉;管恒荣.金属间化合物NiAl的氧化行为与硼含量的关系[J]. 金属学报, 1989,25(4): 120-125

9．张少卿.MB15镁合金的相组成及其微观形态[J]. 金属学报, 1989,25(5): 36-41

10．蒲忠杰;蔡其巩;朱静.TiAl-V金属间化合物的高温变形行为[J]. 金属学报, 1989,25(5): 149-151