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Cu-Cr合金低温时效析出过程的密度泛函理论

冯晶¹, 陈敬超¹, 肖冰², 于杰¹, 李强³, 杜晔平¹

- (1. 稀贵及有色先进材料教育部重点实验室, 云南省新材料制备与加工重点实验室, 昆明理工大学, 昆明 650093;
2. 西安交通大学 材料科学与工程学院, 西安 710049
3. 河南理工大学 材料科学与工程学院, 焦作454000)

摘要:采用雾化法制备过饱和Cu-Cr固溶体, 利用透射电镜观察过饱和Cu-Cr固溶体低温时效富Cr区的显微形貌, 利用能谱仪分析富集区Cr元素的含量, 计算形成不同Cr含量富集区的形成能及合金熵, 采用第一原理解释时效析出过程中合金富集区的电子结构变化。结果表明: 随时间的增加, Cr不断在基体中富集, 时效析出是一个扩散迁移过程; 富集区是一种亚稳态, 有逐渐向稳定态转变的趋势, 即Cr析出是固溶体能量降低的一种方式。态密度的计算证实, Cr含量56.0%时富集区发生结构转变(出现GP区), 体系内原子化学环境发生变化。

关键字: Cu-Cr合金; 时效; 热力学性质; 第一原理

Density functional theory of Cu-Cr alloy during aging precipitation process at low temperature

FENG Jing¹, CHEN Jing-chao¹, XIAO Bing², YU Jie¹, LI Qiang³, DU Ye-ping¹

- (1. Key Laboratory of Advanced Materials of Precious-Nonferrous Metals, Education Ministry of China, Key Laboratory of Advanced Materials of Yunnan Province, Kunming University of Science and Technology, Kunming 650093, China;
2. School of Materials Science and Engineering, Xi'an Jiaotong University, Xi'an 710049, China;
3. School of Materials Science and Engineering, Henan University of Technology, Jiaozuo 454000, China)

Abstract: Supersaturated Cu-Cr solid solution was prepared by atomization. The microstructures of Cr rich zone in Cu-Cr solid solution were investigated by transmission electron microscopy and electron energy disperse spectroscopy. The formation energy and entropy of different Cr soluble enrichment districts were calculated. The electric structure changes of richment zones during aging precipitation process were explained by the first principle. The mechanism of aging precipitation was explained. The results show that the GP zone is presented at relatively low temperature, the concentration of Cr also increases due to the soluble enrichment process. The soluble enrichment is a metastable phase and declines the system

energy. The structure of enrichment zones with 56%Cr is transformed and the environment of atoms in GP zone is charged too.

Key words: Cu-Cr alloy; aging; thermodynamic property; first principle

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地 址：湖南省长沙市岳麓山中南大学内 邮编： 410083

电 话： 0731-8876765, 8877197, 8830410 传真： 0731-8877197

电子邮箱： f-ysxb@mail.csu.edu.cn