Formation of structural disorder in FeNi-based alloys – semi-empirical approach

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Alloys based on FeNi are known to commonly crystallize in bcc or fcc structures, depending on their chemical composition. Additionally, in slowly cooled objects (like meteorites) ordered tetragonal $L1_0$ phase was observed [1]. It shows promising hard magnetic properties, because of its hard uniaxial magnetocrystalline anisotropy. Still, the synthesis of this phase in industrial amount has not been possible yet, mainly because of sluggish diffusion and low ordering temperature [2]. In this work results of the calculations of formation enthalpies for solid solution and amorphous phase in Fe-Ni system were analyzed. Additionally, substitution with Co and Cu was taken into account. These calculations confirm poor glass forming ability of FeNi system and indicate limited influence of Co-substitution. On the other hand, negative heat of mixing of Cu can be treated as a decisive feature for chemical segregation and therefore is a promising candidate when aiming destabilization of the fcc FeNi structure. The latest is critical for the L10 FeNi phase formation.

References:

[1] R. S. Clarke, E. R. D. Scott, Am. Mineral. 65 (1980) 624-630

[2] L. H. Lewis et al., J. Phys. Condens. Matter 26 (2014) 064213

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