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Stability, rigidity and thermal vacancies evolution in Fe—Cr—Mn alloys with C and N additions: DFT and Wagner-Schottky model investigations

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ABSTRACT

The pseudo-potential Density Functional Theory (PP-DFT) combined with the statistical Wagner-Schottky model, are applied to study the Fe-*x*Mn-(26-*x*)Cr—5Mo—3Cu-0.6C-0.7 N austenitic alloys ($x = 6, 9, 12$ and 15 wt%). The obtained results show that the rigidity and the thermal vacancy behavior is very sensitive to the system composition. The overall system stability is found to be governed by the presence of nitrogen. Both carbon and nitrogen favor the vacancy creation at T~1200K and prevent the thermal vacancy activation at T~1600K. Interestingly, beyond 1273K, carbon atom could migrate toward the substitution sites while nitrogen atoms do not leave their favorable octahedral sites.

1. Introduction

Due to the beneficial combination of strength, ductility and good corrosion resistance, austenitic iron alloys are an important class of materials proposed for a wide variety of stainless steel applications, such as biomedical, automotive and mechanical engineering, and nuclear industry [1–4]. Essentially composed with Cr and Ni, these steel alloys have been progressively replaced by Cr—Ni—Mo ones. However, because of their quite high cost price, due essentially to the alloying elements (nickel, chromium), less expensive ones (N, C, Mn … etc) were introduced. Although carbon has long been used for this purpose, its use is not recommended for certain applications because of the risk of corrosion. Nitrogen, a neighboring element of carbon, has fewer disadvantages with respect to corrosion, but it has a low solubility in iron, estimated at about 0.28% at 1323 K for a 18-10 steel [5]. However, by the addition of Mn, it is possible to increase this solubility. Manganese and nitrogen are introduced as austenite stabilizers elements to replace nickel (Ni-free steels), making high nitrogen steel alloys (HNS) more biocompatible and more economical than the conventional ones [6–16].

In solid state, combined addition of C and N is effective in increasing mechanical strength. It reduces the production cost, enhances the wear resistance and improves resistance to pitting and crevice corrosion [6,7,9,12,17]. In general, N slows down the formation of carbides and carbon slows nitrides formation. These two elements act then on the rate of diffusion of Cr, which has a close relationship with the corrosion behavior [11,17,18]. On the other hand, binary and ternary phase diagrams provide several solid solutions including Fe and the other alloying elements (Cr, Mn, Mo, Ti, V) [19]. The substitution of Fe by one or more of them contributes significantly to the improvement of the properties of the steels.

However, little attention has been directed on the modeling of the Cr—Mn austenitic alloyed to C and N [20] and also on the interaction of vacancies with the alloy elements in the austenitic phase (fcc-Fe). Based on a thermodynamic model, M H Wu et al./ [21] show that increasing N content up to 10 at.% at 750 K increases considerably the vacancy concentration, by about eight orders of magnitude when a saturated concentration is reached. The

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