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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-xMn-(26-x)Cr-5Mo-3Cu-0.6C-0.7N austenitic alloys (x 1?4 6, 9, 12 and 15 wt%). The obtained results show that the rigidity and the thermal vacancy behavior isvery sensitive to the system composition. The overall system stability is found to be governed by thepresence of nitrogen. Both carbon and nitrogen favor the vacancy creation at T~1200K and prevent thethermal vacancy activation at T~1600K. Interestingly, beyond 1273K, carbon atom could migrate towardthe substitution sites while nitrogen atoms do not leave their favorable octahedral sites.

Keywords : Fe-Cr-Mon Alloys;, Structural Stability;, Rigidity, Thermal Vacancies, DFT, Wagner-Schottky Model