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Title: Correction to the Wills-Harrison approach: Influence on the Fe-based liquid alloys thermodynamics

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Some years ago, we have developed the procedure for calculating the thermodynamic properties of binary transition-metal liquid alloys [1] on the basis of the Wills-Harrison (WH) model [2]. More recently, in the framework of the WH model the correction due to the non-diagonal coupling (NDC) between d electrons of different atoms was suggested [3]. In the present work, we study an influence of this correction on the thermodynamics of liquid Fe-Co and Fe-Ni alloys in the framework of the calculation formalism developed in Ref. [1]. The heat of mixing and Helmholtz free energy of mixing are investigated at different component concentrations near melting. It is found that the results obtained agree with experimental data better than ones obtained without the NDC correction for both alloys under consideration. This tendency is more powerful for Fe-Co alloy and less for Fe-Ni. This work is supported by the Ural Branch of the Russian Academy of Sciences (project 09-T-3-1012), Russian Ministry of Science and Education (contract 02.740.11.0641), and Russian Program of Scientific Schools (grant 4319.2010.3). [1] N.E. Dubinin, L.D. Son, N.A. Vatolin, J. Phys.: Condensed Matter, v. 20 (2008), 114111. [2] J.M. Wills, W.A. Harrison, Phys. Rev. B, v. 28 (1983), p. 4363. [3] N.E. Dubinin, J.Phys.: Conference Series, in print (2011).