



## ICAMS Special Seminar

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### Ab initio-based mean field theory of site occupation in binary sigma phases

The talk concerns the simulation of the atomic site distribution in binary sigma-phases, which are found in many industrial alloys and usually lead to a destructive effect on the mechanical properties of these alloys. Among them the Fe-Cr  $\sigma$ -phase is the most investigated one due to relevance to different types of steels, where its formation should be avoided due to extreme brittleness. This phase has a low symmetry structure (P42/mnm) with a tetragonal unit cell of 30 atoms divided into 5 nonequivalent sites (2a,4f,8i,8i',8j) denoted as (A,B,C,D,E). One of the most difficult issues for theory as well as for experiment is the description of the  $\sigma$ -phase stability, which first of all implies the accurate determination of the atomic distribution among its five nonequivalent sites. In present work [1,2] we have proposed a simple and powerful approach to calculate the site occupation numbers in binary  $\sigma$ -phases as function of temperature and composition. It is based on the single-site mean-field description of the free energy, where the total energy is expanded in terms of on-site effective cluster interactions. We have shown that the Fe-Cr system exhibits a non-trivial magnetic behavior at high temperatures, which affects the site occupations. The calculated site occupations in the Fe-Cr  $\sigma$ -phase are in very good agreement with available experimental data [3,4]. The structural variation (volume and  $c/a$ ), that might be present due to irradiation and thermal expansion, can lead to an additional atomic redistribution.

The suggested method has been further applied to the Fe-V system and some tests were also performed for the Co-Cr and Re-W sigma-phases. The calculated atomic site occupancies show some general trends, but also some individual features in agreement

with empirical scheme of ordering proposed earlier by Kasper and Waterstrat [5]. The present work has been performed in collaboration with Prof. A. V. Ruban from Royal Institute of Technology, Stockholm.

[1] E. Kabliman, P. Blaha, K. Schwarz, A. V. Ruban, B. Johansson, *Phys. Rev. B* 83, 092201 (2011)

[2] E. Kabliman, P. Blaha, K. Schwarz, O. Peil, A. V. Ruban, B. Johansson, submitted to *Phys. Rev. B* (2011).

[3] H. L. Yakel, *Acta Crystall. B*, 20 (1983)

[4] J. Cieslak, M. Reissner, S. Dubiel, J. Wernisch, and W. Steiner, *J. All. Comp.* 460, 20 (2008)

[5] J. S. Kasper and R. Waterstrat, *Acta Crystall.* 9, 289 (1956)