On behalf of the

Science College CMS

Vienna Computational Materials Laboratory

and Center for Computational Materials Science

we cordially invite you to the following 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 σ-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 ($P4_2/mnm$) 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 σ-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 σ-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 σ-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)

Date: Monday, Oct 10, 2011 16:00

Location: Seminar room 138C (TU Freihaus 9. Stock, gelb)
A-1040 Wien, Wiedner Hauptstaße 8-10