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AB-INITIO HYPERFINE FIELDS IN Fe-Cr

Fe-Cr alloys form the basis of many industrially important steels, in particular, of the stainless steels. In recent years interest on Fe-Cr alloys grew due to the excellent resistance to irradiation induced swelling of ferritic stainless steels, which are expected to be key materials for developing critical structural components in advanced nuclear reactors. Iron-chromium alloys are characterized by extensive mutual solubility in the bcc phase at high temperatures, with small positive enthalpy of mixing and by complex magnetic interactions [1]. All this justifies the investigation of the constitution, thermodynamics and complex magnetic interactions of the bcc Fe-Cr alloys. In this work we focus on the the hyperfine fields at the Fe sites in bcc-based Fe-Cr alloys, determined from first principles calculations. We use the Full-Potential Linear Augmented Plane Wave method (FP-LAPW) as embodied in the WIEN2k code [02]. This method allows the computational of very precise total energies and charge densities in metallic compounds due to its full potential feature and is, one of the most accurate methods for electronic structure calculations in solids, specially metals. Our hyperfine fields are discussed in the light of the theoretical and experimental results in the literature. References [1] Inden, G., C. G. Schön . Thermodynamic self-consistency issues related to the Cluster Variation Method: the case of the BCC Cr-Fe (Chromium - Iron) system. CALPHAD 32 (2008) 661- 668. [02] P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka and J. Luitz, WIEN2k, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties (Karlheinz Schwarz, Techn. Universität Wien, Austria), 2001. ISBN 3-9501031-1-2 Key-words: Fe-Cr alloys, magnetic ordering, WIEN2k, FP-LAPW, intermetallic compounds. Poster Presentation.

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Poster

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