HYPERFINE INTERACTIONS OF ^{57}Fe IN Pt_3Fe – AB INITIO AND MÖSSBAUER EFFECT STUDIES

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9.7 cm

The Pt_3Fe ordered alloy crystallizes in a cubic Cu_3Au-type of structure and shows an antiferromagnetic (AFM) phase transition at T_N=150 K. In the AFM state the Pt_3Fe displays the magnetic structure of (1/2,1/2,0)-type at high and of (1/2,0,0)-type at lower temperatures. The Mössbauer measurements show that, despite cubic crystal structure the electric field gradient (EFG) is present at ^{57}Fe sites. The quadrupolar splitting observed in Zeeman sextet is small and independent on the sample preparation details. The aim of the paper is to elucidate the physical mechanism responsible for the occurrence of the EFG at the ^{57}Fe nucleus in antiferromagnetic Pt_3Fe. With this aim the *ab initio* electronic structure calculations for Pt_3Fe were carried out for paramagnetic, ferromagnetic and both AFM ground states. The calculations were performed applying the Full Potential version of the Linearized Augmented Plane Wave method. Basing on the results of calculations the ^{57}Fe hyperfine parameters were determined and compared with the experimental data. The parameters were analyzed in relation to the electronic structure changes upon the magnetic phase transitions. Our investigations indicated that the AFM transition in Pt_3Fe forces the valence charge density reordering. The process results in the lowering of the local charge density symmetry and is responsible for the occurrence of the electric field gradient at the Fe nuclei in the AFM Pt_3Fe.

13.4 cm

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