HYPERFINE INTERACTION PARAMETERS IN Fe₂₈Al₇₂: ⁵⁷Fe MöSSBAUER SPECTROSCOPY AND AB INITIO STUDY

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It is well established that physical and mechanical properties of Fe-Al alloys are related to their atomic ordering. Mössbauer spectroscopy offers a sensitive microscopic probe to identify the nature of ⁵⁷Fe-atom configurations responsible for various hyperfine fields observed in Fe-Al alloys. The experimental investigations of multicomponent Fe₂₈Al₇₂ alloys of nominal composition 71.64 at % Fe, 28 at % Al and small amounts of other additives (Mo-0.2, C-0.1, Zr-0.05, B-0.01 at%) introduced in order to improve their thermal and mechanical properties were performed with the use of X-ray powder diffraction and Mössbauer effect spectroscopy. We present a method of determining the level of long range ordering in the alloys characterized by superstructure D₀₃. In the presented approach, the possible atomic configurations around ⁵⁷Fe are the basis for reconstruction of Mössbauer spectrum. The degree of ordering is expressed by a sum of populations of chosen atomic configurations characteristic for entirely ordered structure. To control the Mössbauer spectra analysis the complimentary, DFT based, quantum calculations of hyperfine parameters were performed with the use of FP-LAPW method. The hyperfine parameters obtained from the Mössbauer spectra analysis are compared with the results of ab initio calculations performed for the reference system Fe₃Al.

Acknowledgment: The work was supported by the Ministry of Science and High Education in Poland within Grant no. N N507 480938.