HYPERFINE INTERACTION PARAMETERS IN $Fe_{28}Al_{72}$: ^{57}Fe MÖSSBAUER SPECTROSCOPY AND *AB INITIO* STUDY

A. Hanc, J. Deniszczyk, J. Kansy
Institute of Materials Science, University of Silesia, 40-007 Katowice, Poland

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 ^{57}Fe-atom configurations responsible for various hyperfine fields observed in Fe-Al alloys. The experimental investigations of multicomponent $Fe_{28}Al_{72}$ 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 $D0_3$. In the presented approach, the possible atomic configurations around ^{57}Fe 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 Fe_3Al.

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