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Modelling of phase composition of Zr-Fe layered system subjected to thermal annealing

Abzal K. Zhubaev, Gulzat Zh. Omarpatsha, Amangul Sh. Amantayeva, Diana M. Bahtiyarova

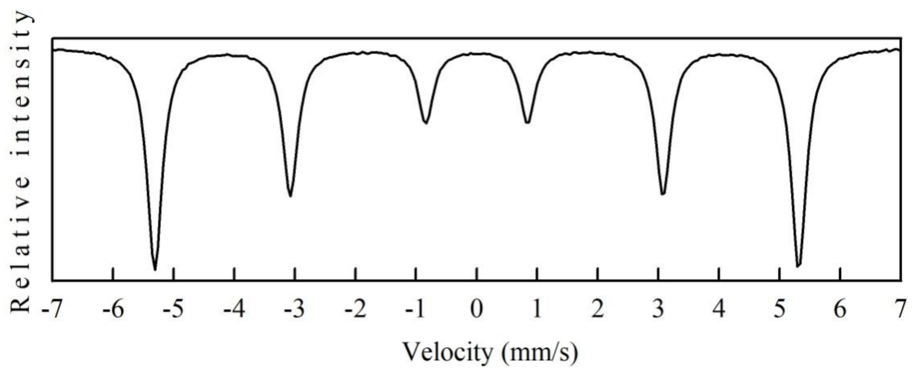
Aktobe Regional State University, Aktobe, Kazakhstan, mosslab.kz@mail.ru

The phase diagram of the Fe-Zr binary system is characterized by low solubility of the components in each other and the presence of intermetallic compounds [1]. The existence of intermetallic phases in the Fe-Zr system was established: $FeZr_3$ (paramagnet with an orthorhombic lattice of the Re_3B type), $FeZr_2$ (paramagnet with an orthorhombic lattice of the $NiTi_2$ type) and Fe_2Zr (ferromagnet, Laves phase with a cubic lattice of the $MgCu_2$ type), and Fe_3Zr (close-packed fcc structure of the type Ti_6Mn_{23}) [2].

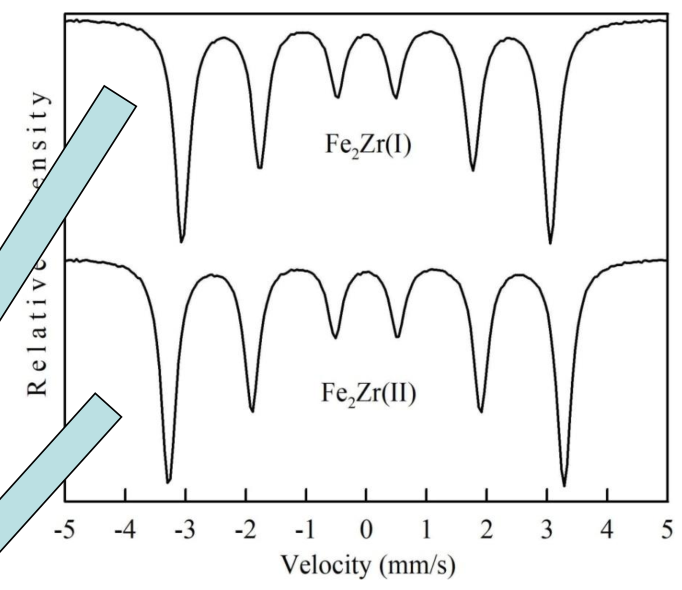
The Mössbauer spectrum of the first paramagnetic phase is a doublet with an isomeric shift δ=–0,151±0,005 mm/s and quadrupole splitting Δ=0,24±0,02 mm/s [3]. The second intermetallic compound [4] in a stable state is a doublet (δ=–0,319±0,005 mm/s and Δ=0,91±0,01 mm/s).

It is known [5] that the Mössbauer spectrum of the Fe_2Zr phase is a superposition of two sextets (with effective magnetic fields at ^{57}Fe nuclei H_n=190±5 kOe and H_n=200±5 kOe) with an intensity ratio of 1:3. This is due to the fact that the Iron atoms in the Fe_2Zr compound occupy nonequivalent positions with different values of the angle α between the direction of the gradient of the axially symmetric electric field and the magnetic field at nucleus. The Fe_3Zr phase is characterized by three sextets with fields H_n=180±5, 224±5 и 241±5 kOe with an intensity ratio of 2:1:1 [6]. The Mössbauer spectrum of the solid solution of Iron in α-Zr is a quadrupole splitting line with an isomeric shift δ=–0,07±0,02 mm/s and a quadrupole splitting Δ=0,32±0,02 mm/s [7].

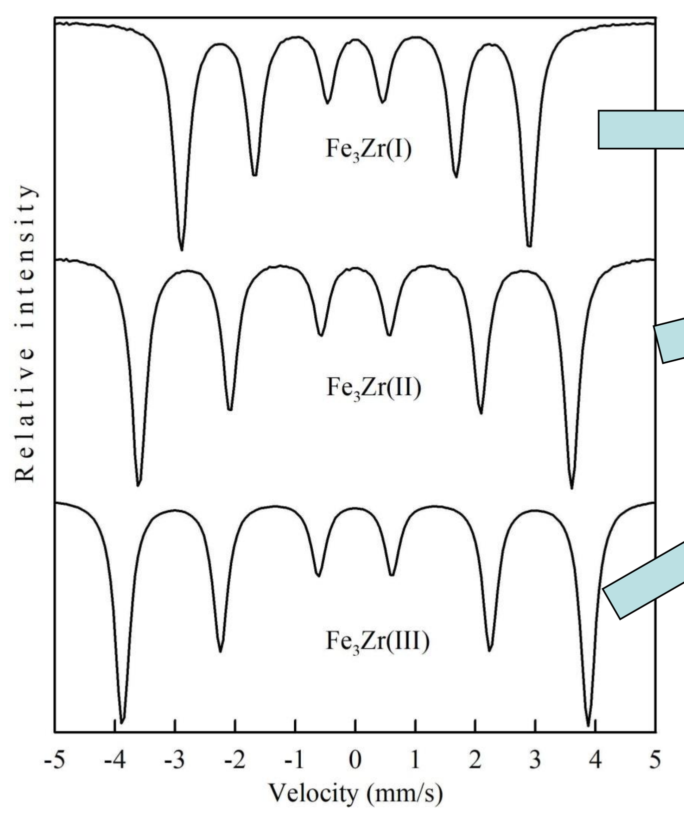
The methods of processing and analysis of Mössbauer data implemented in the form of the MSTools software package [8] were applied in our work. Currently, the MSTools complex consists of ten programs designed to process and analyze both experimental Mössbauer spectra and their parameters. To achieve the goal of the work, we used a model decoding of Mössbauer spectra using a priori information about the object of study (SPECTR) and a comparison of the experimental spectra with the spectra of standard samples (PHASAN).



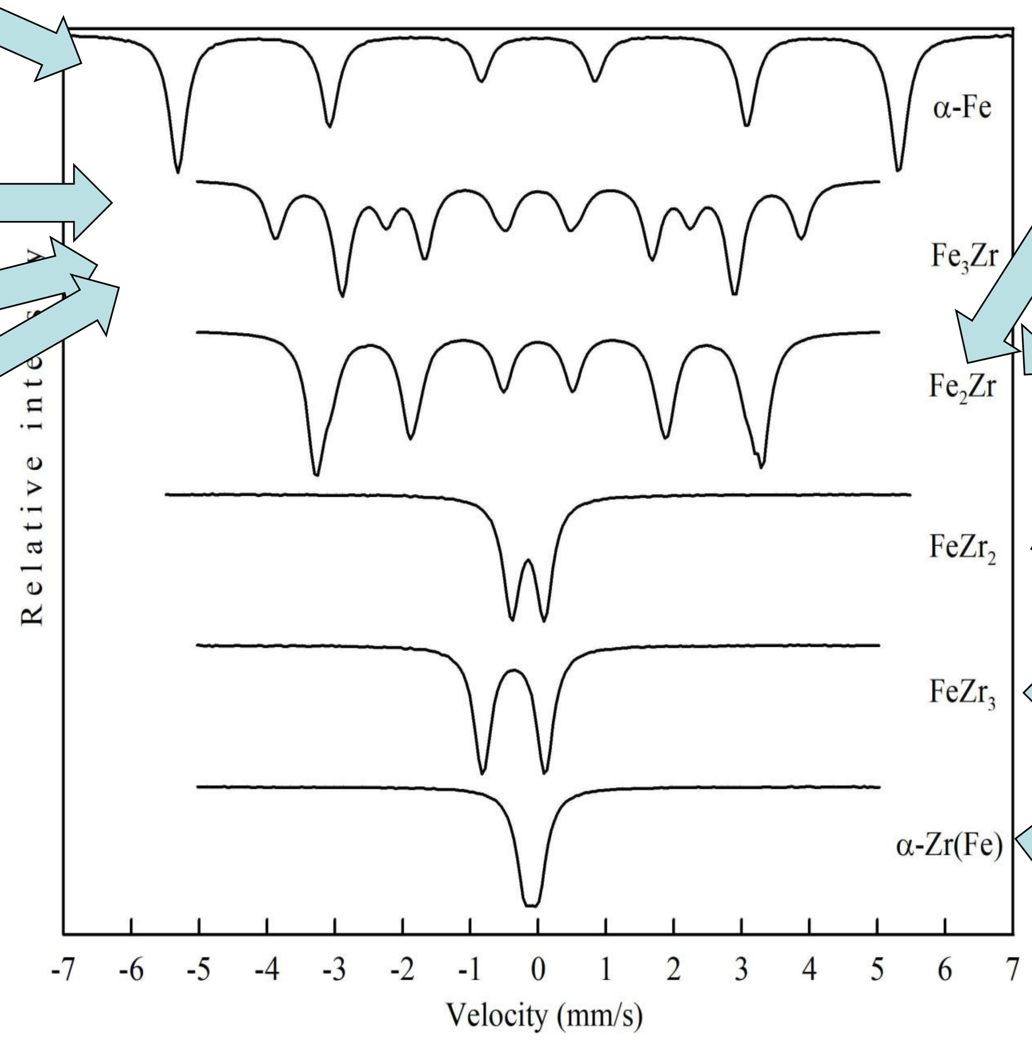
Simulated spectrum of ^{57}Fe nuclei in α-Fe



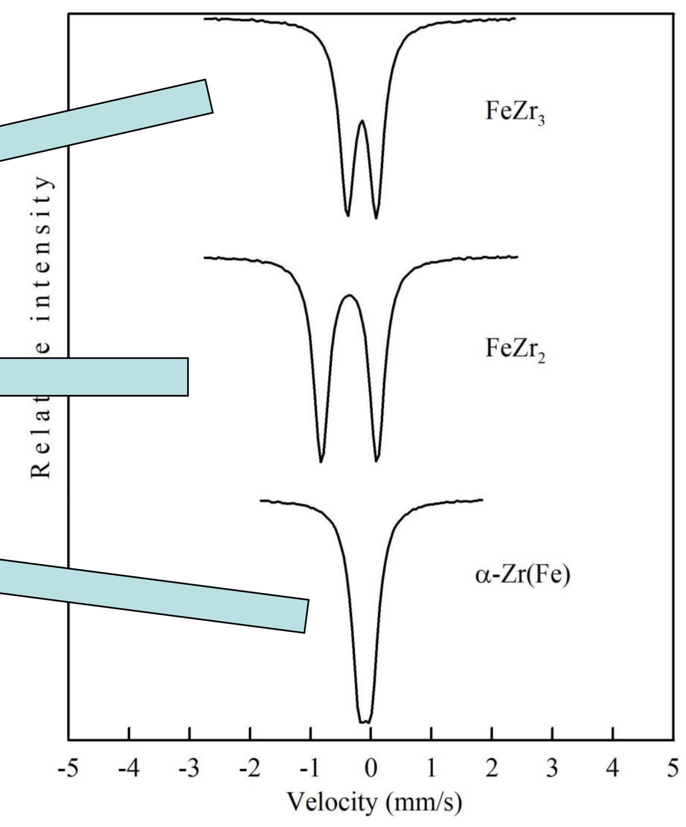
Simulated spectra of ^{57}Fe nuclei in different positions in Fe_2Zr



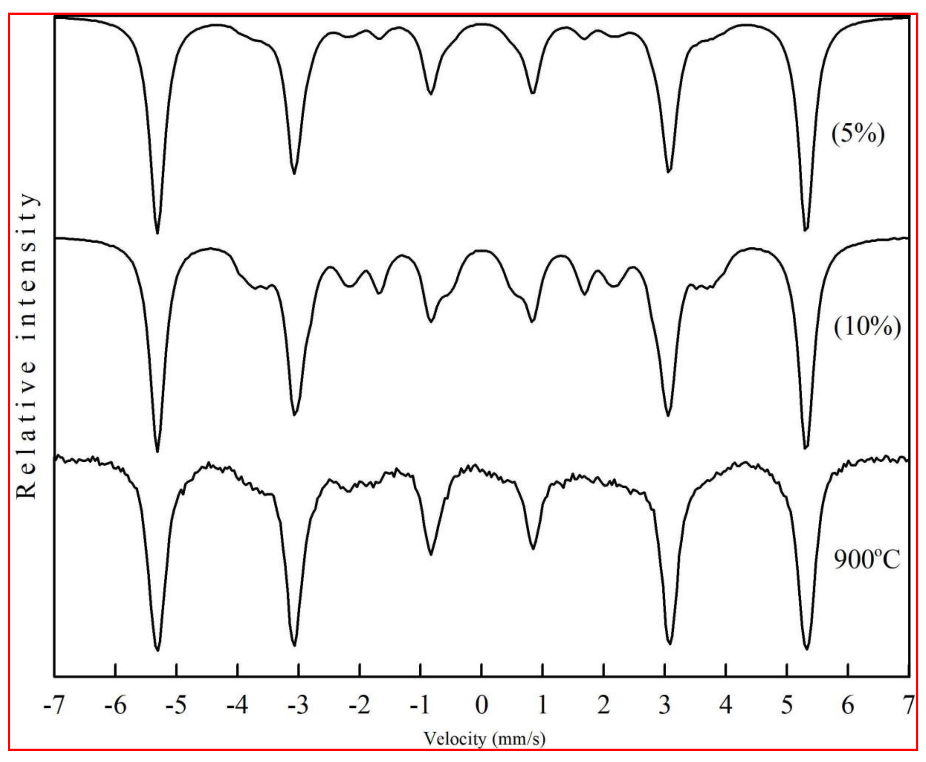
Simulated spectra of ^{57}Fe nuclei in different positions in Fe_3Zr



Model spectra of various phases in the system Fe-Zr



Simulated spectra of ^{57}Fe nuclei in paramagnetic phases



Simulated spectra of the Zr-Fe system with zirconium concentrations of 5% and 10%, and experimental spectra of the Zr(2 μm)-Fe(10 μm) system subjected to isochronous thermal annealing at 900°C for 2 h

Conclusion

As a result of the studies, reference spectra of ^{57}Fe nuclei in various intermetallic compounds and solid solutions of the Fe-Zr binary system were obtained. Using the "lever rule", the relative contributions of the phases were calculated and the spectra with different zirconium concentrations were recreated. Comparison with experimental Mössbauer spectra of the Zr(2 μm)-Fe(10 μm) layered system subjected to thermal annealing at 900°C temperature showed a good correlation.

References

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