

A comparison of crystalline and quasicrystalline Al-Mn-Fe compounds

Kamran Ali · Michael Reissner ·
Walter Steiner · Michael Feuerbacher

© Springer Science+Business Media B.V. 2011

Abstract New complex metallic alloys of the Taylor phase Al₃Mn with 8, 10 and 12% Fe substitution are investigated by ⁵⁷Fe Mössbauer spectroscopy. Two groups of subspectra, with different hyperfine parameters are obtained, and are allocated to Fe sites with only Al nearest neighbors and Fe sites with both Al and Mn in the first shell. No difference between crystalline and quasicrystalline compounds is found indicating that long range periodicity plays a minor role.

Keywords Taylor phase · Spin glass · Complex metallic alloy

1 Introduction

We report on Taylor phase compounds on the Al-rich side of the Al-Mn phase diagram around 70% Al with Fe substitution up to 12 at%. These compounds are so-called ‘Complex Metallic Alloys’, with extreme large numbers of atoms in the unit cell. It was shown that the physical properties of such crystals are mainly determined by the existence of typical substructures, with length scales, which can substantially differ from the lattice constants [1]. A further important characteristic is inherent disorder, caused by partly or mixed occupancy of lattice sites and the occurrence of building blocks in different orientations inside the unit cell. By slightly different heat treatment a decagonal quasicrystal with nearly the same composition could be produced, which gives the possibility to investigate the similarity of both crystalline and quasicrystalline compounds on the very local basis of Mössbauer spectroscopy.

K. Ali · M. Reissner (✉) · W. Steiner
Institute of Solid State Physics, Vienna University of Technology, Vienna, Austria
e-mail: reissner@ifp.tuwien.ac.at

M. Feuerbacher
Institute of Microstructure Research, Forschungszentrum Jülich, Jülich, Germany

2 Experimental

Samples of the orthorhombic Taylor phase Al_3Mn ($Pnma$) with 8, 10, and 12% Fe substitution were produced by levitation induction melting in a water-cooled copper crucible under argon atmosphere followed by thermal annealing for 164 h at 1010°C [2]. For 10% Fe also a sample with decagonal structure could be synthesized. EDX-analysis gave the following compositions: $\text{Al}_{69}\text{Mn}_{23}\text{Fe}_8$, $\text{Al}_{70}\text{Mn}_{20}\text{Fe}_{10}$, and $\text{Al}_{68}\text{Mn}_{20}\text{Fe}_{12}$ for the crystalline and $\text{Al}_{71}\text{Mn}_{19}\text{Fe}_{10}$ for the quasicrystalline compound. Dc magnetic measurements were performed by QD-PPMS-9T-VSM and ^{57}Fe Mössbauer spectra were recorded with a standard constant acceleration spectrometer in transmission geometry between 4.3 K and room temperature. For analysis the full Hamiltonian including electrostatic and magnetic hyperfine interaction is solved [3]. Sample thickness was taken into account after [4].

3 Results

From magnetic measurements spin glass behavior is found for all samples with freezing temperature around 30 K, increasing with Fe concentration. Details of the magnetic measurements are given in [5, 6].

Mössbauer spectra above the freezing temperature are broadened, asymmetric doublets (Fig. 1). They can be fitted by only two subspectra with intensity ratio around 30:70 and line width around 50% larger than the experimental resolution. Quadrupole splitting $eQV_{zz}/4 = 0.15(0.34)$ mm/s, $0.16(0.34)$ mm/s, and $0.15(0.32)$ mm/s as well as center shift $\text{CS}(\text{rel.}^{57}\text{FeRh}) = 0.092(0.069)$ mm/s, $0.083(0.051)$ mm/s, and $0.093(0.071)$ mm/s for the majority(minority) component are obtained at 294 K for the Taylor phases with $x = 8, 10,$ and 12% Fe, respectively. Same values are determined for the decagonal compound. In fitting the spectra by two discrete subspectra instead of distributions, the assumption of a fixed relation between quadrupole splitting and center shift could be avoided. This is surely not the only possibility to fit the data, but gains on reliability as the obtained hyperfine parameters change smoothly with concentration.

Below the freezing temperature the spectra are more complex (Fig. 1). To fit them, both subspectra were divided into three, where the sum of relative area of these three spectra is in fair agreement with that from the high temperature fits. An increase in number of subspectra does not improve the quality of the fit. For each group quadrupole splitting and center shift scatter only within measuring accuracy. Obtained mean hyperfine fields increase slightly with Fe concentration (8.1, 8.1, and 8.4 T for 8, 10, and 12% Fe). This is the same trend as found for the effective magnetic moment [6]. An analysis in terms of hyperfine field distributions gives large contributions at zero field for all samples. Within statistics of the recorded spectra no difference between crystalline and quasicrystalline samples is found (Fig. 1).

4 Discussion

In view of the complex structure—the unit cell of the T-phase consists of 156 atoms with ten different Mn sites—the two groups of subspectra have to be interpreted

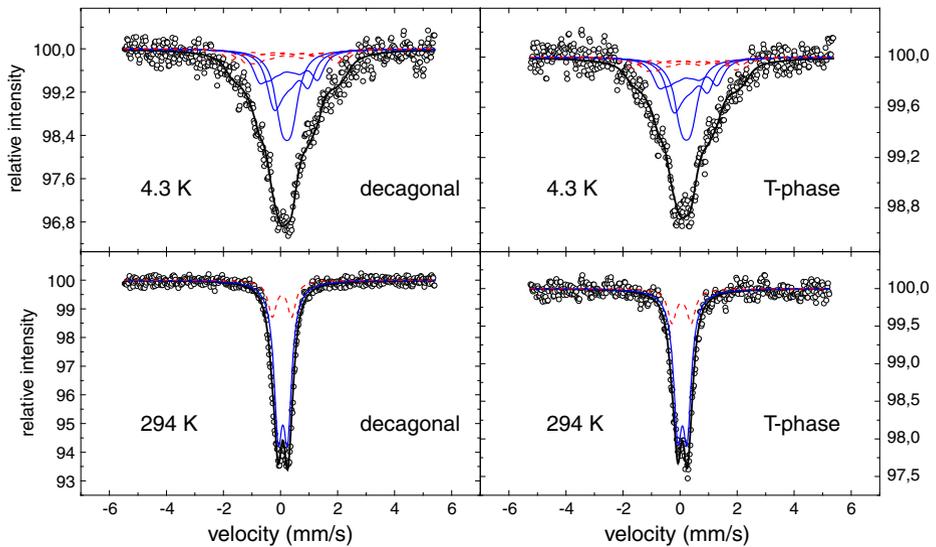


Fig. 1 Comparison of Mössbauer spectra for quasicrystalline (*left*) and crystalline (*right*) Al_3Mn with 10% Fe substitution for temperatures below and above the freezing temperature. The two groups of subspectra are indicated by *solid* and *dashed* lines

to be representatives of two characteristically different groups of crystallographic sites. If one defines the first Mn neighbor shell by the radius following from the sum of the metallic bonds of Al and Mn, one gets, using the occupation numbers given by [7], one Mn-site with only Al atoms in the first shell and a second site with two Mn atoms just at the border of this shell. For all other Mn sites Mn atoms are present in this shell, much closer to the central atom. This consideration defines two groups of Fe-environments for which different hyperfine parameters can be expected. According to our structural investigation and taking into account the concentrations obtained by EDX it was assumed that i) Fe replaces only Mn, ii) that deviations in Al concentration from the ideal $\text{Al}_3(\text{Mn},\text{Fe})$ composition changes only the occupation numbers of mixed Al/Mn sites and iii) that substitution is random. With these assumptions a ratio of the two groups of Fe environments very similar to the intensity ratio obtained for the two groups of subspectra is obtained.

The small difference in center shift for the two groups of Fe environments and the fact that the weighted mean quadrupole splitting and center shift are very similar to the ones obtained for samples with comparable Al concentration but other 3d-elements instead of Mn, like Pd [8], Cu [9] or Ni [10] indicates, that not the Mn-Fe interaction, but the Al(s,p)-Fe(3d) hybridization determines the charge density at the Fe nucleus. Within the investigated concentration interval changes in Fe concentration have only minor influence on the hyperfine parameters. The large contribution with zero field obtained in the hyperfine field distribution of all samples at temperatures below the freezing temperature might be allocated to Fe embedded on those Mn sites, which carry no moment [11]. As the hyperfine parameters for the decagonal sample are within experimental resolution identical with the ones of the crystalline compounds, it can be concluded that for the electronic exchange

interaction those length scales, which are determined by the very similar building blocks forming the T-Al₃Mn phase and the decagonal compound, are dominant. The presence of long range periodic atomic order is of less importance.

Acknowledgements Work performed within the EU Network of Excellence “Complex Metallic Alloys”

References

1. Urban, K., Feuerbacher, M.: *J. Non-Cryst. Solids* **334–335**, 143 (2004)
2. Balanetsky, S., Meisterernst, G., Heggen, M., Feuerbacher, M.: *Intermetallics* **16**, 71 (2008)
3. Kündig, W.: *Nucl. Instrum. Methods* **48**, 219 (1967)
4. Mørup, S., Both, E.: *Nucl. Instrum. Methods* **124**, 445 (1975)
5. Ali, K., Reissner, M., Feuerbacher, M., Steiner, W.: *Journal of Physics: Conference Series* **200**, 032002 (2010)
6. Ali, K., Reissner, M., Feuerbacher, M., Steiner, W.: Solid compounds of transition elements. In: Bolet, J.L., Chevalier, B., Fruchart, D. (eds.) *Book Series: Solid State Phenomena*, vol. 170, p. 127 (2011)
7. Hiraga, K., Kaneko, M., Matsuo Y., Hashimoto S.: *Phila. Mag. B* **67**, 193 (1993)
8. Lawther, D.W., Dunlap, R.A.: *J. Non-Cryst. Solids* **153–154**, 49 (1993)
9. Brand, R.A., Pelloth, J., Hippert, F., Calvayrac, Y.: *J.Phys.:* *Condens. Matter* **11**, 7523 (1999)
10. Dunlap, R.A.: *Phys. Mag. B* **67**, 69 (1993)
11. Hafner, J., Krajčí, M.: *Phys. Rev. B* **57**, 2849 (1998)