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Low-temperature antiferromagnetism in quaternary $Mn_2FeSi_{0.5}Al_{0.5}$ alloys

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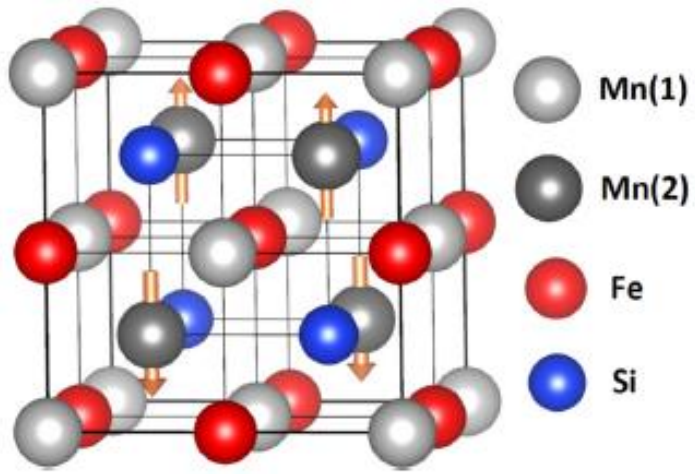
Heusler alloys

- ternary compounds of general formula **X_2YZ** (full-Heusler) or **XYZ** (half-Heusler),
- special class of tunable materials with more than 4000 potential members,
- wide range of applications,
- in present – many theoretical calculations of existing and/or newly proposed compositions,
- applications: microelectronics and spintronics, magnetic shape memory, etc.
- Present fabrication technologies:
    - **ingot metallurgy,**
    - thin films,
    - powder metallurgy,
    - planar flow casting.

Mn-based alloys

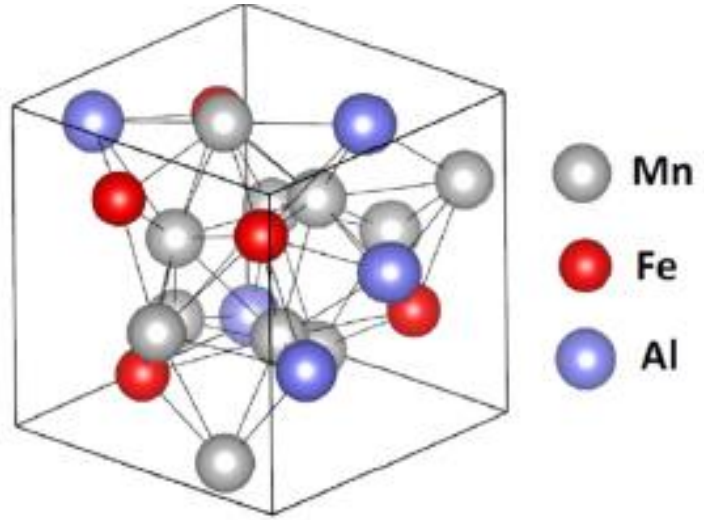
Mn_2FeSi
inverse-Heusler (XA) structure



Unit cell formed by A, B, C, and D fcc sublattices. Corresponding coordinates of A, B, C, and D sites (along the unit cell body diagonal) are: A – (0,0,0), B – (1/4,1/4,1/4), C – (1/2,1/2,1/2), D – (3/4,3/4,3/4). Mn(1) = Mn_A and Mn(2) = Mn_B (Fe_C and Si_D). Arrows indicate possible directions of magnetic moments in antiferromagnetically ordered collinear structures.

O. Zivotsky et al., J. Alloys Comp. 947 (2023) 169672.

Mn_2FeAl
primitive cubic (β-Mn) structure



Pure β-Mn structure consists of 20 Mn atoms that occupy C (8 atoms) and D (12 atoms) fcc sublattices with the coordinates (0.0636, 0.0636, 0.0636) and (0.1250, 0.2022, 0.4522). According to the electronic calculations the structure consisting of 3 Al, 1 Fe, and 8 Mn atoms at D positions and 2 Al, 4 Fe, and 2 Mn atoms at C positions has the lowest total energy.

S. Dash et al., J. Magn. Magn. Mater. 513 (2020) 167205.

Fabrication technology:

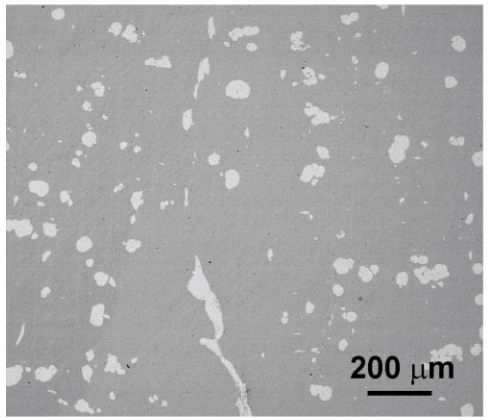
quaternary $Mn_2FeSi_{0.5}Al_{0.5}$ ingots

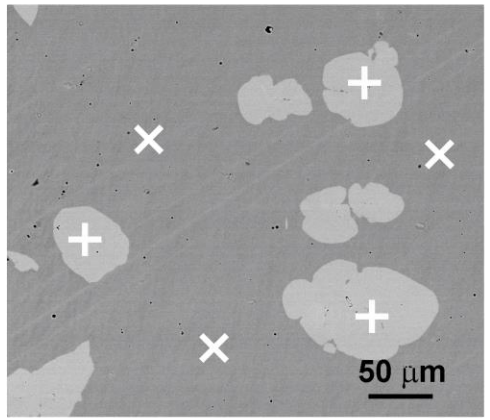
- high purity elements: **manganese (≥ 99.9 wt.%)**, **iron (99.95 wt.%)**, **silicon (≥ 99.9 wt.%)**, and **aluminium (≥ 99.9 wt.%)**,
- cylinder-shaped ingots using an induction furnace Supercast Titan furnace (Linn High Therm, Germany),
- argon protective atmosphere to prevent oxidation,
- re-melting four times to ensure good homogeneity,
- cutting, grinding (SiC sandpapers), polishing,
- homogenization **annealing at 773 K for 100 h,**
- **AC** - as-cast sample, **AN** – annealed sample.

Surface morphology and phase composition

Mn_2FeSi

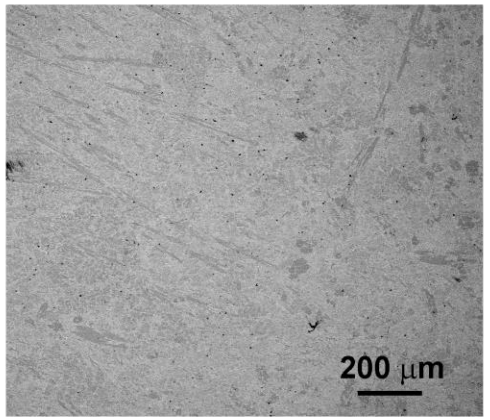
as-cast

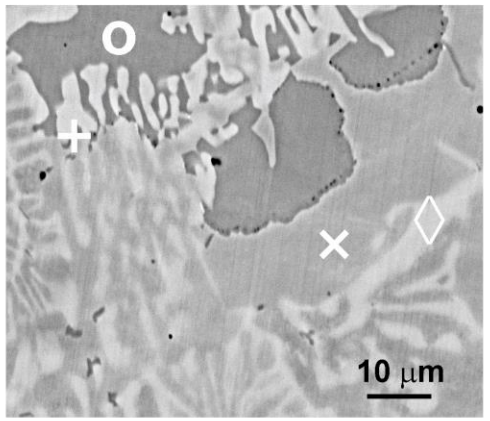




phase	Mn (at.%)	Fe (at.%)	Si (at.%)
mx (×)	48.0 ± 0.2	23.8 ± 0.3	28.2 ± 0.4
pp (+)	52.5 ± 0.4	25.0 ± 0.5	22.5 ± 0.3

annealed

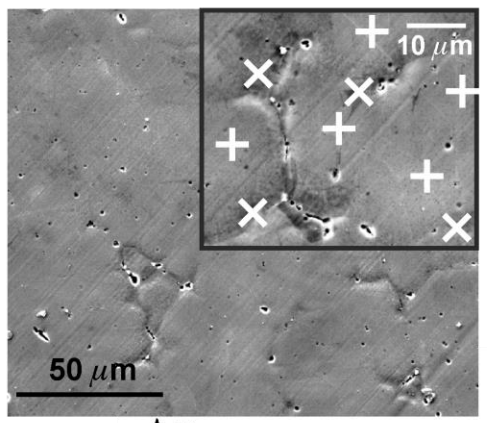




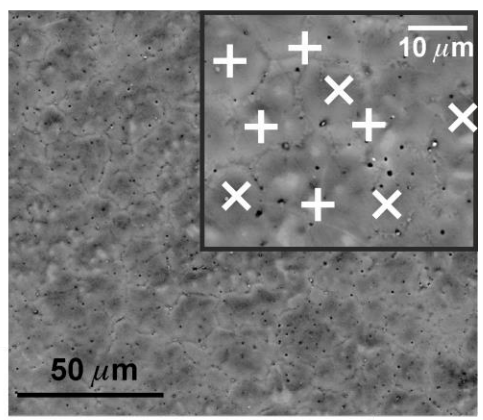
phase	Mn (at.%)	Fe (at.%)	Si (at.%)
1 (×)	47.7 ± 0.3	24.9 ± 0.2	27.4 ± 0.4
2 (+)	56.1 ± 0.3	17.6 ± 0.4	26.3 ± 0.5
3 (o)	42.9 ± 0.4	17.2 ± 0.3	39.9 ± 0.3
4 (◊)	57.6 ± 0.5	19.9 ± 0.6	22.5 ± 0.4

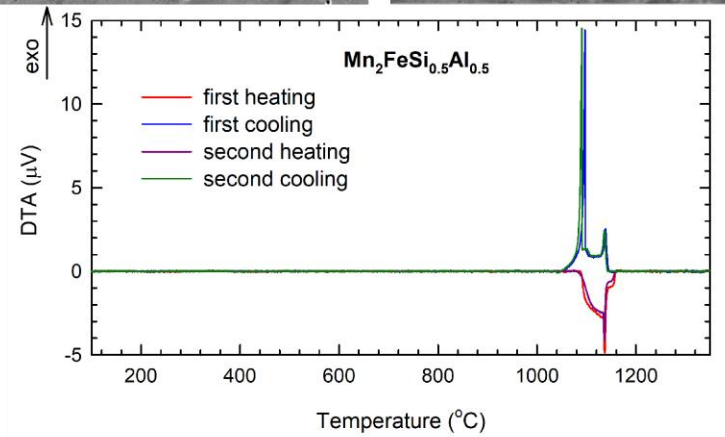
$Mn_2FeSi_{0.5}Al_{0.5}$

as-cast



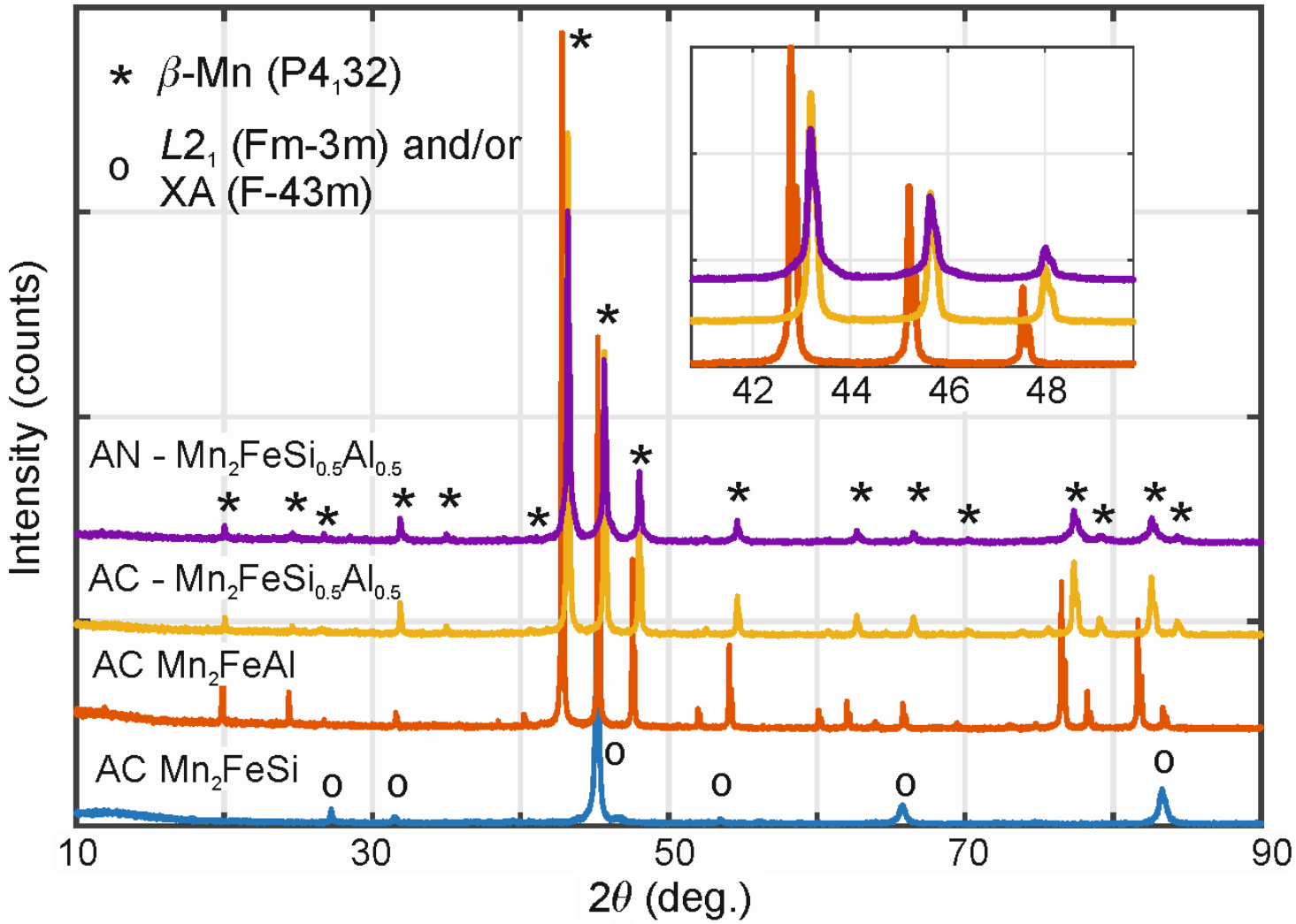
annealed





	phase	Mn (at.%)	Fe (at.%)	Si (at.%)	Al (at.%)
as-cast	dark grey (×)	49.7 ± 0.2	23.3 ± 0.1	18.0 ± 0.2	9.0 ± 0.1
	light grey (+)	48.0 ± 0.3	25.0 ± 0.2	13.6 ± 0.3	13.4 ± 0.2
annealed	dark grey (×)	48.1 ± 0.2	24.5 ± 0.1	16.1 ± 0.2	11.3 ± 0.2
	light grey (+)	46.0 ± 0.3	24.7 ± 0.2	15.6 ± 0.3	13.7 ± 0.3

Structure analysis – X-ray diffraction



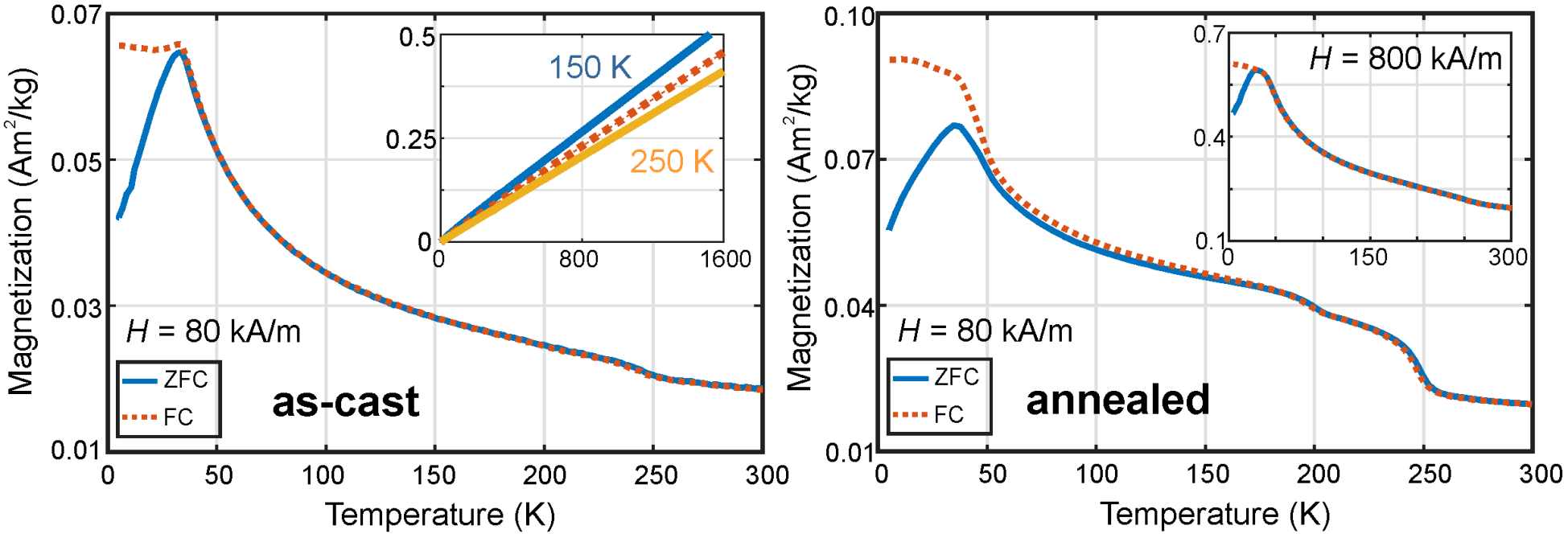
Lattice constants:

Mn_2FeSi: a = 0.5672(3) nm

Mn_2FeAl: a = 0.6339(1) nm

$Mn_2FeSi_{0.5}Al_{0.5}$: a = 0.6274(2) nm

Low-temperature magnetic properties



- antiferromagnetic behavior below Néel temperature ≈ 37 K, paramagnetic above room temperature (RT),
- application of Curie-Weiss law above RT gives negative Curie temperatures ≈ -700 K,
- antiferromagnetic spin fluctuation caused by strong geometric frustration of both systems,
- possible existence of Griffiths phase at 245 K and 190 K.

Conclusions

- quaternary **$Mn_2FeSi_{0.5}Al_{0.5}$** alloys succesfully prepared in the form of induction-melted ingots,
- AC and AN samples showed primitive cubic β-Mn structure comparable to the Mn_2FeAl alloy,
- the SEM and DTA measurements confirmed presence of two phases with an excess of silicon and with close melting points (1363 K, 1407 K),
- antiferromagnetism below 37 K, strong magnetic frustration, paramagnetism at RT,
- ferri-/ferromagnetic contribution detected at AN sample after cooling below 245 K.

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Thank you for your attention

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