Review report on the PhD. thesis "Study of indium doped shape-memory alloy Ni_2MnGa"

by

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The submitted PhD. thesis focuses on the preparation of single crystals of $Ni_2MnGa_{1-x}In_x$ and on the analysis of their properties with respect to the temperature and applied magnetic fields in dependence on various indium doping. This material belongs to the magnetic shape-memory alloys family and is very attractive for applications. The selected topic is actual and relevant in the context of up-to-date research in the field. Scientific quality of the obtained results is supported by the fact that most of the results presented in the thesis have been already published in leading international journals. I consider the overall approach and selected methods used in work to be correct and adequate. The author has shown that he can independently work on given scientific problem, appropriately select the experimental techniques to be used, interpret the results and disseminate them in a form of scientific papers. I especially appreciate the amount of experimental work beginning with the preparation of single crystalline samples and ending in a detailed analysis of the fine structure (twinning and modulation) including extremely difficult and time-consuming in situ X-ray diffraction experiments. It has to be also pointed out that all experimental results are completed by a thorough estimation of the uncertainty of measurement. All factors affecting the results are critically discussed and there is no tendency "to improve" the results neglecting the possible contrarious effect of measuring conditions.

From the formal point of view, the thesis is written in good English with minimum mistakes and typos and with arguments sufficiently supported by cited literature. The graphic design is excellent. Worth mentioning are probably the following incorrectnesses:

- p. 7, Fig. 1.2 – Although the yellow positions are randomly occupied by Mn and Ga atoms, they are considered to be equivalent. According to crystallographic convention, the definition of unit cell requires the smallest repeating unit. Therefore the sketch in Fig. 1.2 represents eight unit cells of B2' structure.
- p. 9 and 22 – Martensitic transformation is a phase transition of the first (page 9) or the second (page 22) kind?
- p. 24, relation (2.13) – There should by B_i in the denominator instead of A_i.
- p. 44 – Figs. 1a and 1b in the line 13 of the 1st paragraph should be probably 4.3a and 4.3b.
- p. 64 – In the Figure caption 6.9 there should be compression instead of tension.

There are a few questions which could be answered:

1. The single crystals were grown without any seed. Surprisingly, for both methods the growth directions were low index crystallographic directions – [111] for Bridgman and [100] for floating zone methods. How many growth procedures were performed and what was the reproducibility of these orientations?

2. The electrical resistivity (Fig. 4.1 on the page 43) was measured in the crystallographic direction [100] of austenite. Is it reasonable to expect any dependence of this parameter on the crystallographic orientation of the sample, i. e. on the direction of measurement?

Issues to be discussed during the thesis defense:

1. p. 41 – The values of FWHM of the symmetric diffraction 400 are listed in Table 3.3. What is the contribution of the instrumental broadening to these widths? Could it be estimated by measuring on a highly perfect crystal, e. g. silicon, performed with the same set-up?

2. p. 25, 26 – It is stated that "In the B2' ordered unit cell... ...the Bragg reflections with all indices odd are extinct". However, the space group of the ordered structure B2 is $Pm\bar{3}m$ (no. 221) (Ref. [49] in the thesis). The space lattice of this type of structure is simple (primitive) cubic (not centered). There is no extinction rule for this space group, i. e. all combinations of diffraction indices are allowed. What is the actual reason of missing intensity for the diffractions with odd indices?

3. p. 71 – The possible effect of the sample surface shift during the tension application is discussed. For the elimination of this effect an exact expression for *sycos* correction was derived. However, utilisation of this formula requires the knowledge of the actual value of shift that is of the order of tenths of mm and is hardly accessible by direct measurement. On the other hand, it is known that the parallel plate collimator standardly used in grazing incidence set-up makes the measurement insensitive to the surface roughness and/or irregularities. Similar effect has the crystal monochromator inserted in the diffracted beam. The use of these elements may probably suppress the effect of the sample surface shift, although the selection of a particular X-ray optical element is always a compromise between the required resolution and the measurable beam intensity. Was this possibility considered by the author?

Finally, I can conclude that the submitted thesis is of high standard and fulfills all criteria given for PhD. theses. I thus do recommend to accept it and after successful defense to award the PhD. doctoral degree to **Mr. Petr Cejpek**.

In Bratislava, August 27 2021 doc. RNDr. Edmund Dobročka, CSc.