Interfaces, Cells and Dendrites:
Investigating the crystal growth parameters in Ni_2MnGa preparation

Supervisor: Ross H. Colman

Magnetic shape memory alloys (MSMAs) are metals that show magnetic field induced reorientation, i.e. by applying a magnetic field, they can reorient their crystal structure and show a significant size change of the crystal [1]. These properties are nearly unique to the family of alloys based on Ni, Mn and Ga. To observe these properties, high quality single crystals are needed.

Frustratingly, Ni-Mn-Ga alloys crystallise incongruently which has two effects:

1. It results in a composition gradient during the growth
2. Can result in a cellular [2] or dendritic crystallisation front, that reduces crystal quality.

The results of a cellular growth front have been found in Ni-Mn-Ga crystals grown at high speed [3], and are missing from crystals grown slowly, confirming the expected behaviour

This project will systematically investigate the crystal growth parameters (speed, temperature gradient) which causes this effect. If time permits, or as an extension to a bachelor project, the magnetic shape memory properties of the grown crystals will then be investigated.

The crystal growth is a multi-step process, first involving the alloying of the metals, followed by preparation of the feed rods, and then growth. We will use an optical floating zone furnace, and potentially a laser floating zone furnace for the growth attempts at various speeds.

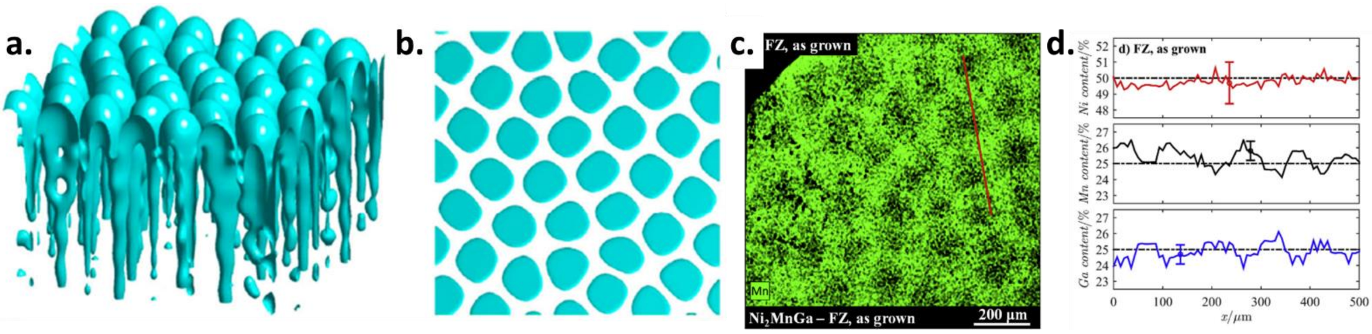

Figure 1a. *A 3D-phase field simulation of a cellular array, showing the solid-liquid interface and **b.** a transverse section of the cells, reproduced from [2]. **c. and d.** shows the observed microscopic composition variation perpendicular to growth direction, due to cellular growth, in rapidly crystalised Ni_2MnGa, with Mn concentrated in inter-cellular regions, reproduced from [3].*

References:

[1] O. Heczko, *Magnetic Shape Memory Effect and Highly Mobile Twin Boundaries*, Mater. Sci. Technol. **30**, 1559 (2014).

[2] S. Chen, G. Guillemot, and C. A. Gandin, *Three-Dimensional Cellular Automaton-Finite Element Modeling of Solidification Grain Structures for Arc-Welding Processes*, Acta Mater. **115**, 448 (2016).

[3] P. Cejpek, L. Straka, M. Veis, R. Colman, M. Dopita, V. Holý, and O. Heczko, *Rapid Floating Zone Growth of Ni2MnGa Single Crystals Exhibiting Magnetic Shape Memory Functionality*, J. Alloys Compd. **775**, 533 (2019).

Improving the crystal growth of magnetic shape memory alloys using a slag.

Supervisor: Ross H. Colman

Magnetic shape memory alloys (MSMAs) are metals that show magnetic field induced reorientation, i.e. by applying a magnetic field, they can reorient their crystal structure and show a significant size change of the crystal [1]. These properties are nearly unique to the family of alloys based on Ni, Mn and Ga. The properties of MSMAs have been studied for ~30 years and are actively being looked at for applications in actuators, micropumps and switching devices.

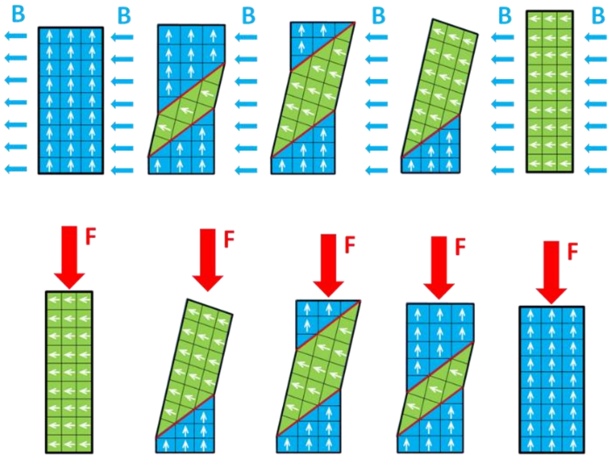

***Figure 1**. Illustration of the reversible nature of sizable strain in single crystalline Ni-Mn-Ga, by twin boundary motion. **Upper**, the MIR effect by application of magnetic field, **lower**, recovery to the original shape by applied force .*

A setback for their applications is the necessity to have high quality single crystals to observe the best and most repeatable properties. We've recently patented an adaptation to the optical floating zone growth technique that reproducibly prepares reasonably high quality crystals, but defects and impurities (usually oxides) can still be included and act as pinning sites to reduce the MSMA properties [2].

A different team previously tested a growth technique that used a slag mixture to reduce oxide contaminants during the growth [3]. This project will attempt to implement the use of the slag into our current growth procedure. It will be tested at both: the pre-alloying stage, where we will use induction melting and quench casting to prepare the polycrystalline alloy rods; and during the growth stage, inside the optical floating zone furnace.

The resulting crystals will be examined by optical microscopy to search for impurities, and the mechanical properties will be tested. In order to do this, the crystals will also have to be oriented, cut and prepared for testing after the growth.

References:

[1] O. Heczko, Mater. Sci. Technol. **30**, 1559 (2014).

[2] R. H. Colman, PV 2019-337 (2019).

[3] K. Rolfs, A. Mecklenburg, J. M. Guldbakke, et al., J. Magn. Magn. Mater. **321**, 1063 (2009).

Searching for new magnetic shape memory alloys

Supervisor: Ross H. Colman, Milan Klicpera, Taras Kovaliuk

Magnetic shape memory alloys (MSMAs) are metals that show magnetic field induced reorientation, i.e. by applying a magnetic field, they can reorient their crystal structure and show a significant size change of the crystal [1]. These properties are nearly unique to the family of alloys based on Ni, Mn and Ga. The properties of MSMAs have been studied for ~30 years and are actively being looked at for applications in actuators, micropumps and switching devices.

Despite extensive study, the research field is now stagnating due to a lack of new compounds that display magnetic shape memory properties.

A few recently investigated materials, such as Fe_3Ga [2], and Ni_2MnGe [3,4] have shown tentative hints of having the possibility of MSMA properties. Single crystals are required to test for these properties, however, and few groups have facilities and experience for growing large crystals of these intermetallics.

This project will involve the preparation and single crystal growth of several target alloys, to test their MSMA potential.

The resulting crystals will be examined by magnetometry and the mechanical properties will be tested. In order to do this, the crystals will also have to be oriented, cut and prepared for testing after the growth.

References:

[1] O. Heczko, *Magnetic Shape Memory Effect and Highly Mobile Twin Boundaries*, Mater. Sci. Technol. **30**, 1559 (2014).

[2] T. M. Inerbaev, A. U. Abuova, A. K. Dauletbekova, F. U. Abuova, G. A. Kaptagay, Z. Zakieva, M. Eltizarova, and A. Barakov, *Magnetic Anisotropy and Stability of Fe3Ga Compounds*, Eurasian J. Phys. Funct. Mater. **5**, 229 (2021).

[3] H. Luo, F. Meng, G. Liu, H. Liu, P. Jia, E. Liu, W. Wang, and G. Wu, *Electronic Structure and Possible Martensitic Transformation in Mn 2NiGe and Ni2MnGe*, Intermetallics **38**, 139 (2013).

[4] T. Kovaliuk, B. Vondrackova, J. Valenta, R. H. Colman, and M. Klicpera, *Evolution of Magnetic and Structural Phase Transitions in Solid Solutions Ni2MnGa1-XGex*, J. Alloys Compd. **894**, (2022).