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Determination of $L2_1$ vs. B2 phase content in Heusler alloys Ni_2MnGa and $Co_2FeGe_{0.5}Ga_{0.5}$ with x-ray diffraction

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Ni_2MnGa and $Co_2FeGe_{0.5}Ga_{0.5}$ are promising members of Heusler alloys because of their application potential. Ni_2MnGa is a shape-memory alloy which can be used for micropumps [1] or actuators [2] and $Co_2FeGe_{0.5}Ga_{0.5}$ has a potential in spintronics [3]. Important properties used for applications are conected to the low-temperature $L2_1$ phase. The high-temperature B2 phase (assuming the formula X_2YZ, the elements Y and Z are mixed together at their positions in unit cell) is for these purposes parasitic and we need to get rid of it. The presence of B2 phase can be observed for example in as cast samples without further heat treatment.

This work presents the determination of $L2_1$ phase content by x-ray diffraction. According to symmetry, we should observe $L2_1$ phase only diffraction with all indices odd or all even (*fcc* symmetry). Higher symmetry of B2 phase discribed with the equally big unit cell leads to the extinction of diffractions which have all indices odd. Proper computation of structure factors shows that diffractions with all even indices remain the same in both phases. Therefore, the ratio of integrated intensities corresponding to diffractions with all indices odd and all indices even should reveal the content of $L2_1$ phase in the sample. However, the whole problematics is more complicated, because it is neccessary to apply all angularly dependend corrections such as polarisation, Lorentz correction, absorption, irradiated volume and primary and secondary extinction.

The results show that this procedure works fine with thin layers and with bulk single-crystals with small mosaicity. If the mosaicity is large enough, it complicates the application of the corrections – especially the irradiated volume and extinction – because it is unclear how big volume of which mosaic block was irradiated. Extinction correction is connected to the size and misorientation of these blocks. Nevertheless, it is clearly visible that good temperature treatment can increase the $L2_1$ content, because overall intensity of sensitive diffractions (all indices odd) increases after annealing procedure (diffraction measured in the same experimental arangement for all cases).

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Thickness distribution of triglyceride crystallites in vegetable fat blends

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The structure of many food products is based on networks of crystalline particles. In oil-continuous products, such as margarine or butter, this network consists of a mixture of small crystallites of triglycerides (also known as triacylglycerols or TAGs) [1]. Product quality is related to the manufacturing process used, since the growth of the fat crystals can be tuned by TAG composition and cooling rates. For a given composition, fat network formation depends on the amount of TAG crystals and their dimensions and is therefore directly related to the surface to volume ratio.

Small Angle X-ray Scattering (SAXS) measurements were performed on both home-lab equipment (D8-Discover, Bruker-AXS) and at the ID02 beamline at the ESRF, Grenoble to obtain information about the thickness of the fat crystallites (domains). Based on the Full Width at Half Maximum (FWHM) of the first order diffraction line the average crystallite thickness is calculated using the Scherrer equation. However, in order to have a better understanding of the structuring capability of the TAGs, knowledge of the thickness distribution of the crystallites is preferred.

Peak shape analysis based on Fourier transformation methods was performed on the X-ray diffraction patterns. We considered the Bertaut-Warren-Averbach [2] method to be a feasible approach to resolve crystallite thickness distributions (CTD) in TAGs where molecules are packed in repeating bi-layers in longitudinal direction. This method, initially developed for metals, was also successfully applied to obtain distributions of domain thickness of layered clay minerals [3]. The proof of principle of BWA method for CTD in fats is presented on a model system consisting of mono-acid TAG (tripalmitate) subject to shock- and slow-cooling. Examples on real-use mixed-acid TAG systems or so-called fat blends are presented as well.

With additional knowledge of the thickness distribution of triglyceride crystallites it might be possible to tune the fat blend composition and to further optimize the processing of food products.

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