

The Influence of Solidification Direction on the CET in Zn-base Alloys

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Zinc gravity casting alloys can be used for general industrial applications where strength, hardness, wear resistance or good pressure tightness is required. Zinc alloys are often used to replace cast iron because of their similar properties and higher machinability ratings.

The composition of hypoeutectic alloys is close to 4%wtAl and their aluminum content is greater than that of eutectic alloys (5%wtAl). All zinc casting alloys have dendritic/eutectic microstructures. However, hypoeutectic alloys solidify with zinc-rich dendrites, whereas hypereutectic alloys solidify with aluminum-rich dendrites.

In a solidification process, the microstructure depends on the alloy characteristics and is mainly a function of the temperature evolution ahead the solid/liquid interphase [1-3].

Among the several phenomena occurring during solidification, like solute segregation or morphology stability, one of the most important ones is dendritic growth. The most important dendrite parameters are the primary, secondary and tertiary arm spacings due to their influence on mechanical properties.

An efficient method to examine the evolution of the dendrite arms is related to the application of steady-state directional solidification with an imposed growth rate, V , and a thermal gradient, G , at the solid/liquid interphase.

In this work, Zn-Al (wt%) alloys were solidified under unidirectional solidification in a device cooled with water, in a vertical upward direction (0°), inclined at 30° and 45° to the vertical and in a horizontal upward direction (90° to the vertical). We determined the position of the transition from columnar to equiaxed structure (CET) through macro and micro-analysis, and significant thermal parameters by recording temperature-time data. The results show that the direction of dendrite growth is about that of the heat extraction and that the angle of inclination of the columnar grains with the longitudinal axis of the alloy sample coincides approximately with the angle of inclination of the furnace.

The relevance of the problem under study is justified on the basis that the solidification variables, including natural convection, affect the structures of the solid and the formation of defects. The solidification variables are also important for modeling prediction of the structure and property of a given cast piece [3-11]. The results also allow a better understanding of the conditions and mechanisms operating in a solidification with different directions.

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Keywords: Solidification, Zn base alloys, CET

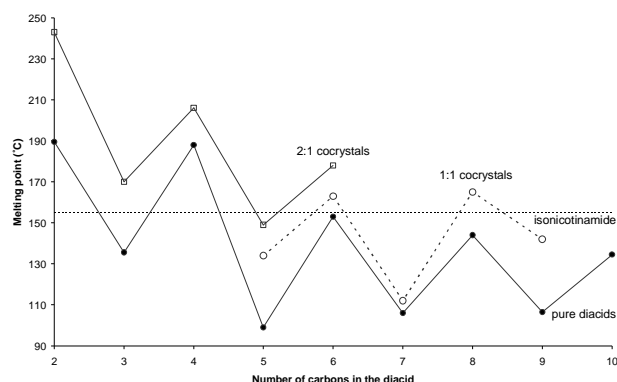
Crystal structures and properties of isonicotinamide: alkanediacid cocrystals

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The tunability of physicochemical properties of crystalline materials through controlled cocrystal formulation is an aim for both the pharmaceutical industry and crystal engineers. Cocrystals are crystalline solids that contain two or more molecular compounds that are solid under ambient conditions and have the potential to provide optimal physical properties whilst retaining the chemical properties of the individual components. The variation in composition and stoichiometry of components in these cocrystals gives us access to a range of tailored structural combinations and as such provides a route to new tunable materials.

In this poster we present the synthesis, characterisation and melting point behavior of three new 1:1 cocrystals of isonicotinamide combined with pimelic, suberic and azelaic acid. These cocrystals demonstrate robust synthon formation whilst mimicking the melting point alternation behavior of pure odd and even chain acids.

All three structures contain hydrogen-bonded chains of alternating acid and amide molecules between which acid-pyridine and acid-amide synthons are formed. Both pimelic acid and azelaic acid cocrystals form structures in which the acid moiety adopts a twisted alkyl backbone conformation similar to that observed in the pure odd alkanediacid materials. The suberic acid cocrystal differs from the other two, retaining both the elevated melting point and the planar acid conformation displayed by even alkanediacid materials in this series [1].



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Properties of metal oxalate materials from electron density. Modelling the building blocks and evaluation of framework interaction

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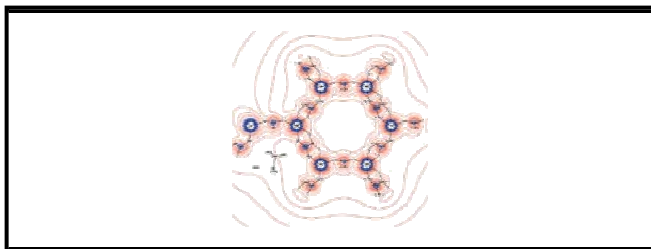
Extensive research work has been carried out in last few decades on the synthesis and characterisation of several metal organic materials including carboxylates, phosphates, and arsenates [1]. To a large extent, the interest is due to the interesting properties possessed by the materials and potential applications, such as electrical conductivity, magnetism, photo mechanism, host-guest

chemistry etc. We focused our attention to metal oxalates, testing the possibility to model electron density of building blocks and obtain at least approximate evaluation of the properties.

In these materials, the oxalate ion often acts as a rigid bidentate ligand which bridge metal centres [2] therefore facilitate the formation of extended structures with dimensionalities ranging from zero to three [3].

New inorganic-organic hybrid structures based on Zinc oxalate structures, which show 1D linear, 2D honeycomb and 3D structures were studied. In order to model the building blocks of these frameworks, we used as benchmark some simple structures like $Zn(C_2O_4)$, $Zn(C_2O_4)(H_2O)$, $Zn(C_2O_4)(C_4N_2H_{10})$, $(HC_2O_4)_2(C_4N_2H_{12})$. All compounds were obtained through hydrothermal synthesis. Electron density distribution was studied through X-Ray diffraction and through density functional theory.

Once the modelling was refined and tested, the electron densities of 1D-2D-3D framework were computed using multipoles restricted to optimized theoretical building blocks. This allows to reconstruct the electron density of more complex structures, often not available in the form of good quality single crystals. The results are utilised for evaluation of material properties such as electrostatic potential (a Zn oxalate honeycomb is plotted in the Figure), the interaction energies between the framework and neutral guest molecules or counter-ions, and the calculation of the active surface areas of the framework [4].



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L.A.31

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Formation of $2NaBH_4/MgH_2$ system from $2NaH/MgB_2$ by hydrogenation

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Borohydrides with a general formula MBH_4 (where M stands for an alkali or an alkali earth metal) are considered as prospective hydrogen storage materials due to a high percentage of hydrogen (up to 20 wt%) [1].

An interesting complex hydride for hydrogen storage is sodium tetraborohydride ($M = Na$). $NaBH_4$ desorbs hydrogen easily [2] but the reversible reaction requires very strong conditions (550 – 700 °C and 30 – 150 bar H_2) [3]. It was found that MgB_2 can facilitate the reversibility reaction [4]. It was shown that formation of $NaBH_4$ does not occur directly, but follows the formation of $MgNaH_3$. But it seems that reaction mechanism strongly depends on the conditions of experiment.

In order to find out the optimal conditions of formation of $2NaBH_4-MgH_2$ system from $2NaH-MgB_2$ and to understand better the reaction mechanism, several experiments were performed. Hydrogen absorption by starting ball-milled compounds ($2NaH-$

MgB_2) was studied at isotherm conditions at several temperatures (400, 425, 450 °C) at 100 bar H_2 pressure. Experiments were performed *in-situ* using synchrotron radiation.

The results indicate different way of $NaBH_4$ and side products formation depending of temperature and hydrogen pressure. Further experimental results will be presented to discuss the optimal conditions for hydrogen absorption in the indicated system.

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Structural studies of the RNA polymerase III transcription factor IIIC

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Transcription in eukaryotes is divided over three different RNA polymerases, termed RNA polymerase (Pol) I, II and III, which have different target genes. Pol III is the most complex of these three polymerases consisting of 17 different subunits compared to 12 and 14 for Pol II and Pol I, respectively. However, the process of polymerase recruitment and transcription initiation in the Pol III system is arguably less complex, especially when compared to Pol II. On most Pol III-transcribed genes, two transcription factors are sufficient to recruit the polymerase (Schramm and Hernandez, 2002). These are known as the RNA polymerase III transcription factors IIIB and IIIC (TFIIIB and TFIIC). On these type 2 (e.g. tRNA) genes, TFIIC gets recruited to the gene-internal B-box through a very strong interaction, followed by binding of this transcription factor to the A-box. Subsequently, promoter-bound TFIIC recruits TFIIIB, and the TFIIIB-TFIIC-DNA complex recruits the polymerase, after which transcription can initiate. We have determined several crystal structures of various parts of TFIIC, and have performed electron microscopy studies of the whole transcription factor.

Schramm, L., and Hernandez, N. (2002). Recruitment of RNA polymerase III to its target promoters. *Genes Dev* 16, 2593-2620.

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