microbatch-style crystallization experiment with a different chemical composition. The MPCS allows the researcher to use the entire protein sample in crystallization experiments for efficient exploration of crystallization phase space by combining sparse matrix with gradient screening in one comprehensive hybrid crystallization trial. Furthermore, individual crystallization optimization trials can be prepared using highly granular gradients of protein and optimization reagents such as precipitation agents, ligands, or cryo-protectants. The MPCS produces Diffraction-Ready crystals that can be removed from the Peel-Apart CrystalCard for traditional cryocooling and diffraction.

Keywords: microfluidic crystallization, nanovolume, *in-situ* X-ray diffraction"

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Three-dimensional void-like defects associated with tin nano-particles in aluminium

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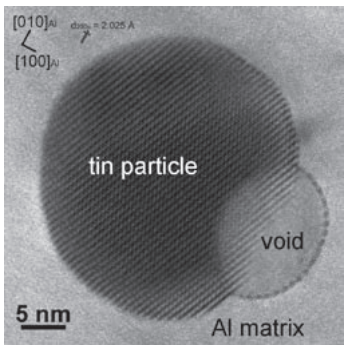
Defects, such as lattice defects (vacancies, dislocations, stacking faults) or extrinsic defects (solute atoms clusters) play a critical role in the nucleation and growth of precipitate phases in precipitation-strengthened aluminium alloys. Defects often act as heterogeneous nucleation sites for phases that nucleate with difficulty. Defects, vacancies in particular, may also influence or even control the kinetics of nucleation and growth. This work reports the finding and characterisation of three-dimensional defects commonly associated with tin nano-particles in aluminium. The shape, structure and composition of the defects and their surroundings were investigated using a variety of transmission electron microscopy imaging, diffraction and analytical techniques. The three-dimensional defects were deduced to contain a significant number of vacancies, hence their description as void-like. These void-like defects were found to occur in isolation at the interface between the tin precipitate and the aluminium matrix. An example of one such void observed at high magnification is shown; in this case tin can be seen to decorate the void-matrix interface.



Keywords: defects, transmission electron microscopy, aluminium alloys

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Microstructure of surface-tailored platinum nanocrystals

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Nanoscaled Pt-based materials have potential applications as electrocatalysts in fuel cells. Fundamental interest in the mechanisms of model reactions has led to the development of synthesis routes allowing a fine tuning of particle shape, mean size and size distribution. However, an effective control of the surface structure seems more important, as the majority of the reactions taking place in fuel cells are structure sensitive or site dependent (1). This fine control over surfaces is allowed by the water-in-oil or by the colloidal routes: single clean-surface nanocrystals with defined shapes and tailored percentages of {100} and {111} surface domains can be produced (2). In particular, the colloidal method allows cubes, octahedra, tetrahedra and cuboctahedra to be preferentially obtained (depending on the Pt precursors and the hydrogen bubbling time), whereas more rounded crystals are formed via water-in-oil. All nanocrystals are almost defect-free and nearly monodisperse, as confirmed by TEM and by X-ray diffraction Whole Powder Pattern Modelling (WPPM)(3). An analysis of the microstructure is proposed, based on the modelling of nanocrystal shape, size distribution, defects and surface effects, following the WPPM and the Debye equation approaches.

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Keywords: nanocrystals, platinum, microstructure

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Crystallite dimensions obtained with Rietveld refinement and Delaunay triangulation

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Crystallite dimensions and morphology of phases were obtained by refining crystalline structures with the Rietveld method. Of special interest was the case where average crystallites were modeled in reciprocal space with a linear combination of normalized spherical harmonics; the coefficients that weighted the harmonics' contribution were refined to fit the breadth of the diffraction peaks. The crystallite dimensions obtained in reciprocal space were used to calculate the corresponding ones in real space, generating a set of vertices that described crystallite surface. These vertices were used to generate a mesh of the surface using the Delaunay triangulation, which made possible to get crystallite surface area, and to generate a Delaunay tetrahedralization that was used to calculate crystallite volume. The density of each phase, determined from the Rietveld refinement, together with the determined volume were used to get crystallite mass and its specific surface area, which, for comparison, can be determined with other experimental techniques. Since in nanocrystalline materials peak breadth is mainly determined by crystallite size and microstrain, the aberrations of the diffractometer can be neglected, which is not the fall for microcrystalline materials.