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Crystal structure of nm-scale precipitates in Al alloys by electron diffraction and DFT calculations

Rene Vissers¹, Calin D Marioara², Sigmund J Andersen², Randi Holmestad¹

¹Norwegian University of Science and Technology, Department of Physics, Hogskoleringen 5, Trondheim, Sor-Trondelag, 7491, Norway,

²Sintef Materials and Chemistry, Hogskoleringen 5, Trondheim, Norway, E-mail: rene.vissers@ntnu.no

The macroscopical properties of Al alloys, such as hardness and formability, are to a large extent determined by their nanostructural properties. During precipitation hardening of Al alloys, several metastable phases are formed as nanometer-scale precipitates. An important aspect in studying the hardening effect of the different phases is the coherence strain between the precipitates and the surrounding matrix. It is essential to obtain an accurate model of the crystal structure of these precipitates, since this will allow for detailed modeling of the precipitate-matrix interface. The crystal structure of several of the hardening phases has been successfully determined, based on quantitative electron diffraction and verified by DFT calculations. Indeed, generally, electron diffraction and DFT calculations would lead to the same selected structure out of a number of candidate models, and structural relaxation in the DFT calculations gave only minor differences with the experimentally determined structure. However, most DFT calculations so far have assumed a 'bulk' precipitate structure, i.o.w. repeating infinitely in 3 dimensions, which was an acceptable approximation in most cases, but has proven to be inadequate for the smallest precipitates. Therefore, in more recent work, it has been decided to include the precipitate-matrix interface in the DFT calculations, where the initial model for the interface structure is based on a combination of electron diffraction and high resolution electron microscopy images.

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Structural studies of spin crossover compounds under extreme environmental conditions

Helena J Shepherd, Andres E Goeta, Michael R Probert

Durham University, Department of Chemistry, University Science Laboratories, South Road,, Durham, England, DH1 3LE, UK, E-mail : h.j.shepherd@durham.ac.uk

Spin crossover (SCO) is the switching between high and low spin states which arises from a variation in temperature or pressure or as a result of light irradiation. The understanding and resultant control of this process is fundamental to the potential applications of these systems in data storage and novel electronic devices. Results of this transition include a dramatic change in the metal-ligand bond distance and often striking changes in the crystal structure. The vast majority of SCO systems studied to date involve mononuclear

iron (II) species that are linked in a crystal through intramolecular interactions. There is an increasing trend towards the study of complexes with higher dimensionality such as 1D-3D coordination polymers and polynuclear metal complexes, largely due to increased cooperativity between iron centres through direct covalent bonding [1]. Application of hydrostatic pressure serves as a tool for modifying the local metal environment in a controlled manner [2]. High pressure studies have been shown to be invaluable in revealing the cooperative nature of these electronic structure transitions, which are accompanied by a significant change in volume. In Durham we are currently developing a set-up which will allow high-pressure low-temperature single crystal diffraction studies to be carried out. This poster will show our first results from single crystal experiments aiming to combine pressure and temperature on a spin crossover material. This research is intended to aid in the understanding of how sample environment impacts on the complex nature of the spin crossover phenomenon.

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Structural stability of the FeCr sigma phase under pressure to 77 GPa

Valentina F. Degtyareva¹, Leonid Dubrovinsky², Aleksander Kurnosov²

¹Institute of Solid state Physics Russian Academy of Sciences, IFTT, Institutskaja ul. 2, Chernogolovka, Moscow region, 142432, Russia,

²Bayerisches Geoinstitut, Universitat Bayreuth, D-95440 Bayreuth, Germany., E-mail: degtyar@issp.ac.ru

The Fe-Cr alloy system contains an intermediate phase of the equiatomic composition called the sigma phase. The crystal structure of the sigma phase is tetragonal with 30 atoms in the unit cell, space group $P4_2/mnm$, lattice parameters $a = 8.7995 \text{ \AA}$, $c = 4.5442 \text{ \AA}$, $c/a = 0.516$, Pearson symbol tP30 [1], whereas pure elements Fe and Cr both crystallize in the body-centered cubic (bcc) structure. The aim of this work was to investigate the stability of the FeCr sigma phase at high pressure. Diffraction studies of the FeCr sample with the sigma phase were performed using diamond anvil cell, image plate detector and synchrotron radiation at the Advanced Photon Source (Argonne National Lab). The highest pressure achieved in this study was 77 GPa. The sigma phase was found to be stable in this pressure range. The equation of state for the tetragonal structure was found to have the values of bulk modulus $K_0 = 217(5) \text{ GPa}$ and $K_0' = 5.8(2)$. Interestingly, the compressibility of the FeCr sigma phase is lower than that of the constituent elements: the bulk modulus K_0 for the bcc phases of Cr and Fe is 161 and 173 GPa, respectively. Structural stability of the sigma phase under pressure found in the present study supports the suggestion that electronic energy is one of the main factors responsible for the existence of this complex, low-symmetry structure. The stability of the sigma phase can be related to the Hume-Rothery effects based on the Fermi surface - Brillouin zone interactions [2]. Partial support from RFBR under grant 07-02-00901 is acknowledged.

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