Structure determination of the precipitates of AlMgSi-alloys by electron diffraction and ab initio calculations, SJ Andersen,[a*] CD Marioara [a], R Vissers[b], AG Frøseth[c,d], P Derlet[c], HW. Zandbergen[b] [a]*Sintef Materials & Chemistry, Appl. Phys, N-7465 Trondheim, Norway,* [b]*NCHREM, Delft University of Technology, Rotterdamseweg 13, 2628 AL Delft, The Netherlands,* [c]*Norwegian University of Science and Technology, Dept. of Phys., N-7491 Trondheim, Norway,* [d]*PSI, Nano-Crystalline Materials Group, CH-5232 Viligen, Switzerland* E-mail: sigmund.j.andersen@sintef.no
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The addition of just 1-2% Mg and Si to aluminium has a profound positive effect on the strength of Al-Mg-Si alloys. The reason is that a high density of very fine coherent, needle-shaped precipitates emerges from solid solution. The needles can have cross-sections below 5 nm^2. They extend along <100> Al directions with lengths ranging from 1-2 nm up to hundreds. High Resolution Electron Microscopy (HREM) and electron diffraction (ED) are methods well suited for structural investigation. By these methods, in some cases supplied by *ab-initio* quantum mechanical (QM) methods, we have determined most precipitate structures of this alloy system: GP-zones [1], β''-Mg_5Si_6 [2], β'-$Mg_{1.8}Si$ [3], U1-$MgAl_2Si_2$ [4], and U2-MgAlSi [4]. QM calculations were used to relax coordinates of U1 and U2. The models are either developed on the basis of *exit waves*, HREM images or on the other precipitate structures, and aided by ED. When QM relaxed coordinates cause improvement in the calculated ED patterns, an atomic structure could be confirmed by ED refinements. The structures are related to each other, as well as to pure Si and Al. GP-zones and β'' take monoclinic (C2/m) super-cells in Al. U2, β' and B' (unfinished study) are orderings of Mg and Al on {111} type Si-planes parallel with {100} type Al-planes. β' ($P6_3$) and B' show extra reflections along **c,** which can be explained in terms of a modulation along c of the Si 00z atoms. For example, the average structure of β' (a=715 pm, c=405 pm) was refined to 000 (Si1), 2/3 1/3 1/2 (Si2) and 0.6152 0.6954 0 (Mg) with the occupancy of Si1 being 2/3. A tripling of the unit cell along c (i.e. z=0, 1/3 and 2/3 for both Si2 and Mg) together with the modulation -235-372-235- (pm) of the S1-atom, will explain the super-reflections, account for the occupancy, and prevent too close S1-S1 atoms. The modulation may be given as z= 0.07 and 0.2634, but three equally possible, incommensurate strings exists. When a crystal contains similar proportions of the sets, super-reflections are absent [3]. Acknowledgements [5].

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