# Oral Contributions

**[MS17-03] Identification and structure solution of ordered $U(Al_x,Si_{(1-x)})_3$ phase.**

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Binary and ternary alluminides of uranium has been investigated thoroughly for several decades. Industrial importance of these alloys stems from the fact that during processing – Al-based alloy, used for cladding of U (fuel in nuclear reactors), undergoes heat treatment which stimulates the diffusion among the fuel and the cladding. The interface between these materials is not stable under service conditions. In the U-Al phase diagram there are many intermetallic phases which form and may undergo phase transitions. These changes usually degrade the material under subsequent irradiation. One of the commonly used means for the stabilization of U-Al interface is an addition of Si. This addition stabilizes the $UAl_3$ phase, which is less brittle than the $UAl_4$ phase, and has isotropic cubic structure (vs. anisotropic orthorhombic structure of $UAl_4$) so it is more resistant to swelling under irradiation [1,2]. Matter of $U(Al,Si)_3$ crystal structure stability drove many researchers to investigate the $UAl_3$-$USi_3$ quasi-binary phase diagram. Since both $UAl_3$ and $USi_3$ phases are isostructural (possessing $AuCu_3$ structure type), one would have expected an isomorphous phase diagram up to 900°C [suggested in 3]. Investing lower temperature range, miscibility gap was reported to exist at 600°C [4] and in 1992 this phase diagram was revisited again and miscibility gap was identified at T=900°C [5], contradicting [3]. During our study of the $UAl_3$-$USi_3$ quasi binary phase diagram, new stable $U(Al_x,Si_{(1-x)})_3$ phase with x= 0.42 was identified. The alloys containing this phase exhibited also original (disordered) cubic $U(Al,Si)_3$ compound. Due to the close structural relation of the new phase to the original one – structure solution of the later using solely traditional X-ray diffraction methods was unsuccessful. The structure of the new $U(Al_x,Si_{(1-x)})_3$ phase was determined using a combination of electron crystallography and powder X-ray diffraction methods as tetragonal (*I4/mmm* (No.121) space group), with lattice parameters of a=8.346(9), c= 16.808(4)Å. Its unit cell has 64 atoms and can be described as an ordered variant of the $U(Al,Si)_3$ solid solution, due to the ordering of Al and Si atoms at the non-U sites. The ordering can be also explained and atom positions re-calculated by means of Bärnighausen tree which was constructed using the original $U(Al,Si)_3$ structure as an aristotype.

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