Poster Presentations

[MS19-P06] Site Preference and Ordering Induced by Au Substitution in the γ-Brass Related Complex Au–M–Zn (M=Cr, Mo) Phases

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The crystal chemistry of the ternary Au-M-Zn (M=Cr, Mo) alloys were studied by synthesis, single crystal X-ray diffraction, and electron structure calculations. The binary phases-CrZn17 or MoZn20.44 [1] are disordered exhibiting a complex interplay of occupational and positional disorders. The inclusion of Au proves to be very site specific, and at the limiting composition $Au_{10}M_4Zn_{89}$ (M=Cr, Mo), structures are completely ordered. Electronic structure calculations of Au10M4Zn89 (M=Cr, Mo) by using the tight-binding linear muffin-tin orbital atomic-spheres approximation (TB-LMTO-ASA) method, indicate that the observed chemical composition and atomic distributions lead to the presence of a pronounced pseudogap at the Fermi level in the electronic density of states curves and this is consistent with the Hume-Rothery interpretation of γ-brasses, in general. [2,3]
This presentation will discuss about the synthesis, crystal and electronic structure calculations of the ternary Au-M-Zn (M=Cr, Mo) alloys.

References

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