Poster Presentation

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Rh_8Cd_{43}: a rhombohedral variant of cubic Rh_8Mg_{44}

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γ-brass phases are a class of Hume-Rothery phases that attract attention due to their intricate structures, close relation with quasicrystals (QCs) and challenges towards understanding the underlying stabilisation mechanism. Our recent study of the γ-brass-region of Rh-Cd system was inspired by a previous report- by Westgrenet al. – which mentioned that in analogy to some other related systems, a cubic γ-brass-type phase may exist in the Rh-Cd binary system. Our investigation has uncovered three new γ-brass related phases: (a) rhombohedral phase at 15.7 atomic % of Rh, (b) a monoclinic phase at approximately 15 atomic % of Rh (c) a complex cubic phase at approximately 11 atomic % of Rh. The fully ordered compound Rh8Cd43 (at 15.7 atomic % of Rh) crystallizes in the rhombohedral space group R $3\bar{}$m (166) and contains 306 atoms per unit cell. This new compound is the first example of a rhombohedral distortion of a (2aγ)3 - superstructure of cubic γ-brass, in particular, it is closely related to Rh7Mg44. The structure contains 19 crystallographically independent sites: five rhodium and fourteen cadmium sites. The structure of Rh8Cd43 is mostly tetrahedrally close packed. The two main building units in the structure of Rh8Cd43 are the 38-atom modified Pierce cluster and unions of three double sphenocoronae. The two main building units form 3D-networks. The electronic structure of Rh8Cd43 shows that the phase is stabilized by a Hume-Rothery mechanism.

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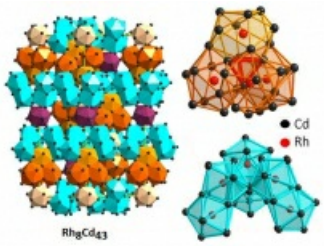

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