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Crystal structure of κ -Ag₂Mg₅

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Abstract

The structure of κ -Ag₂Mg₅ has been refined based on X-ray powder diffraction measurements ($R_{wp} = 0.083$). The compound has been prepared by combining mechanical alloying techniques and thermal treatments. The intermetallic presents the prototypical structure of Co₂Al₅, an hexagonal crystal with the symmetries of space group $P6_3/mmc$, and belongs to the family of kappa-phase structure compounds. The unit cell dimensions are $a=8.630(1)$ Å and $c=8.914(1)$ Å. Five crystallographically independent sites are occupied, Wyckoff positions $12k$, $6h$ and $2a$ are filled with Mg, another $6h$ site is occupied with Ag, and the $2c$ site presents mixed Ag/Mg occupancy. The crystal chemistry of the structure and bonding are briefly discussed in the paper.

Keywords: Intermetallics, Structure, Crystal chemistry, X-ray diffraction, Mechanical alloying and milling

1 Introduction

The kappa-phase structure compounds constitute a crystallographic family based on the structure of W₁₀Co₃C_{3.4} [1]. These compounds crystallize in the hexagonal system, space group $P6_3/mmc$. The metal atom substructure of this prototypical structure is that of Mn₃Al₁₀, and the different kappa-phase structure compounds are obtained by filling the trigonal prismatic ($2c$) or the octahedral ($6g$) interstices of this “host lattice” by p elements or transition metals. If only the trigonal prismatic interstices are filled, the Co₂Al₅ prototypical structure is obtained. On the other hand, if no more than the octahedral interstices are occupied the Mo₁₂Cu₃Al₁₁C₆ structure is obtained. Some compounds have both interstices filled [1].

During an experimental study conducted to analyze MgH₂ destabilization by the formation of Ag-Mg alloys we have identified an intermetallic compound denoted for simplicity Ag₂Mg₅ that crystallizes with the Co₂Al₅ structure. Up to now, only eleven compounds with this prototypical structure have been reported [2-3], together with numerous RE₁₀TMCd₃ and RE₁₀TMAl₃ (RE: rare-earth metal, TM: transition metal) ternary compounds with *anti*-Co₂Al₅ structure recently identified [4-5]. Interestingly, four of the Co₂Al₅ structure compounds contain Mg and show some regularity in the periodic table of the elements, namely: Ir₂Mg₅ [6], Rh₂Mg₅ [7], Pd₂Mg₅ [3], and the ternary compound Ir_{2.096}Mg_{1.980}In_{2.924} [3]. The existence of the intermetallic Ag₂Mg₅ follows this trend. To the best of our knowledge this compound has been only previously mentioned in a PhD thesis [8] and is not included in the Ag-Mg equilibrium phase diagrams [9-11]. We present here the refinement of its structure, based on X-ray diffraction experiments on powders.

2 Experimental and refinement details

The compound was prepared by combining mechanical alloying techniques and thermal treatments. A mixture of magnesium and silver with molar ratio Mg:Ag = 5.25:2 was mechanically alloyed in a planetary mill (Fritsch Monomill Pulverisette 6) under pure argon (99.999 %)

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