

论文

Pd替代对Ti-Zr-Ni准晶合金结构的影响

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摘要:

针对 $Ti_{45}Zr_{38}Ni_{17}$ 与 $Ti_{40}Zr_{40}Ni_{20}$ 准晶合金用X射线衍射仪、透射电子显微镜与金相等手段研究了不同含量的Pd替代对其结构的影响。在吸铸态下, 前一个合金形成了二十面体准晶相(IQC)与少量配位数为8的bcc β -(Ti, Zr)相, 用2%Pd (原子分数, 下同)对合金的Ti或Zr组元替代, 抑制了 β -(Ti, Zr)相析出并促使配位数为14的 $MgZn_{12}$ 结构的简单六方C14 Laves相生成。而后一个合金中IQC相则与少量简单六方 α -(Ti, Zr)共存, 在2%Pd替代后 α -(Ti, Zr)消失, 生成了单一的IQC相, 但当Pd替代量增加到6.7%或13.3%时, 配位数为12的IQC相急剧减少而C14相大量析出, 并在 $Ti_{40}Zr_{26.7}Ni_{20}Pd_{13.3}$ 合金中生成了单一C14相。结果表明, 添加中等尺寸的Pd原子有利于提高Ti-Zr-Ni合金的原子密堆性, 使合金趋于生成高配位数的Laves相, 这种相的Fermi面与Brillouin区的相互作用不显著, 偏离了电子相的稳定机制。

关键词: 准晶 Ti-Zr-Ni合金 Pd添加 Laves相

EFFECT OF Pd SUBSTITUTION ON THE STRUCTURES OF Ti-Zr-Ni QUASICRYSTALLINE ALLOYS

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Abstract:

Quasicrystals are a kind of special crystals, combining aperiodicity with long-range translational order and displaying a strong potential of applications. However, the forming law of quasicrystals, especially icosahedral, which have drawn a lot of attention since the discovery of the first quasicrystal, are not clearly known. A general knowledge, derived from the past work, is that the quasicrystal belongs to Hume-Rothery phase with special electron concentration per atom (e/a), and furthermore needs meeting the topological packing of atoms. Based on this, certain criteria named by e/a -constant line, e/a -variant line and cluster line, et al., have been used to design novel quasicrystals, especially in ternary alloy systems. But, as indicated in the previous work, these rules would not work very well in pseudo-ternary or quaternary systems built on Ti-Zr-Ni quasicrystals with the addition of Co or Cu. In order to further specify the quasicrystal formation in multi-component systems, in the present study an investigation was conducted in an alloy system, based on $Ti_{45}Zr_{38}Ni_{17}$ and $Ti_{40}Zr_{40}Ni_{20}$ alloys with the addition of Pd, because Pd is the neighbourhood of Ni in the element table like Co and Cu and has the atom size and e/a between Ti (or Zr) and Ni. Using XRD, TEM and OM, it is found that in the suction cast alloys, the icosahedral quasicrystal (IQC) phase is formed in the coexistence of a little bcc β -(Ti,Zr) in $Ti_{45}Zr_{38}Ni_{17}$ alloy and of a bit hexagonal α -(Ti,Zr) in $Ti_{40}Zr_{40}Ni_{20}$ alloy. And after 2%Pd (atomic fraction) substitution for Ti and Zr, a $MgZn_{12}$ -type Laves C14 hase with coordination number of 14 is precipitated along with the disappearance of β -(Ti,Zr) with coordination number of 8 in the former alloy, while only a complete IQC phase with coordination number of 12 is yielded in the latter alloy. However, as the substitution is increased up to 6.7% or 13.3% in $Ti_{40}Zr_{40}Ni_{20}$ alloy, the formation of IQC is prevented and the C14 phase occurs instead till a single C14 phase form in $Ti_{40}Zr_{26.7}Ni_{20}Pd_{13.3}$ alloy. The results show that the Pd addition in Ti-Zr-Ni alloys would promote closer atom packing, being beneficial to the formation of Laves phase because of the weak interaction between Fermi surface and Brillouin zone in Hume-Rothery phase like IQC.

Keywords: quasicrystal Ti-Zr-Ni alloy Pd addition Laves phase

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