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Abstract
Single grains of icosahedral $Cd_{84}Yb_{16}$ quasicrystalline phase were characterized using high resolution transmission electron microcopy (HRTEM) technique. Image reconstruction of the obtained multiple through-focal series for both the two and five-fold axes are consistent with the local cluster structure of concentric polyhedra consisting of Cd tetrahedron (1/3 occupied icosahedron), Cd dodecahedron, Yb icosahedron and a Cd icosidodecahedron. Edge-sharing of the clusters can result in complete tiling of the 2-D projections. Simple matching rules are being investigated to construct a 3-D model.

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ABSTRACT

Single grains of icosahedral $Cd_{84}Yb_{16}$ quasicrystalline phase were characterized using high resolution transmission electron microcopy (HRTEM) technique. Image reconstruction of the obtained multiple through-focal series for both the two and five-fold axes are consistent with the local cluster structure of concentric polyhedra consisting of Cd tetrahedron (1/3 occupied icosahedron), Cd dodecahedron, Yb icosahedron and a Cd icosidodecahedron. Edge-sharing of the clusters can result in complete tiling of the 2-D projections. Simple matching rules are being investigated to construct a 3-D model.

INTRODUCTION

Understanding the unique structure of QC and what gives rise to the aperiodic structure has been an open question since quasicrystals were first discovered by Dan Shechtman in 1984[1]. Whether the rare-earth quasicrystals are based upon any cluster model has been openly debated and remains uncertain. Recently, M. J. Kramer *et al*. studied the local atomic structure of R-Mg-Zn ternary QC and identified the atomic positions[2], showing that the face centered icosahedral quasicrystals are based upon Bergman-like clusters and the rare-earth provides a unique probe to determine the atomic structure[3]. However, the occupants of those sites have not been uniquely determined. All stable quasicrystals (QC) consist of at least three elements before the first binary icosahedral cadmium-ytterbium ($Cd_{5.7}Yb$) quasicrystalline reported in 2000 by Tsai *et al*.[4] and Guo *et al*.[5]. Stable binary phases (aperiodic and related crystalline) provide an intriguing opportunity to gain better insight into their structural versus chemical stabilities, which has been elusive in ternary and higher order systems. The complexity of performing site occupation determinations in a binary compound is considerably reduced compared to the ternary. Therefore, a binary system will be the best candidate to study the basis for the construction of crystallographic model of quasiperiodic structure. The general simplicity of a binary system presents numerous advantages in both computational and experimental investigations of structure.

In this paper, we will try to investigate the local atomic structure of a binary icosahedral $Cd_{84}Yb_{16}$ quasicrystal[6] using high resolution transmission electron microcopy (HRTEM) and simulation techniques, in an attempt to provide an insight into the role of short range order in controlling the stability of quasicrystalline compounds.

EXPERIMENTAL DETAILS

Bulk single grain of icosahedral $Cd_{84}Yb_{16}$ quasicrystalline was prepared using the

Bridgman method. HRTEM foils were firstly electron discharge machined from larger grains on the order of 0.75 cm^3 and then mechanically thinned to ~200 μm. The samples were cut to circular plates of 3 mm in diameter and 300 μm in thickness and were electrolyte-polished to make final HRTEM specimens. Special care had to be undertaken to minimize air exposure due to rapid surface oxidation. Examination was performed along the two and five-fold axes of the primitive icosahedral structure. A Philips CM30 TEM with a point-to-point resolution of 0.18 nm operated at 300kV was employed for HRTEM investigations.

RESULTS AND DISCUSSION

The alloy studied in the present paper, i.e., $Cd_{84}Yb_{16}$, is very close to the stable $Cd_{5.7}Yb$ quasicrystal reported by Tsai *et al.*[4]. According to the study by Takakura *et al.*[7], the compound of cubic Cd_6Yb (space group $Im\bar{3}$) serves as the approximant to the quasicrystal ($Cd_{84}Yb_{16}$) and the Cd_6Yb has the same structure as the Cd_6Y (space group $Im3$)[8] except for the distribution of fractional Cd sites located in the void. Therefore, based on this assumption, the crystal structure of Cd_6Y is employed to construct the local structure of the QC approximant phase (Cd_6Yb) in the present paper.

Tsai *et al.*[4] and Takakura *et al.*[7] suggested that the structure of the approximant alloy, cubic Cd_6Yb, consists of a body-centered-cubic packing of clusters that have atomic shells with icosahedral symmetry around their center, i.e., the first shell consists of 4 Cd atoms forming a tetrahedron around the cluster center, the second consists of 20 Cd atoms forming a dodecahedron, the third consists of 12 Yb atom forming an icosahedron and the fourth is an icosidodecahedron obtained by placing 30 Cd atoms on the edges of the Yb icosahedron, as shown in Figure 1a. The cluster consists of 66 atoms in total.

Based on the above information, our reconstructed cluster models are shown in Figure 1b. This figure illustrates that the approximant single cluster projected along two specific crystalline directions which are equal to the 5-fold and 2-fold of the QC structure, i.e., [01τ] and [001]. The longest atom distances of the successive shells are calculated as 0.3 nm, 0.863 nm, 1.1 nm and 1.278 nm, respectively.

Figure 2a is a typical HRTEM image obtained along the 5-fold direction of the $Cd_{84}Yb_{16}$ quasicrystal with corresponding selected area electron diffraction pattern (SAEDP) as inset. By overlaying a series of through-focus HRTEM images and further Fast Fourier Transformation (FFT) operation, a clean FFT-inverted image is shown in Figure 2b. The reason to overlay a series of through-focus HRTEM images is to obtain more detailed structure information. A reconstructed QC approximant cluster with projection along QC 5-fold direction ([01τ] of the cluster) is fitted in Figure 2b based on both calculated cluster size and the scale of HRTEM image. Smaller red balls represent Cd atoms and large green balls are Yb atoms. It can be seen that those Cd atoms of icosidodecahedron shell fit the bright spots quite well. In order to clearly show the packing of QC clusters in the HRTEM image, which may give a better understanding on the QC

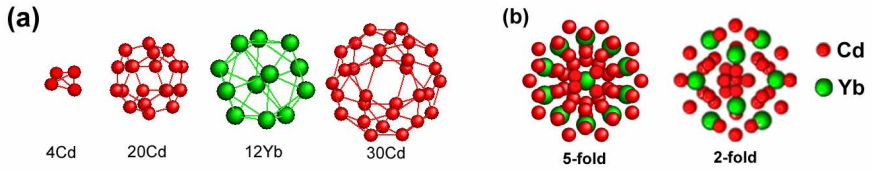

Figure 1 The model of successive atom shells of the Cd_6Yb structure (a) and the associated cluster structure of these concentric shells form in the 5 and 2-fold orientations.

structure, seven clusters represented by Yb icosahedron shells are also fitted in the figure in matching the HRTEM images, which shows two typical kinds of relationships among the quasicrystal clusters, i.e., edge sharing and overlay of the quasicrystal cluster. Figure 2c is the reconstructed three-dimensional basic b.c.c. approximant structure projected along [01τ] direction, containing 9 clusters. In order to clearly describe the structure relationship between the reconstructed approximant and the real quasicrystal, only Yb atoms of the icosahedron shell are drawn. Thinking of the projection of the QC structure from three-dimensional space to two-dimensional plane, the HRTEM image of QC (Fig. 2a) results from the packing of QC clusters. With a comparison, the relationship among the approximant clusters in the bcc structure shown in Figure 2c is not equal to that among the real QC clusters in Fig. 2b. The packing of clusters in the QC structure is different from that in the bcc approximant structure. We assume that the real QC structure results from distorted QC approximant bcc structure.

Figure 3a shows a typical HRTEM image obtained along the 2-fold direction of the $Cd_{84}Yb_{16}$ quasicrystal with corresponding SAEDP as inset. A FFT-inverted HTREM image is shown in Figure 3b. Similarly, a reconstructed QC approximant cluster projected along [001] direction (equal to the 2-fold direction of QC) is fitted into Figure 3b. Five clusters represented by Yb icosahedron shells are also fitted into the figure and match the HRTEM images, indicating the relationships among quasicrystal clusters, i.e., edge sharing and overlay of the quasicrystal clusters. Figure 3c shows the three-dimensional reconstructed b.c.c. approximant structure projected along [001] direction. Only Yb atoms of icosahedron shell are presented. Comparing the packing of QC clusters (Fig. 3b) and the approximant bcc clusters (Fig. 3c), we can see that these figures further suggest that the real QC structure results from distorted QC approximant bcc structure.

Before the report of $Cd_{84}Yb_{16}$ quasicrystal, stable quasicrystalline can be only found in those alloys contain three or even more elements. The stability of this binary QC phase must be strongly related to its local order structure. Considering the similarity between the local structure of a QC and of its bcc approximant, i.e., the same cluster, the local structure may not be the crucial factor forcing quasiperiodicity. It is suggested that the long-range order, controlled by the electronic band structure, as well as the configurational entropy related to the special degrees of freedom of a quasiperiodic systems are the driving forces, which will be studied further.

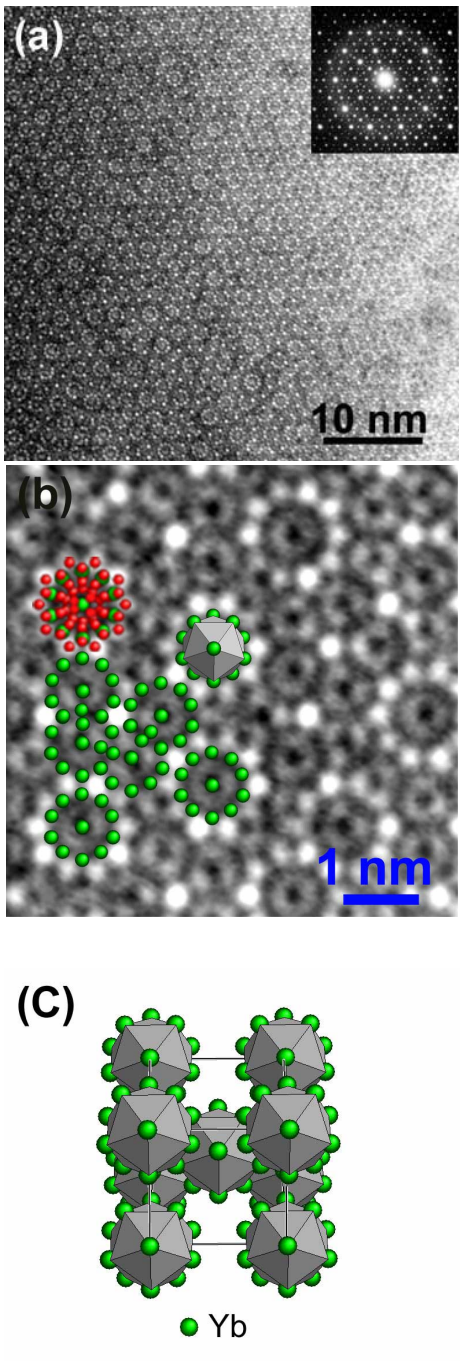

Figure 2 HRTEM image (a), the QC cluster reconstruction on ıe 5-fold inverted FFT image (b) and reconstructed approximant structure projected along 5-fold direction (c).

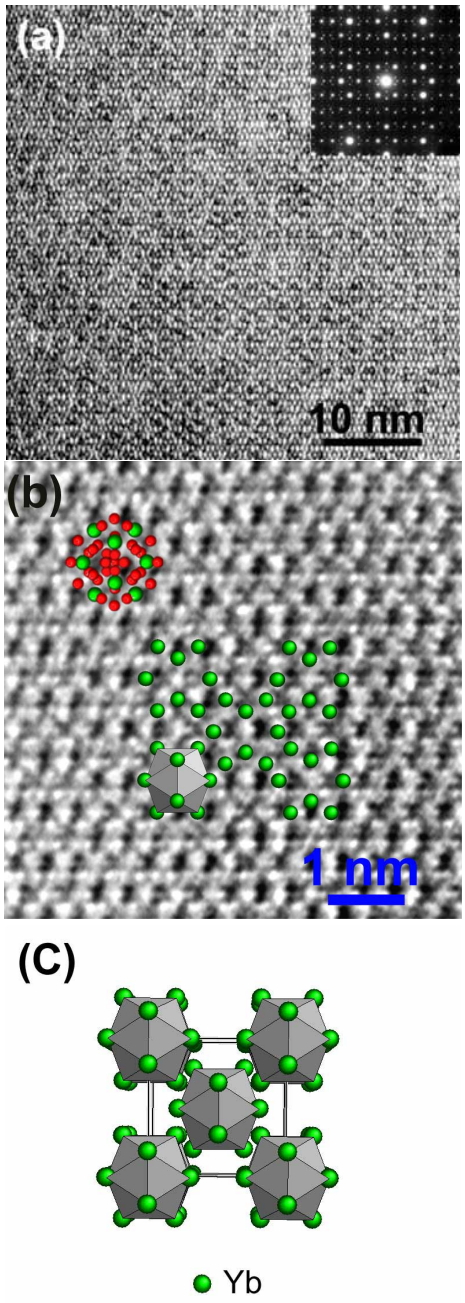

Figure 3 HRTEM image (a), the QC cluster reconstruction on the 2-fold inverted FFT image (b) and reconstructed approximant structure projected along 2-fold direction (c).

CONCLUSIONS

1. The local order structure of single grain binary $Cd_{84}Yb_{16}$ quasicrystalline can be reconstructed using the approximant model of Cd_6Yb. The approximant model is a b.c.c. structure with 9 clusters. Each cluster consists of four successive shells, i.e., Cd tetrahedron (1/3 occupied icosahedron), Cd dodecahedron, Yb icosahedron and a Cd icosidodecahedron.
2. Distorted approximant structure contributes to the real quasicrystalline structure.
3. Two basic relationships, i.e., edge-sharing and overlaying, among clusters are found to match the real QC structure. HRTEM images of both 5-fold and 2-fold of QC can be explained using the distribution of multiply clusters.
4. Local order of the clusters contributes to the stability of this binary quasicrystalline.

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