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Evidence of a stable binary CdCa quasicrystalline phase

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Quasicrystals with a primitive icosahedral structure and a quasilattice constant of 5.1215 Å have been synthesized in a binary Cd–Ca system. The thermal stability of the quasicrystal has been investigated by in situ high-temperature x-ray powder diffraction using synchrotron radiation. It is demonstrated that the binary CdCa quasicrystal is thermodynamic stable up to its melting temperature. The linear thermal expansion coefficient of the quasicrystal is 2.765×10⁻⁵ K⁻¹.


Since the discovery of the icosahedral phase (i phase) in rapidly quenched Al-based alloy systems, 1 there have been extensive studies on quasicrystals. 2–8 More than ten stable quasicrystals containing at least three metallic elements have been prepared. 9 Recently, Tsai et al. 10 reported that stable quasicrystals are found in the binary CdYb system. Here we report the formation of quasicrystals in the binary CdCa system and verify the thermodynamic stability of the novel quasicrystals by performing in situ high-temperature x-ray powder diffraction using synchrotron radiation.

The Cd₈xCa₁₀₀₋ₓ (x = 80–90 at. %) alloys were prepared from the elements (Alfa with 99.9 purity) in a sealed quartz tube with a vacuum of around 10⁻⁵ mbar at 923 K for a few hours. The structure of as-solidified alloys was studied by a Philips PW 1820 x-ray powder diffractometer with Cu Kα radiation. Some selected samples were measured by in situ high-temperature x-ray powder diffraction using synchrotron radiation at beamline I711 at the MAX II synchrotron in Lund, Sweden, utilizing a Huber G670 imaging plate Guinier camera. The wavelength, 1.513 852 Å, was determined using a Si standard. 11 The powder sample, ground from the recovered sample, was placed in an amorphous quartz capillary, pumped down to 10⁻⁵ mbar and then sealed, and rotated during data collections. The diffraction patterns were all collected in the range 30°–50° in 2θ steps of 0.005°, and accumulated for 5 min. An oven was used for high temperature measurements in steps of 30 K. The temperature at sample was calibrated using the known temperature dependence of lattice parameter for pure silicon powder at the sample position. 12

Figure 1 shows an x-ray powder diffraction pattern recorded at 295 K from an as-solidified Cd₈₂Ca₁₈ alloy using Cu Kα radiation. A primitive icosahedral structure was found to be the most promising indexing scheme. The icosahedral Miller indices are generated by cyclic permutations of (q₁, q₂, q₃) = (±1 ± δ, 0). 2 Six independent vectors are expressed by: q₁ = (1, δ, 0); q₂ = (1, −δ, 0); q₃ = (0, 1, δ); q₄ = (0, 1, −δ); q₅ = (δ, 0, 1); and q₆ = (−δ, 0, 1), where δ is the golden mean, 1.618. As an example, the (110 000) peak is found at \( q = Q₀(q₁ + q₂) = (2, 0, 0) \) and \( Q₀ = 2π/\alpha \), where a is the quasilattice constant. The quasilattice constant at room temperature is found to be \( a = 5.1215 \) Å. The peak (2θ ≈ 33°, q ≈ 2.32 Å⁻¹) is a choice for the basic (100 000) reciprocal lattice vector. It is found that binary CdCa quasicrystals together with tiny Cd, Cd₈Ca, or Cd₈₁Ca₄₃ phases are formed in the as-solidified Cd₈₂Ca₁₈ (x = 81–86 at. %) alloys. To ascribe the stability of the binary CdCa quasicrystals, a large number of in situ high-temperature x-ray powder diffraction measurements for several quasicrystal alloys in a temperature range from 295 to 973 K (above melting temperature) were performed. Figure 2 exemplifies in situ x-ray powder diffraction patterns recorded for the as-solidified Cd₈₂Ca₁₈ sample at various temperatures using a wavelength of 1.513 852 Å. At 303 K, the pattern can be indexed with the CdCa quasicrystal phase together with a broadened peak for the Cd phase at 2θ ∼ 37.8°. With increasing temperature, the peaks for the Cd phase (2θ ∼ 31.2° and 37.8°) become narrow while peaks for quasicrystals just slightly shift to lower angles due to thermal expansion. At 573 K, new peaks at 2θ ∼ 33.5°, 34.3°, 38°, and 39.6°, indexed to the Cd₈Ca phase, appear while the peaks for the Cd phase almost disappear. This infers that the reaction between Cd (melting point is around 594 K) and any Ca-containing components occurs to form the Cd₈Ca phase. Both quasicrystal and Cd₈Ca phases coexist up to 783 K. At 843 K, the quasicrys-

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FIG. 1. X-ray powder diffraction pattern recorded with Cu Kα radiation for the as-solidified Cd₈₂Ca₁₈ alloy.
and a tiny solid Cd$_5$Ca$_{14}$ phase. At 903 K, the sample is in the liquid state. When the liquid phase resolidifies, the quasicrystals reappear, as indicated in the pattern recorded at 313 K. The results obtained from our in situ x-ray powder diffraction measurements strongly demonstrate that the binary CdCa quasicrystals formed here constitute a thermodynamic stable phase up to their melting point. Figure 3 shows the linear thermal expansion of as-solidified Cd$_{83}$Ca$_{17}$ quasicrystals.

In conclusion, binary CdCa quasicrystals have been synthesized and their thermodynamic stability has been investigated by in situ high-temperature x-ray powder diffraction using synchrotron radiation. It is found that the quasicrystalline phase is stable up to its melting temperature. The quasi-lattice constant increases linearly with temperature, $a = 5.0791 \pm 1.4155 \times 10^{-4} \text{T}$, having a thermal expansion coefficient of $2.765 \times 10^{-5} \text{K}^{-1}$ at 300 K. The stable binary CdCa quasicrystal will be a good candidate for the determination of the basic atomic structure of quasicrystals.

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11. The pure silicon powder, marked 640°C, was provided from the National Institute of Standards and Technology (NIST) with certified lattice parameter for a temperature of 295.5 K of 5.431194 6 0.000009 2 Å.