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Structural stability of binary CdCa quasicrystal under high pressure

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The structural stability of a binary CdCa quasicrystal with a primitive icosahedral structure has been investigated by *in situ* high-pressure x-ray powder diffraction at an ambient temperature using synchrotron radiation. It is demonstrated that the icosahedral quasicrystalline structure of the sample is intrinsically stable up to 47 GPa. The bulk modulus at zero pressure and its pressure derivative of the icosahedral CdCa quasicrystal is 68.1 ± 2.0 GPa and 4.3 ± 0.2, respectively. The compression behavior of different Bragg peaks is isotropic, indicating no pressure-induced anisotropic elasticity in the stable binary icosahedral CdCa quasicrystals. *© 2001 American Institute of Physics.* [DOI: 10.1063/1.1408902]

Recently, Tsai *et al.*[1] reported that stable quasicrystals were found in a binary CdYb system. Subsequently, Guo *et al.*[2] and Jiang *et al.*[3] have found binary CdCa quasicrystals. The thermodynamic stability of the CdCa quasicrystals was verified by *in situ* high-temperature x-ray powder diffraction using synchrotron radiation.[3] It was demonstrated that the binary CdCa quasicrystals are thermodynamically stable up to their melting temperature at an ambient pressure. The linear thermal expansion coefficient of the quasicrystal is $2.765 \times 10^{-5}\,\mathrm{K}^{-1}$. Here, we report the structural stability of the binary CdCa quasicrystals under pressure up to approximately 47 GPa by *in situ* high-pressure x-ray powder diffraction (XRD) at an ambient temperature using synchrotron radiation.

$\mathrm{Cd}_x\mathrm{Ca}_{100-x}$ ($x = 80-90$ at %) alloys were prepared from the constituent elements (obtained from 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 the as-solidified alloys was studied by a Philips PW 1820 x-ray powder diffractometer with Cu $K\alpha$ radiation. Some selected samples were measured by *in situ* high-pressure (up to 47 GPa) energy-dispersive XRD using synchrotron radiation by beamline F3 at Hasylab, Germany using the Bragg angle 5.033. High pressures were produced at room temperature in a diamond anvil cell of the Holzapfel–Syassen type.[4] The powder sample and a small ruby chip were enclosed in a hole of diameter 0.2 mm in an inconel gasket. A 16:3:1 methanol:ethanol:water solution was used as the pressure-transmitting medium. The actual pressure was determined from the wavelength shift of the ruby line using the nonlinear pressure scale of Mao *et al.*[5]

Figure 1 shows a standard XRD pattern recorded at 295 K from an as-solidified $\mathrm{Cd}_{84}\mathrm{Ca}_{16}$ alloy using Cu $K\alpha$ radiation. A primitive icosahedral structure was found to be the most promising indexing scheme. The icosahedral Miller indices are generated by cyclic permutations of $(q_x, q_y, q_z) = (\pm 1, \pm \delta, 0)$.[6] Six independent vectors are expressed by: $q_1 = (1,\delta,0)$; $q_2 = (1,-\delta,0)$; $q_3 = (0,1,\delta)$; $q_4 = (0,1,-\delta)$; $q_5 = (\delta,0,1)$; and $q_6 = (-\delta,0,1)$, where δ is the golden mean, 1.618. As an example, the (110 000) peak is found at $q = Q_0(q_1 + q_2) = (2,0,0)$ and $Q_0 = 2\pi/a$, where a is the quasilattice constant. The quasilattice constant at room temperature is found to be $a = 5.1215$ Å. The peak ($2\theta \approx 33°$, $q \approx 2.32$ Å^{-1}) is a choice for the basic (100 000) reciprocal lattice vector. It is found that binary CdCa quasicrystals together with tiny Cd and unknown phases are formed in the as-solidified $\mathrm{Cd}_x\mathrm{Ca}_{100-x}$ with compositions of $x = 81-86$ at % alloys. The average grain size of the quasicrystals in the samples is approximately 50 nm. To investigate the stability of the binary CdCa quasicrystals at high pressure at ambient temperature, a large number of *in situ* high-pressure energy-dispersive XRD measurements for several quasicrystal alloys in a pressure range from 0 to 50 GPa were performed. Figure 2 exemplifies *in situ* XRD patterns recorded for the as-solidified $\mathrm{Cd}_{83}\mathrm{Ca}_{17}$ sample at various pressures. The patterns can be indexed to the primitive icosahedral structure together with one peak from Cd and another peak caused by the detector (see caption of Fig. 2). The Bragg peaks for the quasicrystal shift monotonously to higher energy (or lower d-spacing values) when the pressure

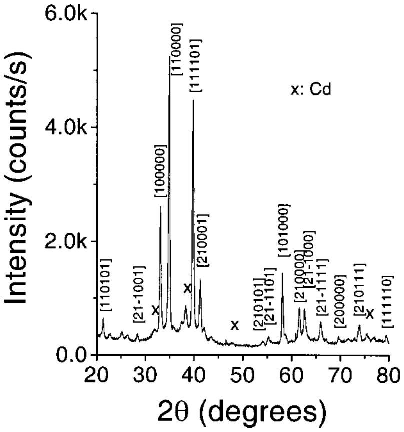

FIG. 1. XRD pattern recorded with Cu $K\alpha$ radiation for a stable binary icosahedral $\mathrm{Cd}_{84}\mathrm{Ca}_{16}$ quasicrystal is shown.

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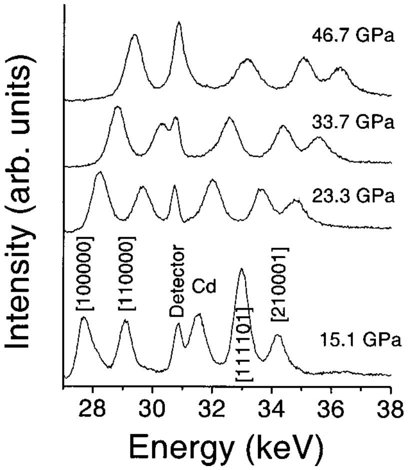

FIG. 2. *In situ* energy-dispersive XRD patterns recorded at various pressures of a stable binary icosahedral $Cd_{83}Ca_{17}$ quasicrystal are shown. The peak, marked as "detector," is due to a damage in the detector provided by the experimental station. It always appears at approximately the same energy (even for no incident x rays).

increases, as shown in Fig. 3 for four Bragg peaks. Although none of the existing peaks disappear, no new peaks appear either, so that the alloy remains having the icosahedral structure up to at least 47 GPa. A question of particular interest is whether the sample exhibits anisotropic elasticity. To address this question, we have plotted the compressibility, assuming $V(P)/V(P=0)$ is equal to $[d(P)/d(P=0)]^3$, for the four Bragg peaks (110 000, 111 101, 210 001, and 101 000), as shown in Fig. 4. It is seen that the data points obtained from the four Bragg reflections fall on the same curve in the $V(P)/V(P=0)$ diagram. The curve can be described by the Birch–Murnaghan equation of state using the zero-pressure bulk modulus (B_0) and its pressure derivative (B_0') as fitting parameters.[7] The result of the fit is $B_0=68.1\pm2.0$ GPa and $B_0=4.3\pm0.2$. The B_0 value for the stable binary icosahedral CdCa quasicrystal is lower than those for icosahedral Al-based, Ti-based, and Zr-based quasicrystals.[8] It is clear from Fig. 4 that the compressibility is equivalent in all directions within experimental uncertainty. We conclude that there are no distinguishable anisotropies in the stable binary icosahedral CdCa quasicrystals.

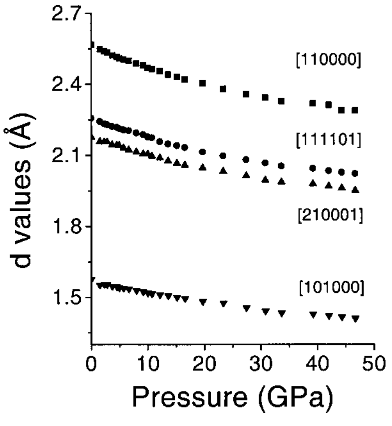

FIG. 3. Pressure dependence of the *d* spacing for four Bragg peaks of the stable binary icosahedral $Cd_{83}Ca_{17}$ quasicrystals is shown. Squares denote the [110 000] peak, circles: the [111 101] peak, triangle-up: the [210 001], and triangle-down: the [101 000] peaks.

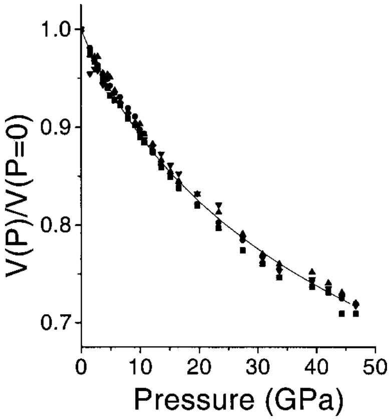

FIG. 4. Pressure dependence of $V(P)/V(P=0)\equiv[d(P)/d(P=0)]^3$, for four Bragg peaks of the stable binary icosahedral $Cd_{83}Ca_{17}$ quasicrystals is shown. The solid line is the fit of the Birch–Murnaghan equation to all the data points. Squares denote the [110 000] peak, circles: the [111 101] peak, triangle-up: the [210 001], and triangle-down: the [101 000] peaks.

In conclusion, the effect of pressure (up to approximately 47 GPa) on the structural stability of the binary CdCa quasicrystals has been investigated by *in situ* energy-dispersive XRD at ambient temperature using synchrotron radiation. It is found that the icosahedral quasicrystalline structure in the sample is intrinsically stable up to at least 47 GPa. The bulk modulus at zero pressure and its pressure derivative of the icosahedral CdCa quasicrystal are 68.1 ±2.0 GPa and 4.3 ± 0.2, respectively. The compression behavior of different Bragg peaks is isotropic, indicating no anisotropic elasticity in the stable binary icosahedral CdCa quasicrystals induced by pressure.

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