X-ray measurements of the compressibility of an $Al_{5.1}Li_3Cu$ quasi-crystal

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X-ray measurements of the compressibility of an $Al_{5.1}Li_3Cu$ quasi-crystal

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Abstract. The bulk modulus of $Al_{5.1}Li_3Cu$ has been measured over the pressure range up to 7 GPa from x-ray measurements of the d-spacings of five reflections. The result for the bulk modulus is $K_0 = 70.5 \pm 4.7$ GPa and for its pressure derivative $K_0' = 4.6 \mp 1.2$. This value for the modulus is consistent with the value of 70 given by Akahama *et al* but remains in disagreement with the ultrasonic measurements of between 53 and 58 GPa given by Reynolds *et al*.

1. Introduction

Since the observation of icosahedral symmetry in rapidly cooled Al_6Mn, quasi-crystals have been the subject of considerable experimental and theoretical activity. The elastic properties of icosahedral crystals are of particular interest. In an ultrasonic study of the mechanical properties of large-grained $Al_{5.1}Li_3Cu$, Reynolds *et al* [2] obtained the bulk moduli $K_0 = 53$ GPa and $K_0 = 58$ GPa for two different directions of the propagation of sound waves: along twofold and fivefold axes, respectively. They found that the elastic properties of the Al–Li–Cu quasi-crystal are isotropic within experimental error.

The starting point for the present investigation is a result obtained by Akahama *et al* [1]. In that work the pressure-induced amorphization of icosahedral Al–Li–Cu (i-Al–Li–Cu) was studied using the x-ray diffraction technique. These workers made a qualitative estimation of the bulk modulus and the reported value was 70 GPa. This result disagrees with that of Reynolds *et al* [2]. Nevertheless, we think that such a value is possible. According to Akahama *et al* [1], the pressure behaviour of interplanar distances of the quasi-crystal under a low pressure (below 7 GPa) is similar to that of aluminium, and the bulk modulus of aluminium is equal to 73 GPa [3].

In this paper we present our experimental results on the compression of (i-Al–Li–Cu) under a high pressure. The experiment was supposed to answer the two following questions. Is the compression isotropic? What is the bulk modulus of Al–Li–Cu? We found that the compression is isotropic within experimental error ($\mp0.5\%$) and the zero-pressure bulk modulus K_0 is 70.5 ∓ 4.7 GPa. There is a difference between our result and the results from ultrasonic measurements, and a comparison is presented in table 1.

2. Experimental procedure and results

The sample of (i-Al–Li–Cu) was prepared by induction melting of high-purity metals under an argon atmosphere. The cooling rate was about $10\,°C\ s^{-1}$. Chemical analysis of the

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Table 1. Data from the ultrasonic and high-pressure measurements. ρ, density of the sample; v_L, longitudinal velocity of sound; v_T, transverse velocity of sound; v_R, Rayleigh velocity of sound; velocities: K_0, bulk modulus.

Sample	ρ (g cm^{-3})	v_L (10^5 cm s^{-1})	v_T (10^5 cm s^{-1})	v_R (10^5 cm s^{-1})	K_0 (GPa)	Reference
$Al_{5.1}Li_3Cu$ twofold	≃2.4[a]	6.4	3.8	≃3.6[b]	53	[3]
Single-grain fivefold		6.1	3.7		58	
Multigrain Al_6Li_3Cu with impurities Al, $R(Al_5Li_9Cu)$ and $T(Al_2LiCu)$	2.52	6.94	—	—	—	[4]
Al_6Li_3Cu Single-grain	—	—	—	3.73	—	[5]
Al_6Li_4Cu Single-grain	—	≃6.2[c]	—	—	—	[6]
Al_6Li_3Cu	—	—	—	—	70	[1]
$Al_{5.1}Li_3Cu$	2.34[d]	—	—	—	70	This work

[a] We estimated this value from given data.
[b] Calculated in [5] and used to compare results.
[c] This value was found by extrapolating a given experimental curve up to room temperature.
[d] *Measured with a picnometer, taking into account the fraction of Al.*

Table 2. X-ray (filtered Cu-Kα radiation) data for $Al_{5.1}Li_3Cu$ with FCC Al: I_{obs}, observed intensity; vw, very weak; w, weak; m, medium; s, strong; vs, very strong.

Line ($n_1n_2n_3n_4n_5n_6$)	d (10^{-1} nm)	I_{obs}	Line ($n_1n_2n_3n_4n_5n_6$)	d (10^{-1} nm)	I_{obs}
110000	5.905	w	311111	1.927	w
111000	4.238	s	321111	1.755	vw
111100	3.682	w	322101	1.641	w
111110	3.458	vw	Al(220)	1.429	w
211111	2.382	m	332002	1.400	m
Al(111)	2.332	m	333101	1.328	vw
221001	2.264	vs	422211	1.308	vw
Al(200)	2.016	w	433101	1.192	vw
222100	1.994	s			

prepared sample indicated that the composition of the sample was 66.96 wt% Al, 8.34 wt% Li and 24.7 wt% Cu. According to the phase diagram given in [7], i–Al_xLi_3Cu exists in the aluminium concentration range $5.0 < x < 5.2$. Thus, there was about 14 wt% of pure aluminium together with i–$Al_{5.1}Li_3Cu$. The zero-pressure powder x-ray diffraction data (filtered Cu Kα radiation) revealed that the alloy contained a fraction of FCC Al (table 2). Diffraction lines of the quasi-crystal were indexed in accordance with [8]. The measured i–(Al–Li–Cu) peak positions agree very well with the positions reported in [7].

The experiments described here were conducted using x-ray powder diffraction from an i–Al–Li–Cu quasi-crystal in a high-pressure diamond anvil cell. To obtain hydrostatic pressures up to 10 GPa an alcohol mixture (methanol:ethanol = 4:1) was used as a pressure-transmitting medium. The pressure was determined from the wavelength shift of the ruby R_1 fluorescence line. The details of the experiment have been described in [9]. The x-ray powder diffraction measurements required about 80 h exposures with photofilm using Mo Kα radiation from a rotating-anode fine-focus tube operating at 1.25 kW (50 kV; 25 mA).

A collimated x-ray beam was filtered with the Zr filter. The radius of the Debye camera was 57.3 mm. The distance from the sample to the film was determined before experiment from the diffraction pattern of NaCl as the internal standard within the measurement error of ∓0.08%. We waited for a day or two before beginning the exposure and we used the value of pressure measured after exposure. As a rule, the pressure changed by no more than 0.4 GPa. This was due to the mechanical properties of the high-pressure cell (mainly the internal friction).

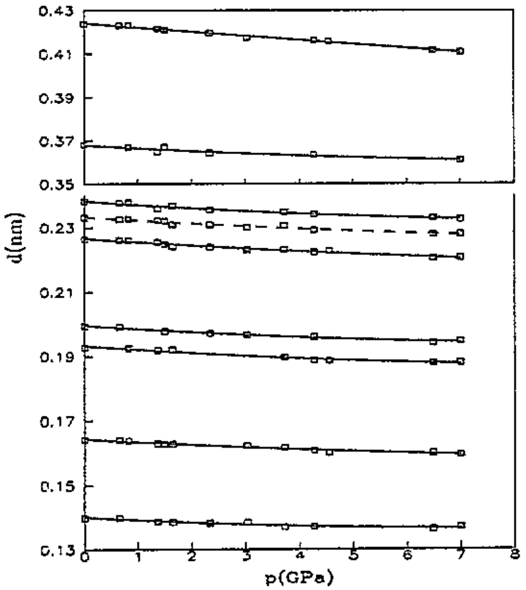

Figure 1. Pressure dependence of d-values for the quasi-crystal (——) and for Al (– – –). Note the similar behaviours of the reflections for both solids.

The i–(Al–Li–Cu) results reported here are for the eight icosahedral peaks observed, namely (111000), (111100), (211111), (221001), (222100), (311111), (322101) and (332002), and the FCC Al results are for the Al(111) peak. Figure 1 shows the dependence of d-values for the quasi-crystal and the aluminium on the pressure. The data were taken both as the pressure was increased and as the pressure was decreased. No hysteresis in the positions of the diffraction lines was observed. To obtain the volume versus pressure curve $V(p)$, the relationship between the d-spacings and the volume is required. For systems with icosahedral symmetry the compression must be isotropic and $V(p)$ will be proportional to $[d(p)]^3$. We calculated the ratios $d/d(221001)$ of measured d-spacings) versus pressure for several lines. As shown in figure 2, the observed ratios are constant within the measurement error ∓0.5%. Since the observed i–(Al–Li–Cu) compression under pressure was isotropic, the relative volume $V(p)/V(0)$ was calculated by averaging the ratios $[d(p)/d(0)]^3$. The error in the d-values for the first two diffraction lines was very large. The weak peak (311111) could not be reliably determined under pressure. So, the average ratios $[d(p)/d(0)]^3$ were calculated taking into account the d-values of the (211111), (221001), (222100), (322101) and (332002) lines. The resulting pressure–volume data for i–(Al–Li–Cu) are shown in figure 3.

According to the Birch–Murnagham equation of state [10]

$$p = \tfrac{3}{2}K_0(x^{-7/3} - x^{-5/9})[1 - \tfrac{3}{4}(4 - K_0')(x^{-7/9} - 1)]$$

where $x = V/V_0$, K_0 is the bulk modulus and K_0' is its pressure derivative, we determined the zero-pressure bulk moduli and their first pressure derivatives for the quasi-crystal, namely

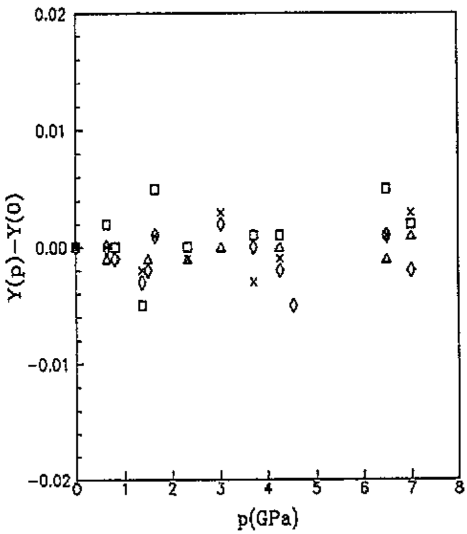

Figure 2. Plots of the ratios $Y(\rho) = d[n_1n_2n_3n_4n_5n_6](\rho)/d[221001](\rho)$ of the measured d-spacings for lines (211111) (□), (222100) (Δ), (322101) (◊) and (332002) (×). The observed ratios are constant within the experimental error.

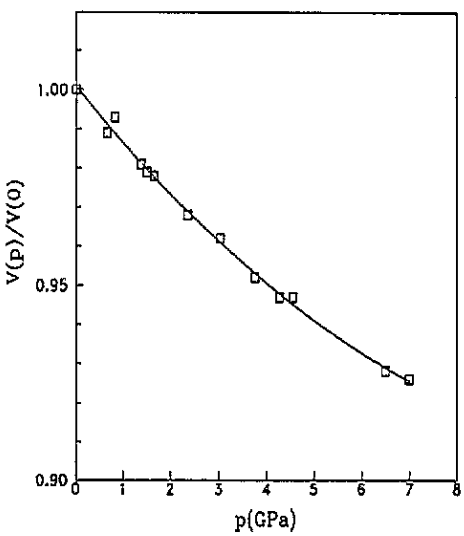

Figure 3. The measured pressure–volume data for $Al_{5.1}Li_3Cu$. The resulting bulk modulus at the zero pressure is $K_0 = 70 \pm 4.7$ GPa and its first pressure derivative $K_0' = 4.6 \pm 1.2$.

$K_0 = 70.5 \pm 4.7$ GPa and $K_0' = 4.6 \pm 1.2$, and for Al, namely $K_0 = 75 \pm 8$ GPa, and $K_0' = 5 \pm 2$. The K_0 and K_0' determined for aluminium are in a good agreement with the known equation of state for Al [3].

3. Conclusion

The measured linear compression of the several observed i–(Al–Li–Cu) peaks was isotropic within the measurement error. The isotropy of compression indicates that the pressure does not break the icosahedral symmetry. The volume compression of an Al–Li–Cu quasi-crystal is well described by the finite-strain equation of state. The measured zero-pressure bulk modulus is in a disagreement with the modulus determined from the ultrasonic measurements by Reynolds *et al* [2].

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