Quasicrystals at extreme conditions: The role of pressure in stabilizing icosahedral $Al_{63}Cu_{24}Fe_{13}$ at high temperature

VINCENZO STAGNO[1, 2, 3], LUCA BINDI[4], CHANGYONG PARK[5], SERGEY TKACHEV[6], VITALI B. PRAKAPENKA[6], H.-K. MAO[1,7], RUSSELL J. HEMLEY[1], PAUL J. STEINHARDT[8], YINGWEI FEI[1]

Supporting Information

Table S1. Experimental conditions and results from diamond anvil cell experiments

run	P_{Neon} (GPa)	d-spacing (Å) of (8,4)	a_{6D}(Å)	V(Å^3)
-	-	*8.94*	*12.64*	*2021*
$^{+}$QC_6	3.50	-	-	-
QC2_10	5.30	8.8029	12.4492	1929
$^{+}$QC2_11	7.20	-	-	-
QC2_14	12.70	8.6673	12.2574	1842
QC2_17	16.80	8.6016	12.1645	1800
QC2_19	17.10	8.5917	12.1505	1794
QC2_22	20.12	8.5524	12.0949	1769
QC2_20	20.30	8.5486	12.0895	1767
QC2_23	24.40	8.4933	12.0113	1733
QC2_25	24.50	8.4913	12.0085	1732
QC2_27	28.00	8.4609	11.9655	1713
QC2_26	29.50	8.4424	11.9394	1702
QC2_28	29.65	8.4361	11.9304	1698
QC2_30	32.50	8.4187	11.9058	1688
QC2_32	34.00	8.3831	11.8555	1666
QC2_34	35.60	8.3505	11.8094	1647
QC2_36	37.60	8.3460	11.8030	1644
QC2_37	40.00	8.3113	11.7540	1624
QC3_38	41.30	8.2955	11.7316	1615
QC3_42	44.50	8.2872	11.7199	1610
QC3_43	45.50	8.2834	11.7145	1608
QC3_41	45.90	8.2792	11.7086	1605
QC3_45	50.00	8.2380	11.6503	1581
QC3_44	51.30	8.2289	11.6374	1576
QC3_47	44.00	8.2822	11.7128	1607
QC3_49	39.00	8.3091	11.7508	1623
QC3_50	36.50	8.3594	11.8220	1652
QC3_53	33.20	8.3834	11.8559	1667
QC3_54	31.50	8.4234	11.9125	1690
QC3_55	30.60	8.4314	11.9238	1695

QC3_56	27.25	8.4858	12.0007	1728
QC3_57	23.30	8.5363	12.0722	1759
QC3_59	18.55	8.5926	12.1518	1794
QC3_60	14.35	8.6495	12.2322	1830
QC3_61	13.68	8.6486	12.2310	1830
QC3_62	9.10	8.7049	12.3106	1866
QC3_63	7.05	8.7793	12.4158	1914
QC3_64	5.99	8.8234	12.4782	1943
QC3_65	3.00	8.8816	12.5605	1982
QC3_66	2.07	8.9154	12.6083	2004
$^{+}$QC3_67	0	-	-	-
*QC_P_05	3.10	8.8622	12.5330	1969
*QC_P_06	5.40	8.8092	12.4581	1934
*QC_P_07	10.00	8.7221	12.3349	1877
*QC_P_08	14.50	8.6429	12.2229	1826
*QC_P_09	18.50	8.5797	12.1335	1786
*QC_P_10	25.20	8.5356	12.0712	1759
*QC_P_11	28.20	8.4949	12.0136	1734
*QC_P_13	32.00	8.4243	11.9138	1691
*QC_P_14	36.00	8.3627	11.8267	1654

Numbers in italics are parameters at ambient conditions reported by Bindi et al. 2011. ($^{+}$) For this runs the (8,4) peak could not be observed. (*) indicates in situ high resolution angle dispersive X-ray diffraction measurements. Uncertainties in the pressure determination are within 0.5 GPa and propagate from the uncertainty in the lattice parameter of the pressure marker. Uncertainties relative to the six-dimensional lattice parameter of i-AlCuFe are generally less than 1%.

Single crystal X-ray diffraction measurement

Single crystal X-ray diffraction measurements were performed on quasicrystalline powder recovered after being exposed at high pressure and temperature using diamond anvil cell (see main text). Since the cell broke in the attempt to increase pressure during in situ measurements, most of the grains were diamond fragments and scattered pieces of the rhenium gasket. A total of 7 grains between 11 μm and 24 μm were extracted and initially studied by powder diffraction to verify the presence of potential QC. An automated CCD-equipped Oxford Diffraction Xcalibur Ultra-PX diffractometer (Cu*K*α radiation) was used with ultra-high exposition times (from 30 to 48 hours). A fragment of 18 μm in size consisting of an aggregation of several fragments all aligned in the same direction (along with other impurities consisting of diamonds and rhenium) was selected for further single crystal X-ray diffraction studies. The results are summarized in

Figure S3 where it appears evident that the analyzed fragment retained icosahedral symmetry after high pressure and (likely) high temperature.

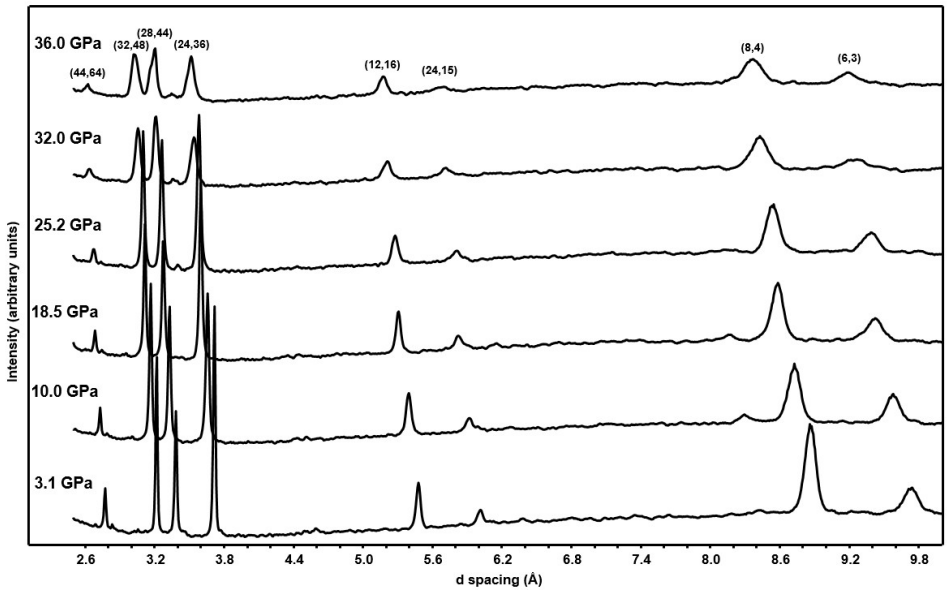

Figure S1. Variation of the *d*-spacing from selected high-resolution XRD profiles (sample detector distance ~478 mm; wavelength, 0.5167 Å) at different pressures. Broadening is observed with increasing pressure, which is likely due to local changes in atomic configuration. Two additional peaks are visible (24, 15) and (8, 4).

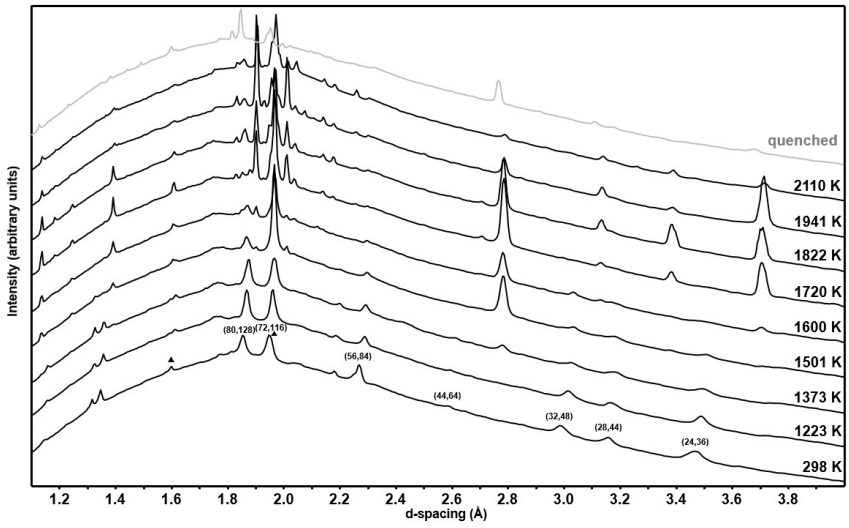

Figure S2 XRD patterns collected from a different point of the sample than in Figure 5 heated up to 2110 K. It can be seen that the diffraction pattern of the quenched sample appears different from that of i-QC.

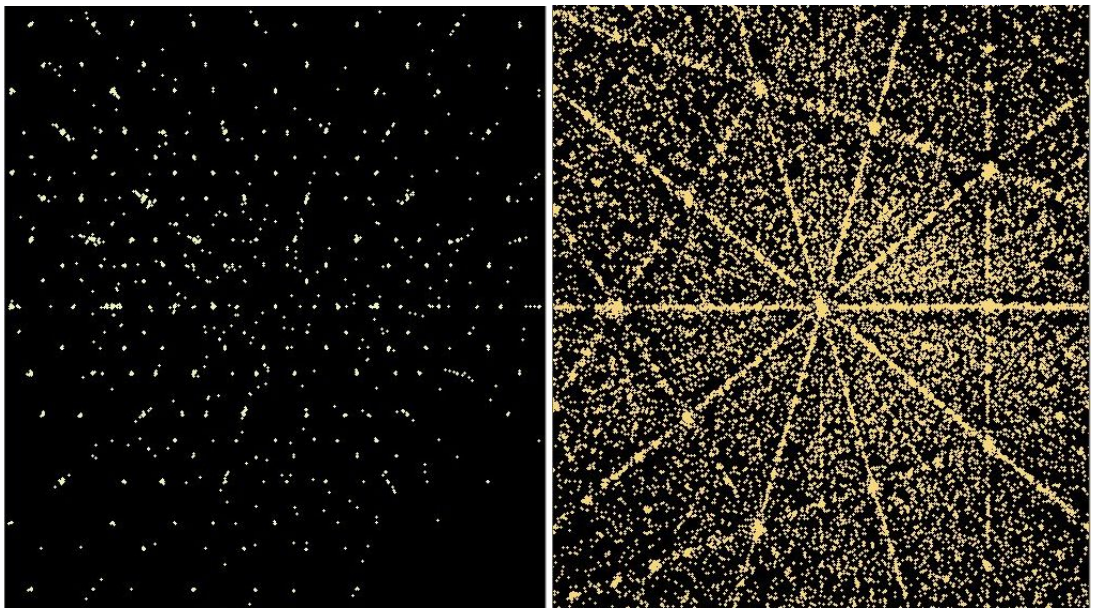

Figure S3 Left panel: The collected reflections in the Ewald sphere are projected down the five-fold axis. Additional spots are probably due to diamond or gasket material but most of the reflections are in excellent agreement with the diffraction pattern along the 5-fold axis of an icosahedral material. Right panel: Gnomonic projection of the same collected X-ray reflections that clearly shows the five-fold symmetry of the QC.