ESRF

Experiment title:
Decagonal quasicrystals at high pressure

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9

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Report:

Until now quite a few *in situ* studies on quasicrystals are known to the literature. Most of them are based on powder experiments on icosahedral phases (see e.g. [1] and references therein). As it was shown by a former high-temperature experiment at SNBL, ESRF, a phase transition of the Ni-rich d-Al-Co-Ni (so-called Edagawa phase) is only detectable by the disappearance of weak superstructure reflections and changes in the shape of the diffuse scattering [2]. Therefore, the use of single crystals is an essential requirement for detailed structural investigations on possible structural transitions of quasicrystals. In a feasibility study using in-house equipment and synchrotron radiation at SNBL, ESRF, it was shown that by use of adequate experimental parameters, diffraction images with comparable details are obtainable with and without diamond-anvil cell [3]. The Edagawa-phase was found to be stable up to the maximum pressure used, 10.7 GPa.
Datasets of preoriented single crystals of decagonal Al-Co-Cu, Al-Ni-Ru, and Al-Co-Ni (basic Ni-rich phase) were measured at about 2, 6, and 10 GPa on the mar IP scanner ($30\,° \le \varphi_{tot} \le 60\,°$, $\Delta\varphi = 0.5\,°$) by the use of the ETH-DAC. To minimize the unwanted scattering of the gasket, the beam diameter was reduced to about $100 \times 100\ \mu m^2$.
Like the Edagawa phase, decagonal d-Al-Cu-Co shows very well structured diffuse scattering within and between the Bragg layers. Figure 1 shows the reconstructed reciprocal-space layers of a decagonal Al-Cu-Co quasicrystal. The quality of the reconstructed images allows a detailed comparison of weak Bragg peaks and diffuse scattering phenomena at ambient and high pressure. Figure 2 shows enlarged regions of the zero reciprocal-space layer shown in

Figure 1 at ambient pressure and 10.9 GPa. Up to 10.9 GPa, no significant changes in the shape of the diffuse scattering or Bragg peak broadening was observed, indicating the structural stability of this compound within the investigated pressure range.

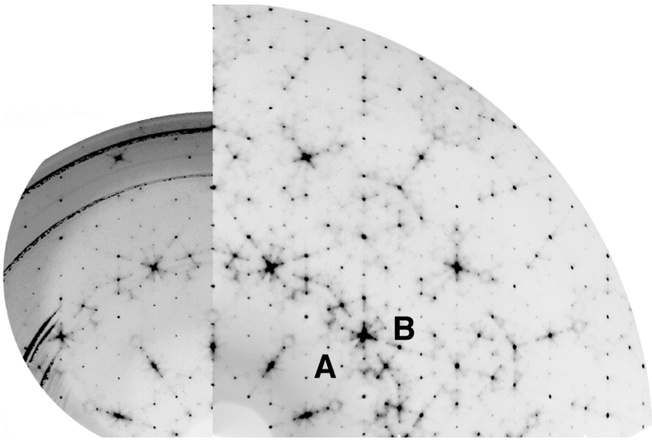

Figure 1. Comparison of reconstructed reciprocal space layers of d-Al-Cu-Co with (left images) and without diamond anvil cell. (Left zero, right first quasiperiodic layer) [1].

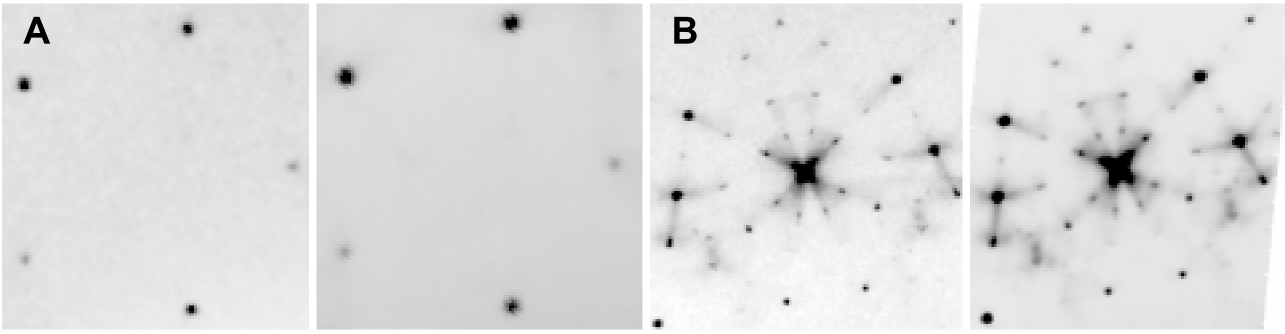

Figure 2. Details of the reconstructed zero reciprocal space layer of d-AlCuCo with (left images) and without diamond anvil cell. (Left: area around A in Figure 1. Right: around B) [1].

To reconstruct layers of reciprocal space, the knowledge of the orientation matrix is necessary [4]. For decagonal quasicrystals showing well structured diffuse scattering, a suitable matrix for the reconstructions can be found by geometric considerations. The problem is more complex for decagonal quasicrystals showing only weak or less structured diffuse scattering. State-of-the-art indexing algorithms fail due to the high amount of structured backgound (caused by diamond-anvils, gasket, and backing-plates) and the small amount of quasicrystal-reflections, indexable by integers. Ongoing data analyses focuses therefore on the indexing, determination of the orientation matrices and lattice parameters, and the reciprocal-space reconstructions of d-Al-Ni-Ru and d-Al-Ni-Co (basic decagonal phase).

[1] Krauss, G., Steurer, W.: Why study quasicrystals at high pressures? In *High-Pressure Crystallography* (Eds. A. Katrusiak and P.F. McMillan), Kluwer Dordrecht, 2004, pp. 521-526. *in press*

[2] Steurer, W., Cervellino, A., Lemster, K., Ortelli, S., Estermann, M.A.: Ordering principles in decagonal Al-Co-Ni quasicrystals. *Chimia* 55 (2001) 528-533.

[3] Krauss, G., Miletich, R. Steurer, W.: Reciprocal-space imaging and the use of a diamond-anvil cell: a single-crystal high-pressure study of a quasicrystal up to 10.7 GPa. *Phil. Mag. Lett.* 83 (2003) 525-531.

[4] Estermann, M.A., Steurer, W., Diffuse scattering data acquisition techniques. *Phase Transit.* 67 (1998) 165-195.