High-energy X-ray Diffraction Study of Phason Disorder in Icosahedral AlPdMn

W. Schweika, D. Hupfeld, T. Brückel
Institute of Solid State Research (IFF), Forschungszentrum Jülich, Jülich, Germany

Introduction

Since quasicrystals were discovered by the end of 1984, their structural features have attracted much attention. The stability of AlPdMn makes it an excellent candidate for such studies. While the typical low mosaicity indicates an exceptionally high structural quality even for large, single grains, relative strong diffuse scattering indicates that disorder is an essential part of the structure. Note that the structure of this quasicrystal phase is still not very well known, and the relative strong diffuse scattering could be one intrinsic reason for this problem. A detailed theoretical prediction of diffuse scattering related to phason disorder was given within the elasticity theory of Jaric and Nelson [1], showing also that this "Huang"-like diffuse scattering is inversely proportional to q^2, where q is the reduced scattering vector. The possible peculiar anisotropies that arise from possible elastic instabilities have been analyzed by Widom [2]. Neutron and x-ray scattering experiments confirmed this diffuse scattering near Bragg peaks [3].

The present study is pioneering in that it uses high-energy x-rays in combination with an image-plate detector to investigate the diffuse scattering in large regions of the reciprocal space, with enormous gains in efficiency and quality. The aim is to determine phason coupling constants from the diffuse scattering and explore the benefits and feasibility of a promising new technique.

Methods and Materials

A large single crystalline sample of icosahedral $Al_{0.705}Pd_{0.21}Mn_{0.085}$ of high quality was grown by the Czochralski method. A 5-mm-thick piece was cut to both sides normal to one of the axes of twofold symmetry. The classical method of measuring x-ray diffuse scattering in reflection geometry and using a single detector is very demanding with regard to positioning time, particularly when a large section of the reciprocal space needs to be explored. In addition, this method prevents the naturally high Q-resolution of synchrotron radiation from being used efficiently. In a recent experiment on the diffuse scattering of AlPdMn quasicrystals, Capitan et al. [4] used an area detector in reflection geometry (an image-plate and/or a charge-coupled device [CCD] camera are appropriate) at the European Synchrotron Radiation Facility (ESRF). However, large differences in the x-ray intensities were measured for two quasicrystals of similar composition. These appear to be inconsistent with our results and related to systematic errors and corrections for the reflection geometry.

Applications of high-energy x-rays have several advantages. Because of their high penetration, the measurements are performed in transmission geometry. By using a small wavelength, a much larger section of the reciprocal space is covered. The intensity is largely enhanced because of the thickness of the sample, and systematic corrections are of minor importance. Also, the experimental setup is quite simple. In order to avoid over-illumination due to intense Bragg peaks, the sample was oriented normal to a basal Bragg plane of the crystal such that a relatively flat section of the Ewald sphere near the basal reciprocal lattice plane was measured.

The experiment was performed at the high-energy-side station of the Midwest Universities Collaborative Access Team (MU-CAT) beamline at the APS. With an incident energy of 94.6 keV, a distance of 1.6 m between the sample and image-plate detector, and a small tungsten beam stop, the covered Q range is as large as $0.1\ \text{Å}^{-1} < Q < 5.2\ \text{Å}^{-1}$. The largest Q component parallel to the incident beam is at the highest scattering angles $Q_z = 0.26\ \text{Å}^{-1}$. Although the undulator gap was not optimized for the side station, collecting the data for the image shown in Fig. 1 took only 1 min.

Results and Discussion

There is a characteristic modulation of diffuse intensities that is particularly strong near Bragg peaks and is proportional to q^{-2}, where q is the distance to the Bragg point. Thermal diffuse scattering would have the same Q dependence; however, as can be found from modeling and has been proven by neutron scattering experiments, these intensities are essentially related to static phason disorder rather than phonon disorder. The pronounced anisotropy found in the diffuse scattering pattern can be described in detail on the basis of the theory of quasicrystalline elasticity. Thus a single parameter — the ratio of phason coupling constants $K_1/K_2 = 0.6$ — is sufficient. This value shows that this icosahedral quasicrystal is close to its boundary of stability. The present data can also be used to determine the relative Bragg intensities from the diffuse scattering. Contrary to existing databases of Bragg peaks measured with both x-rays and neutrons, this diffuse scattering is free of extinction effects, and corrections play

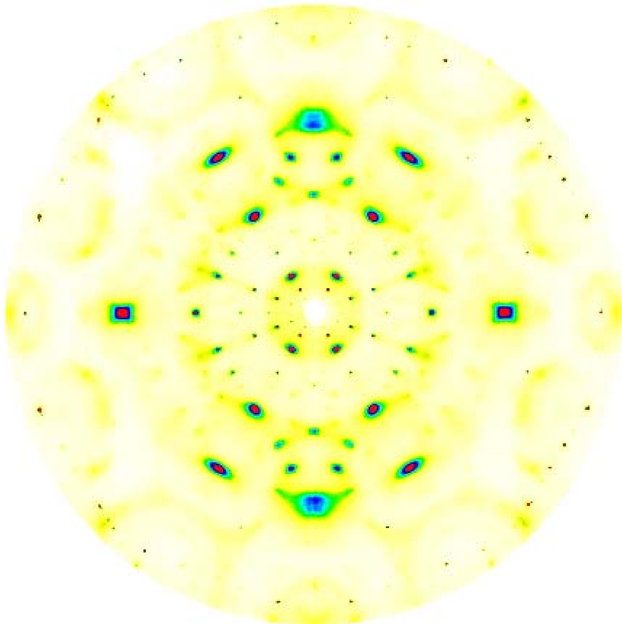

FIG. 1. High-energy x-ray diffuse scattering of icosahedral AlPdMn at room temperature.

a much weaker role. It will be important to test actual quasicrystalline models. While the pure phason disorder clearly dominates the overall diffuse intensities, the data should allow for a quantitative determination of the strength of phason-phonon coupling. This part of the data analysis is still in progress.

Acknowledgments

Use of the APS was supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences (BES), under Contract No. W-31-109-ENG-38. The MU-CAT sector at the APS is supported by the DOE BES through Ames Laboratory under Contract No. W-7405-ENG-82.

References

[1] M. V. Jaric and D. R. Nelson, Phys. Rev. B **37**, 4458 (1988).
[2] M. Widom, Philos. Mag. Lett. **64**, 297 (1991).
[3] M. de Boissieu, M. Boudard, B. Hennion, R. Bellissent, S. Kycia, A. Goldman, C. Janot, and M. Audier, Phys. Rev. Lett. **75**, 89 (1995); M. Boudard, M. de Boissieu, A. Letoublon, H. Hennion, R. Bellissent, C. Janot, Europhys. Lett. **33**, 199 (1996); A. Letoublon, M. de Boissieu, M. Boudard, L. Mancini, J. Gastaldi, B. Hennion, and M. Mori, Phil. Mag. Lett. **81**, 273 (2001).
[4] M. J. Capitan, Y. Calvayrac, A. Quivy, J. L. Jouland, S. Lefebvre, and D. Gratias, Phys. Rev. B **60**, 6398-6404 (1999).