Quasi-Brillouin zones and s-p band dispersion observed in photoemission from the 2fold surface of decagonal AlNiCo

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In spite of considerable progress in the understanding of the structural properties of quasi-crystalline alloys, an explanation of their fascinating physical properties in terms of the nature of their electronic states remains elusive[1]. The conventional picture of Bloch waves, so successful in interpreting the properties of regular crystals, is obviously problematic since the basis of Bloch wave behavior, i.e. translational symmetry, is absent in quasicrystals. Hence, cluster-like localized states have been put forward in theoretical treatments, in analogy to the cluster concept of the quasicrystal geometric structure. We have recently shown that signatures of band-like states are observed in decagonal AlNiCo quasicrystals by means of photoemission from the tenfold surface[2]. The observation of band-like states, which exhibit a free-electron like dispersion with the parallel and normal component of the electron wave vector $k_{\parallel}$ and $k_{\perp}$, can be understood within a picture of quasi-Brillouin zones in which only those reciprocal lattice vectors with a large structure factor associated act as centers for higher-order Brillouin zones[3]. Here we show that this concept provides a consistent description of the electronic states along both the periodic and quasiperiodic directions of decagonal AlNiCo. Planes of atoms are stacked periodically along the tenfold axis, while within the planes the atoms are ordered quasiperiodically; this is sketched schematically in the top left side of Figure 1. Normal to the tenfold axis are two inequivalent 2-fold symmetric directions (named "P" and "E" in the inset of Figure 1), and our photoemission experiments were performed on these two, which are represented by arrows passing through the planes and vertices of the fictitious decagon in the Figure; they form an angle of 18° with one another. All data were recorded on beamline 7.0.1, and were recorded by rotating the sample in the polar and azimuthal directions with analyzer and light incidence fixed, with subsequent symmetrization; the azimuthal range was large enough to avoid artefacts from the symmetrization process. The images were constructed by subtraction of a polynomial background to enhance the weak features in the s-p band region.

The concept of quasi-Brillouin zones is based on the relation between the diffraction pattern and the influence of the dominant Bragg planes on valence electron dynamics in the quasicrystal. Quasicrystals possess diffraction patterns characterized by (countably infinite) sharp spots, with a hierarchy of decreasing intensity. This suggests that one may, to a first approximation, take only the location of the
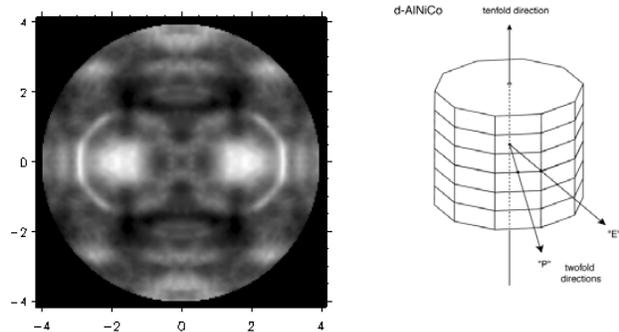

Figure 1: Distribution of photoelectron intensity from two inequivalent 2-fold surfaces of AlNiCo at a binding energy of 6 eV below E_F. The horizontal direction is the quasi-periodic and the vertical the periodic direction. The inset shows a schematic diagram of the symmetry axes in d-AlNiCo

most intense spots in reciprocal space as centers of higher order Brillouin zones. If we consider an s-p band with a free-electron-like dispersion, we expect spherical constant energy surfaces in k-space. By sampling the intensity distribution at a specific binding energy below the Fermi level E_F, as a function of parallel wave vector $k_\parallel^x$ and $k_\parallel^{y'}$ (in terms of polar and azimuthal angle of electron emission), we expect ring-like features from the cut through these spherical surfaces. Such rings, centered at specific points in $k_\parallel$-space, are in fact observed (Fig. 1). They arise from s-p-like states in the AlNiCo valence band, dispersing in a parabolic manner. The top image (from the "E" surface) shows two rings on either side of the center $(k_\parallel^x, k_\parallel^y)=(0,0)$, while the bottom (from "P") has one ring centered on (0,0) and two rings on either side. This demonstrates that bulk states are sampled, since the rotation of the bulk direction exactly corresponds to the displacement of the ring structures in the k-space images.

The above analogy between the diffraction and quasi-Brillouin zones can in fact be made by directly comparing our electron diffraction image from the "P" surface and the corresponding $k_\parallel$-space distribution of s-p state intensity in Figure 2. The low energy diffraction (LEED) pattern shows a rhombic arrangement of intense spots, as shown by the white lines; a similar arrangement connects the centers of the ring patterns in the photoemission image. The fact that the rings in the horizontal plane are strongest, while those centered around the top and bottom corner are weaker may be related to the photoemission transition matrix element. The image actually contains more detailed information which goes beyond the simple interpretation in terms of s-p states which disperse in a parabolic fashion; note, for example, that the rings seem to overlap in the center of the $k_\parallel$ space image, and that there are secondary rings above and below the strongest features. The energy which is sampled here is already close to the onset of the Co and Ni d-band region, where a more complex dispersion is expected.
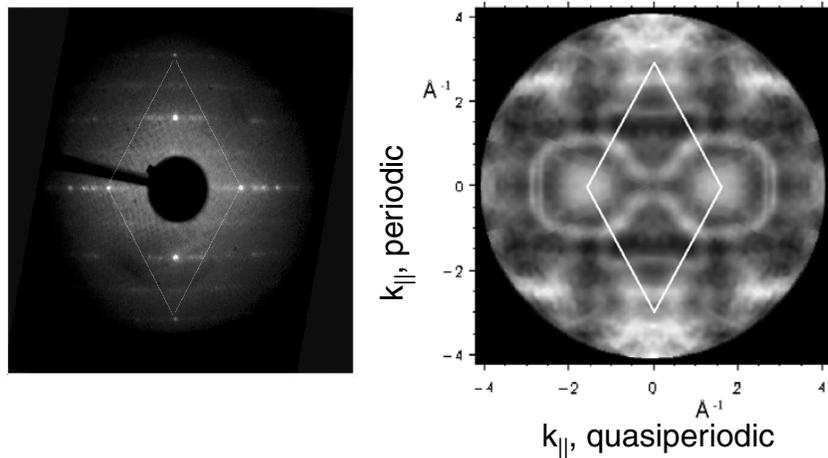

Figure 2: a.) LEED pattern of a twofold surface of d-AlNiCo at 100 eV kinetic energy. B.) Photoemission intensity map from d-AlNiCo at a binding energy of 4.5 eV below E_F, recorded at a photon energy of 99 eV. The rhombic pattern connecting the prominent LEED diffraction spots and the centers of the rings in the photoemision

References

1. "Physical Properties of Quasicrystals", ed. Z.M.Stadnik, Springer Series in Solid State Sciences 126, (1999).
2. E.Rotenberg, W.Theis, K.Horn, P.Gille, Nature **406**, 602(2000)
3. K.Niizeki, T.Akamatsu, J.Phys.Cond.Mat. 2, 2759(1990)