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Atomic Structure of Quasicrystal Studied by Spherical Aberration Corrected 300kV-STEM

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Phason is a unique elastic degree of freedom specific to quasicrystals, and may cause structural disorders at specific atomic sites. Using annular dark-field scanning transmission electron microscopy (ADF-STEM), we have recently shown that some particular Al atoms in the decagonal $Al_{72}Ni_{20}Co_8$ reveal significantly large Debye-Waller factors at high-temperature [1]. These anomalous DW factors can be related to phason fluctuations within the context of hyperspace crystallography; that is, these anomalous Al sites are shown to be generated from the *edge* portions of the occupation domains. Local DW anomalies may enhance short-range diffusional atomic jumps between their neighbour sites, and slow phason dynamics can be achieved *only* when these local atomic jumps are correlated across certain length-scale. Diffusional jumps result in the 'quenched phason disorders' that are detectable by experimental measurements on the quenched sample.

ADF-STEM provides atomic-resolution images by effectively illuminating each atomic column one-by-one. To a good approximation, the imaging is incoherent and can be described by a convolution between the scattering object and the probe-intensity function. Within this context, the resolution of STEM is simply determined by the size of the electron probe, and improving a spherical aberration (Cs) of objective lenses promises to achieve at least sub-Ångstrom resolution [2]. It is noteworthy that its potential benefits for the ADF-STEM may turn out to be much greater than those for the conventional TEM of phase-contrast, because incoherent imaging is much less sensitive to chromatic instabilities (Cc).

We describe the details of quenched phason disorders in the decagonal $Al_{72}Ni_{20}Co_8$ by an Cs-corrected 300kV-STEM (VG-HB603U with Nion corrector, at ORNL). It is quite obvious that the image becomes much clearer after Cs correction; significantly, even the Al atomic columns, not only the heavier Ni or Co columns, are now seen clearly as weak bright spots under the scattering amplitude sensitive Z-contrast mode. This is a remarkable effect of Cs-correction, provided a better signal-to-noise ratio which has been realized by suppressing secondary-maxima that exist in uncorrected probe tails. Structural details can be directly addressed by a simple deconvolution procedure on the incoherent ADF-STEM images. Deconvolution using maximum entropy (ME) algorithm [3] gives a safest, least possible structure that fits the experimental image. Figure 1 shows the result after ME-deconvolution on Cs-corrected 300kV-STEM image. Impressively, the Al atomic sites that are expected to be half-occupied and separated by less than 1Å (phason-related atomic sites) now emerge out clearly, as indicated by arrows. We will describe significant distributions of substitutional and occupational disorders across an entire quasiperiodic structure, for those not only the transition metal sites but also the Al sites.

REFERENCES
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[2] S.J. Pennycook, B. Rafferty and P.D. Nellist, Micrc. Microanal., **6** (2003) 343.
[3]_DeConvHAADF : commercially available software from HREM Research Co. (www.hremreserach.com)._We acknowledge K. Ishizuka for helpful discussions on deconvolution processing.

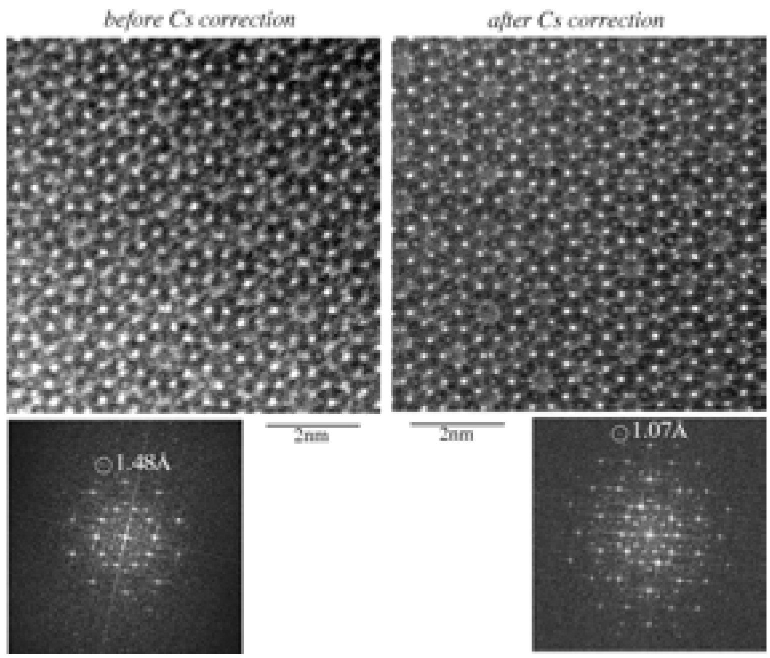

Figure 1. ADF-STEM images of an $Al_{72}Ni_{20}Co_8$ quasicrystal, obtained by the VG-HB603U (left) before and (right) after the Cs-corrector is installed. The corresponding Fourier transform patterns are shown below.

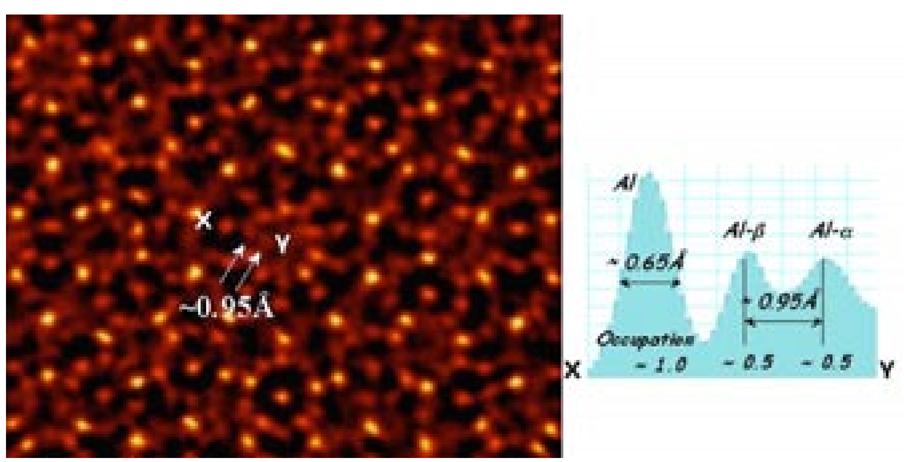

Figure 2. Maximum-entropy deconvolution processed Cs-corrected STEM image of an $Al_{72}Ni_{20}Co_8$ quasicrystal. The intensity profile across X-Y is shown right.