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Local Symmetry and Phason Fluctuations of an Ideal Al-Ni-Co Quasicrystal Studied by Atomic-resolution HAADF-STEM

Eiji Abe[*, **] S. J. Pennycook[*] and A. P. Tsai[**]

[*] Oak Ridge National Laboratory, Solid State Division, P.O. Box 2008, Oak Ridge, TN37831-6031 USA
[**] National Institute for Materials Science, Aperiodic Solids Research Team, 1-2-1, Sengen, Tsukuba 305-0047, Japan

Quasicrystals are solids with symmetries forbidden to ordinary crystals. The central issues have been to locate atoms in such a non-periodic, complicated structure. The decagonal quasicrystals are built up by a periodic stacking of quasiperiodic planes (a two-dimensional quasicrystal), so that atomic-resolution imaging along the tenfold symmetry axis provides a direct interpretation of the quasiperiodic atomic structure.

An important key structural feature recently raised concerns local symmetry of quasicrystals [1-4], namely, the true symmetry of their basic building block - *atomic cluster*. In the case of decagonal quasicrystals, the cluster had been believed to posses a tenfold symmetry axis. The $Al_{72}Ni_{20}Co_8$ is one of the best quasicrystalline compounds with nearly-perfect quasiperiodic atomic order close to its ideal stoichiometry. Atomic-resolution phase-contrast and Z-contrast images are shown in Figs. 1a and b, in which some decagonal clusters with a diameter of about 2nm are outlined to guide the eye. Viewing carefully the cluster interiors, one notices a striking feature that the contrasts appear to break tenfold symmetry at the core of the clusters [2-4]; the triangle of brightest spots representing Ni or Co is intuitive in the Z-contrast image, and the triangle modulations in the phase contrast are found to be mainly due to slight shift (~0.95Å) of Al atoms from the tenfold symmetry positions. The overall quasiperiodic structure can be interpreted according to the quasi-unit-cell picture [2,3] in which the symmetry-breaking decagonal clusters are allowed to overlap with their neighbors according to well-defined rules.

Originating from its high-symmetry, a unique elastic degree of freedom – termed *phasons* – can be defined specific to quasicrystals. This extra degree of freedom may cause a local anomaly of the Debye-Waller (DW) factor at the specified atomic sites. Here we employ the HAADF-STEM to map directly the change in thermal diffuse scattering (TDS) intensity distribution in the quasicrystal, through an *in-situ* high-temperature observation of the decagonal $Al_{72}Ni_{20}Co_8$. We find that, at 1100K, a local anomaly of thermal vibrations monitored by anomalous HAADF-contrasts occurs at the core of some decagonal clusters (FIG.2), the long-range distribution of which is not random but quasiperiodically well-correlated on a length scale of 2nm [5]. Quite interestingly, we are able to explain this feature by assuming an anomalous temperature (DW) factor for the Al atoms those sit at the phason-related sites defined within the framework of hyperspace crystallography [5]. We check the DW factor effect on HAADF image contrast by changing the angular range of the detector. The origin of some phason-related structural disorders will also be discussed.

References

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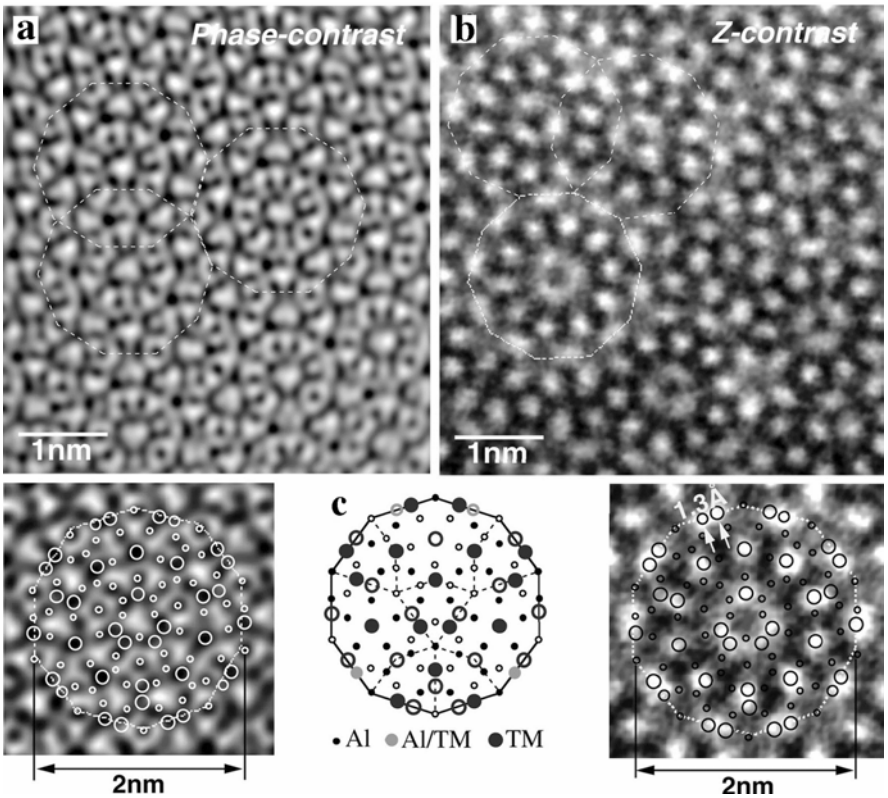

FIG. 1. Atomic-resolution (a) phase-contrast (JEM-4000EX with Cs=1.0mm) and (b) Z-contrast (JEM-2010F with Cs =0.5mm) images. (c) Atomic model of the $Al_{72}Ni_{20}Co_8$, where all possible atomic positions derived from the three variations [3] of the cluster are shown. TM denotes the transition metals; Ni or Co.

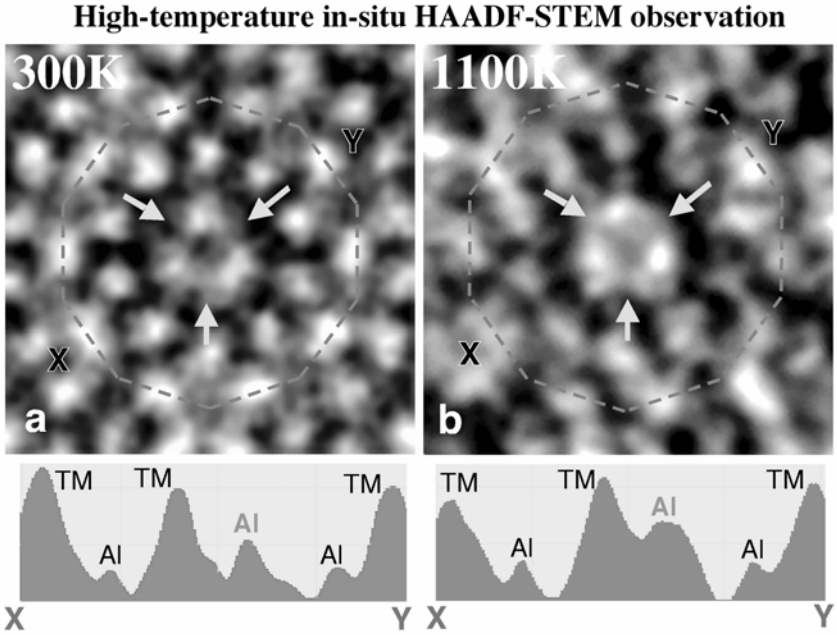

FIG. 2. HAADF images and intensity profiles across a 2nm-cluster at (a) 300K and (b) 1100K. Significant contrast enhancement can be seen at the core of the cluster at 1100K, as indicated by arrows. This temperature-dependent contrast change is fairly well explained by an anomalous Debye-Waller factor for the Al atoms, related to *phason* fluctuations.

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