s3.m11.o5 **Modulations in Complex Structures – Two Case Studies.** Lidin, Sven[1], Pay-Gomez, Cesar[1], Boström, Magnus[2] [1]*Inorganic Chemistry, Arrhenius Laboratory, Stockholm University,* [2]*MPI Chemische Physic fester Stoffe, Dresden. E-mail: Sven@inorg.su.se*

Keywords: Incommensurate; Intermetallic

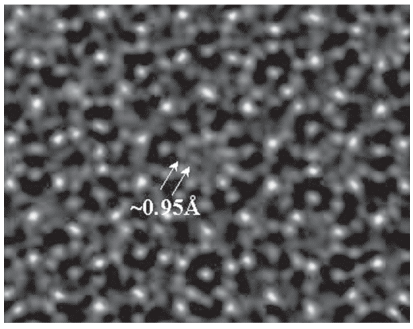
There is something very appealing about rendering complex approximations to incommensurately modulated structures simple by using the super space formalism to present them in a clear and succinct form. There are however cases when the basic structure itself is quite complex, and this makes analysis a little more involved. First of all, the solution of the underlying parent structure is far from straight-forward, and secondly, the identification of the primary cause of the modulation is more difficult. We present here two cases that present such problems, the structures of ht-Sb_2Zn_{3-x} and that of $Ce_{13}Cd_{58}$. The first structure belongs to a class of compounds that form between the zinc group metals and the pnictides. They typically consist of rigid pniktide frameworks and interstitial Zn and Cd, and the ordering of Zn/Cd forms complex commensurate superstructures. In the compound ht-Sb_2Zn_{3-x} the Sb network is modulated due to a slight icosahedral mismatch, and the combination of the two effects leads to a very complex arrangement indeed. The second compound, $Ce_{13}Cd_{58}$ is a ortho-hexagonal approximant to the stable binary $CaCd_{5.7}$ type quasi crystals. Here the incommensuration is driven by two coupled mechanisms, the exchange of a Cd_2 dumbbell by a single Ce atom, and the ordered partial occupancy of Cd_8 cubes.

s3.m12.o1 **Direct Imaging of Phason-Related Disorders in Decagonal Al-Ni-Co By Scanning Transmission Electron Microscopy**. Eiji Abe[a] and Stephen J Pennycook[b], [a]*National Institute for Materials Science, Japan,* [b]*Oak Ridge National Laboratory, USA. E-mail: abe.eiji@nims.go.jp*

Keywords: Quasicrystals; Electron Microscope; Atomic Structure

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 negibor 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.

We describe the details of quenched phason disorders in the decagonal $Al_{72}Ni_{20}Co_8$ by recently developed super- resolution STEM (aberration correction of the objective lens has successfully achieved the sub-Ångstrom resolution). Because ADF-STEM provides the incoherent images that can be well described by a convolution between the scattering object and the probe-intensity function., atomic structures can be directly addressed by a simple deconvolution procedure. Deconvolution using maximum entropy (ME) algorithm gives a safest, least possible structure that fits the experimental image. Figure 1 shows the result after ME-deconvolution on aberration-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.



[1] Abe, E., Pennycook, S. J. & Tsai, A. P. (2003). *Nature* **421**, 347.
Fig.1 STEM image (processed) of a decagonal $Al_{72}Ni_{20}Co_8$.