Short-Term Visit in Kyoto (Prof. Hiroshi Kageyama Group)

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Funded by the Mixed-Anion ASPIRE programme, we had the opportunity to be hosted by the Kageyama group in Kyoto University for two weeks (4/7-4/18). We are part of Professor Goodwin's group and are specialised in scattering and structure solutions. As part of the ASPIRE programme we are applying these techniques to new, mixed anion compounds that show short-range ordering and correlated disorder.

The objectives of this trip were two-fold. First, to discuss possible collaborations and research plans with the researchers from the Kageyama laboratory. There are many different avenues of research within this group and we think there should be many possible areas for productive collaboration. The second, more immediate goal, was to rationalise the structure of HfZnSb, where the diffuse scattering measurements showed signs of non-random ordering.

From the first day, we discussed possible projects with Professor Hiroshi Kageyama, Associate Professor Tong Zhu, Associate Professor Suguru Yoshida and Assistant Professor Daichi Kato. We had the honour of being the first to sign Professor Kageyama's ASPIRE project Daruma. It was also very interesting to attend the group's kenso where we were impressed by the wide array of both experimental and theoretical research. Talks ranged from oxynitride exploration via topochemical reactions, calculation of phase diagrams using DFT and oxyhydride exploration. We also had the opportunity to give respective talks on our own research. Although our research themes may seem different, we believe there is significant overlap in applying our techniques and methodology to the mixed-anion systems of the Kageyama group. The use of a slack channel during the kenso to facilitate questions (and allowing it to be posed in any language), is a brilliant idea. It makes it very easy for all to participate and contribute to these research meetings. We also noted how the questions were geared to constructive steps that the researcher could implement readily.

Fig 1. The signing of the Daruma.

Fig 2. Lunch with Prof. Kageyama, Assistant Prof. Kato and Dr Mahato.

Throughout our stay, we were generously hosted in one of the main offices and had the pleasure of many fruitful discussions with the group members as well as several lunches with Professor Kageyama which we were particularly appreciated. Possible future collaborations discussed include an order/disorder switching (and lack-thereof) in PhD student Shumma Kozaki's systems containing Sb—Sb bonds, the changes in symmetry with temperature of the mixed $Bi_{2-x}Sb_xYO_4Cl$ system of PhD student Artem Gabov and the correlations in the dynamics of systems with Associate Professor Tong Zhu.

For our second aim, we think we have a relatively good model for the diffuse scattering, and therefore the short-range ordering of HfZnSb. The Zn-Sb layers are not random, with the short-range ordering driven by minimisation of local strain; slight Zn—Zn repulsion and atomic displacements and relaxation. This model can of course be improved, but the diffuse match indicates that the main features are captured well by these interactions.

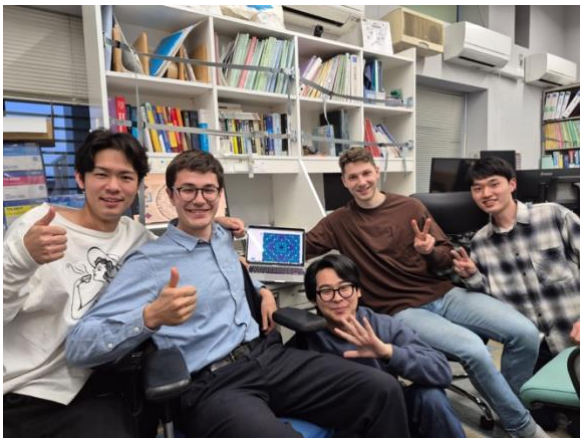

Fig 3. Celebrating with Shumma, Kotaro and Ryotaro our HfZnSb model.

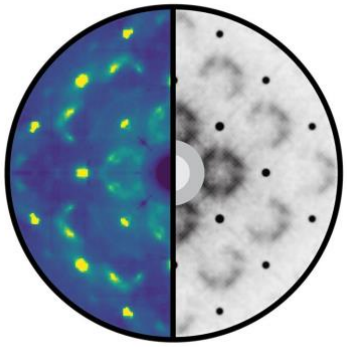

Fig 4. The current diffuse match comparing experiment with simulated.

We are extremely grateful to the ASPIRE program for supporting our visit to Kyoto and to the Kageyama group for generously hosting us. We had an extremely productive and enjoyable time here and will both look back fondly on our stay in Kyoto.

誠にありがとうございました.