Session X - Thursday, September 3 - late afternoon

PL9

STACKING DISORDER IN NATURAL CLAYS AND OTHER LAMELLAR STRUCTURES

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Layered minerals and materials are ubiquitous and characterized by the frequent occurrence of stacking defects. In particular, interstratification (or mixed layering), or intimate intergrowth of layers differing by their layer thickness and/or internal structure, and stacking faults, both random and well-defined, are especially common. These defects strongly impact the reactivity of lamellar materials. In addition, they may record the conditions of mineral (trans)formation.

Determining their nature, abundance, and possibly their distribution is thus an essential step of their structural characterization in the scope of understanding their reactivity. Over the last decades, modelling of X-ray diffraction profiles has proved to be a unique and precious tool allowing such a detailed structural identification of defective lamellar structures. This presentation will outline how our understanding of defective structures and mixed layers has improved over the last decade or so and describe some of the new perspectives opened by this improvement.

S10-L1

TWINS REVISITED: QUINARY TWINS AND BEYOND

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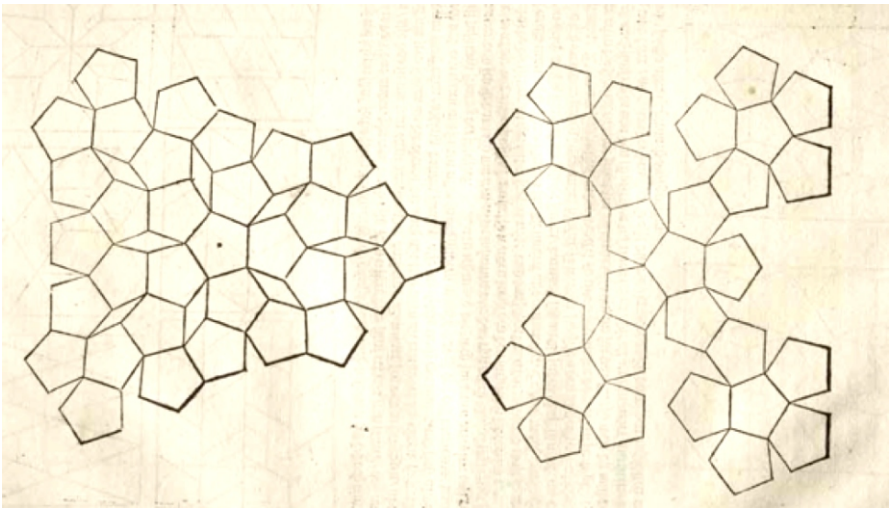
We define twin as being an external operation between two identical crystals that share a fraction of the atomic structure with no discontinuity from one crystal to the other. This includes merohedral twins, twin by reticular merohedry as well as coherent twin by contact where only the habit plan is shared by the two adjacent crystals (epitaxy). Interesting and original cases appear when the invariant substructure is built with positions belonging to a same Z-module (irrational projection in d-dim space of a N-dim lattice, with N > d) as, for example, the quinary twin structure (C5-module) first drawn by Albrecht Dürer (De Symmetria... Humanorum Corporum 1525).

We will show that the Dürer twins, once defined in 5-dim space, is a pure merohedral twin, in the sense of Georges Friedel, leaving the 5-dim lattice invariant. This analysis will be generalized to the Cn-modules.



Original drawings of pentagonal structures created by A. Dürer (De Symmetria... Humanorum Corporum 1525).

S10-L2

A HIGH-ENTROPY ALLOY CAN BE A SUPERCONDUCTOR: AN ANALYSIS OF THE PHYSICAL PROPERTIES OF $Ta_{34}Nb_{33}Hf_8Zr_{14}Ti_{11}$

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High-entropy alloys (HEAs) [1,2] are a modern alloy design strategy that utilizes the disorder of solid solution phases to stabilize new and unique structures. They are based on the observation that in a random mixture consisting of four or more principal elements (elements in similar concentrations, from 5% to 35% each) the entropic term in the Gibbs free energy $G = H - TS$ can be sufficiently large to stabilize simple structures (bcc, fcc, simple hexagonal) with randomly filled sites rather than more complex intermetallics. While studies have found technologically favourable structural and mechanical properties [1], the physical properties have not been particularly interesting – low electrical and thermal conductivity (due to large scattering on disorder) and standard para- or ferromagnetism [3].

The physical properties of $Ta_{34}Nb_{33}Hf_8Zr_{14}Ti_{11}$ have, however, turned out to be much more intriguing [4] as this alloy is *the first HEA known to exhibit a transition to a superconducting (SC) state*. Our sample had composition $Ta_{34}Nb_{33}Hf_8Zr_{14}Ti_{11}$ (EDS spectroscopy) and its structure was average body-centered cubic with lattice parameter a = 3.36 Å (determined by powder XRD). Since the lattice properties – namely, the lattice parameter and Debye temperature – conform to Vegard's rule of mixtures, we have interpreted the mixing to be completely random. The measured electrical resistivity, heat capacity and magnetic measurements indicate that $Ta_{34}Nb_{33}Hf_8Zr_{14}Ti_{11}$ is a type II superconductor with a critical temperature of T_c 7.3 K, a lower critical field $_0 H_{c1}$ 32 mT and an upper critical field of $_0 H_{c2}$ 8.2 T. Further analysis of the specific heat gives us an energy gap in the electronic density of states (DOS) at the Fermi level of 2 2.2 meV and an indication that $Ta_{34}Nb_{33}Hf_8Zr_{14}Ti_{11}$ is close to a BCS-type phonon-mediated superconductor in the weak electron-phonon coupling limit. Moreover, due to the large amount of disorder we are tackling with a "dirty" superconductor. While the transition from normal to superconducting state is associated with a decrease in energy, this decrease is not sufficient to compensate the weakening of the entropic stabilization mechanism at low temperature and stabilize $Ta_{34}Nb_{33}Hf_8Zr_{14}Ti_{11}$. Therefore we predict that $Ta_{34}Nb_{33}Hf_8Zr_{14}Ti_{11}$ is metastable at room temperature and below (albeit extremely long-lived).

To conclude, let me state two open questions regarding superconductivity in HEAs. Firstly, how wide (or narrow) is the composition range for HEA superconductors and does it enable us to optimize their properties? Secondly, the mechanism behind this superconductivity is not yet understood - what is it?

1. J.W. Yeh, et al., *Adv. Eng. Matter*., **6,** (2004), 299.
2. J.W. Yeh, *Ann. Chim. Sci. Mat.*, **31**, (2006), 633.
3. M.H. Tsai, *Entropy*, **15**, (2013), 5338, and references therein.
4. P. Koželj, S. Vrtnik, A. Jelen, S. Jazbec, Z. Jagličić, S. Maiti, M. Feuerbacher, W. Steurer, and J. Dolinšek, *Phys. Rev. Lett.*, **113**, (2014), 107001.

S10-L3

ORDER AND COHERENT DIFFRACTION

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We are generally taught that a crystal is disordered if its diffraction pattern consists in Bragg reflections and diffuse scattering. However, more insight in diffraction theory shows that the diffraction pattern of a crystal can exhibit diffuse scattering while the crystal is perfectly ordered. This is the case of the Rudin-Shapiro sequence, whose pair correlation function is similar to a random sequence one.

In this paper, we show that this property is true only for infinite systems. Indeed, finite and thus real crystals exhibit **speckles patterns**, which can be measured by coherent diffraction. With the help of the Rudin-Shapiro sequence, we demonstrate that the intensity distribution of such patterns contains information on high-order correlation functions, which are irrelevant in infinite crystal diffuse scattering pattern. The effect of dimensionality is also explored.

This surprising result indicates that the concept of order should be revisited in the light of coherent beams.

S10-L4

STRONG ELECTRON CORRELATIONS IN A TWO-DIMENSIONAL HUBBARD MODEL ON THE PENROSE LATTICE

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Recently, interesting low-temperature properties have been observed in the quasicrystal $Au_{51}Al_{34}Yb_{15}$ and its approximant $Au_{51}Al_{34}Yb_{14}$. In the former compound, the specific heat and susceptibility exhibit power-law behaviour with a nontrivial exponent at low temperatures. In contrast, the approximant with the periodic structure shows conventional heavy fermion behaviour. These findings suggest that electron correlations and the quasiperiodic structure play a crucial role in stabilizing quantum critical behaviour at low temperatures. Therefore, it is desirable to clarify how electron correlations affect low temperature properties in quasiperiodic systems.

To clarify how electron correlations affect low temperature properties in strongly correlated quasi-periodic systems, we study the repulsive Hubbard model on two-dimensional Penrose lattice. The model Hamiltonian is given as

$$H \quad t(c_i\ c_j \quad h.c.)\ \ U \quad n_i\ n_i$$
$$\langle i,j\rangle,$$

where $\langle i,j\rangle$ denotes nearest neighbour site, c_i (c_i) is the creation (annihilation) operator of a fermion at the *i*th site with spin , n_i $c_i\ c_i$ t is the hopping integral, and U is the Coulomb interaction. First, we study Mott transitions in this model [2] by means of the real-space dynamical mean field theory (RDMFT) [3] which incorporates local electron correlations. We find that geometrical structure in the system induces nontrivial renormalization in the metallic state close to the Mott transition point. As the temperature decreases, intersite correlations as well as local correlations should be important, and the theoretical approach beyond DMFT is necessary to discuss low temperature properties. Here, we make use of the real-space dual fermion approach [4], which enable us to investigate intersite correlations in quasi-periodic system. We then study how magnetic correlations develop at low temperatures.

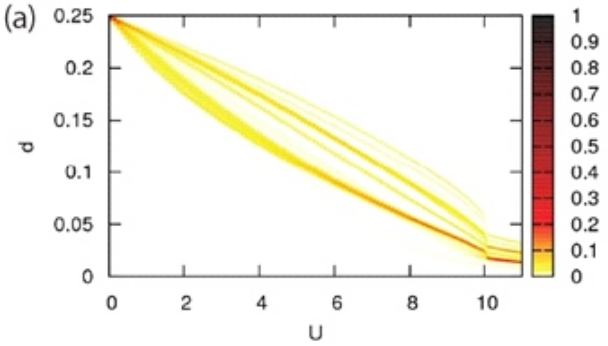

Figure 1. Density plot of double occupancy as a function of interaction strength U/t in the half-filled Penrose-Hubbard model with 4481 sites when $T/t = 0.05$.

1. K. Deguchi., *et al*., *Nat. Mater.* **11**, 1013-1016 (2012).
2. N. Takemori, and A. Koga., *J. Phys. Soc. Jpn.* **84**, 023701 1-5 (2015); N. Takemori, and A. Koga., *J. Phys.: Conf. Ser.* **592** 012038 (2015).
3. A. Georges et al., *Rev. Mod. Phys* **68**, 13 (1996).
4. A. N. Rubtsov et al., *Phys. Rev. B* **77**, 033101 (2008).