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Shifts:	**Local contact(s)**: Luigi Paolasini & Alexei Bosak	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Daniel Chaney*, University of Bristol

Sophie Rennie*, University of Bristol

Gerard Lander*, European Commission Joint Research Centre Institute for Transuranium Elements

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Exploring the phonon dispersion of γ-(UMo) with grazing incidence IXS

D. Chaney[1, 2], S. Rennie[1], L. Paolasini[2], A. Bosak[2], G. H. Lander[3] and R. Springell[1]

[1] *University of Bristol, Tyndall Avenue, Bristol, BS8 1TL, UK, email: daniel.chaney@bristol.ac.uk*
[2] *European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble, France*
[3] *Institut Laue-Langevin, 71 Avenue des Martyrs, 38000, Grenoble, France*

The U-Mo system has been studied for at least 50 years since it was identified as potential low enriched fuel for research reactors, which require a high flux, avoiding the use of high-enriched ^{235}U and the associated proliferation risk. The phase diagram suggests that for compositions between 15 at.% and ~30 at.% Mo the *bcc* structure (which for pure U is stable only above 775°C) may be stabilized at room temperature [1]. However due to the lack of single crystal samples, and perhaps also the complexity of the system, there has been little recent work on the fundamental character of the system.

Building on previous work [2], epitaxial films have been grown and characterized at Bristol, utilizing a Nb buffer deposited on A-plane sapphire to provide the required epitaxial match. Thicknesses between 75 and 300 nm for compositions of 22, 23, 29 and 35 at.% Mo have been synthesized with the epitaxial relationship $(110)_{Nb}||(110)_{U-Mo}\ [110]_{Nb}||[110]_{U-Mo}$.

These films have been part of three different synchrotron experiments. The first was a study of the *diffuse x-ray scattering* to determine the correct crystallographic structure. In agreement with Yakel [3] the structure between 22 and 30 at% Mo is a modification of the γ (*bcc*) structure denoted γ^s. Importantly, in this structure, there is *short-range disorder* with the structure described by doubling the original γ (*bcc*) unit cell and allowing some atoms to be displaced an amount δ from their special positions. The resulting *average structure* is based on the $I\bar{4}3m$ space group. The diffuse signal arises due to deviations from the ideal

structure and is a factor of ~100 weaker compared to the ideal *bcc* reflections, and thus often missed using conventional x-ray scattering techniques

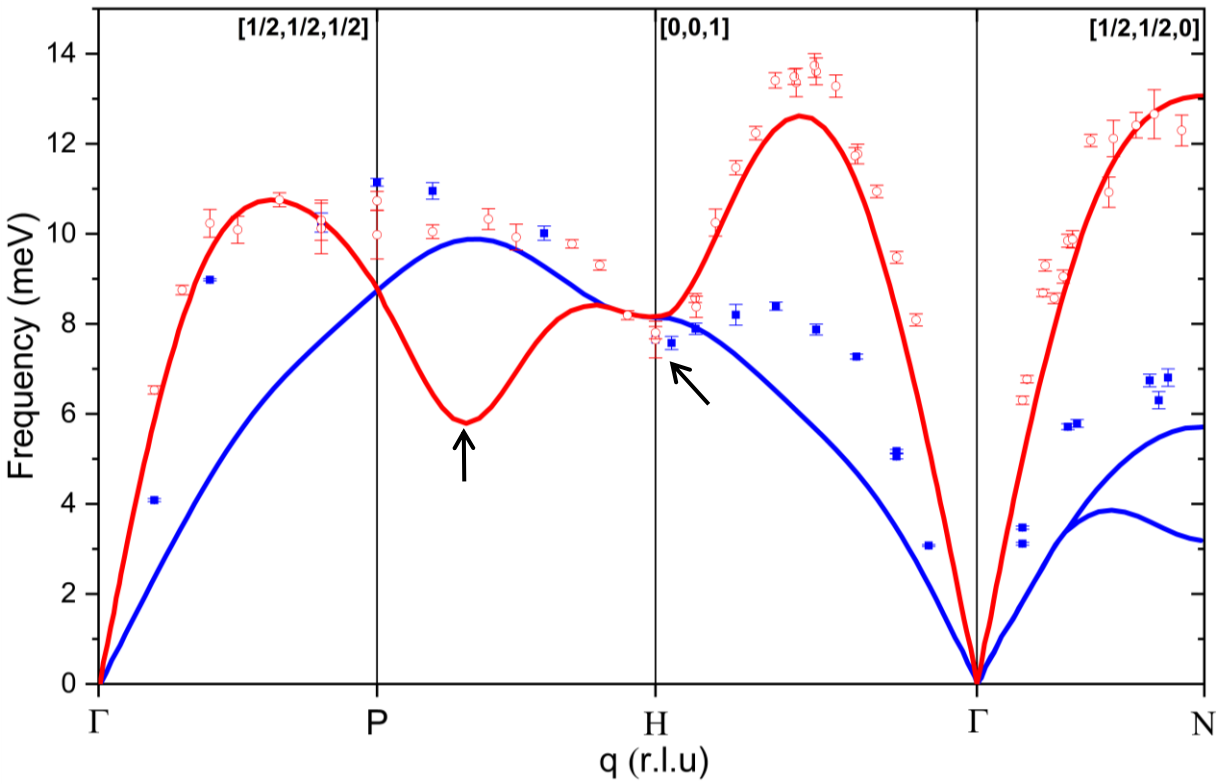

Fig.1 Theoretical dispersion shown as solid lines, experimental points as open red circles and filled blue squares for LA and TA modes respectively. Arrows are discussed in text.

Subsequently inelastic x-ray scattering studies have been performed at the ID28 beamline to explore the phonon dispersion in the 29 at.% Mo film using grazing-incidence techniques [4]. All major symmetry directions have been explored for both the longitudinal (LA) and transverse (TA) acoustic branches and generally compare well with first-principle calculations [5]. Notable differences (indicated by arrows) include the presence/absence of softening at the H and 2/3[1,1,1] positions respectively. Both provide an insight into the underlying electronic structure of the system. A strong variation in linewidth is also reported and is attributed to the short-range disorder. The IXS studies will form the basis of the current presentation with results discussed in the context of the first study.

References:
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