## **Dr Colin Carlile, Director, Institut Laue-Langevin.**

17 March 2005

Dear Director,

## Resignation as Instrument Group Leader for Diffraction

I respectfully request that you replace me as Diffraction Group Leader at your earliest convenience. I find that unfortunately I no longer represent your views on the future development of diffraction instruments at the ILL, and I believe that you would be better served by some one else.

Over the past year, IGLs and the ILL Science Division, at the request of the Science Council, have been working on proposals for future instrumentation at ILL. We collected numbers of user groups, proposals, publications, highly cited papers, and formulated suggestions for the future evolution of instruments. A broad consensus was reached, the results were presented to the Science Council 6 months ago, and final versions of our papers were completed earlier this year. In my paper, on http://www.ill.fr/dif/AlanHewat/ I remarked that only one thermal beam tube (H11) was available for Diffraction in addition to the thermal guides. I stressed the importance of an additional thermal beam, and an upgrade to modern super-mirror guides, as has already been started for the SALSA strain scanner project, VIVALDI and D1A/D1B.

Yet this week, in my absence, a radical last minute proposal was drafted for immediate submission to the Science Council. As you wrote, you strongly prefer a proposal to convert ILL thermal guides to cold guides fed by a 3<sup>rd</sup> cold source. You will know that our group already gave up one of our two thermal beam tubes for the construction of the 2<sup>nd</sup> cold source, forcing us to build all of our high performance thermal instruments on the single remaining beam tube H11. You will know that thermal neutrons are essential for atomic resolution, and that our continuous reactor source has a clear advantage over pulsed sources such as SNS for medium resolution, high flux instruments, according to the arguments for DRACULA accepted by the last two ILL Instrument Committees, and endorsed by the Science Council.

In this letter I will set out alternative proposals for the future evolution of ILL beam positions. I will argue that super-mirror thermal guide tubes represent a unique advantage for ILL, and that the two existing cold sources should be sufficient for our future development. I will argue that instead of constructing a 3<sup>rd</sup> cold source, which will be expensive and further complicate reactor operation, we should ensure that existing guides are rebuilt to the highest standards, avoiding the disasters represented by the failures of the H112 cold guide, the D11 replacement cold guide, the large intensity loss in the LADI guide, and most recently the implosion of the CENG super-mirror guide. Good guides are essential; new guides are not. Already we have shown that by replacing just part of the H22 guide we have obtained a gain of 40% at thermal wavelengths; the total gain is expected to be 400% with the complete H22 super-mirror guide in place. It is naturally much more difficult to obtain such large gains with cold guides.

New super-mirror thermal guides are also of interest to the 3-axis and the TOF groups. A new high flux 3-axis machine could be built with very low background on a new H23 thermal guide. The troubled IN4 spectrometer would best be re-located far from the reactor on a thermal super-mirror guide, where again the background would be reduced and the chopper configuration would not be limited by reactor safety. New super-mirror thermal guides will of course be of great benefit for unique Diffraction instruments such as the new SALSA strain scanner and the VIVALDI image plate machine, as well as for "workhorse instruments" like D1A and D1B which contribute so much to ILL's publication and student training programme.

Moving IN4 to a super-mirror thermal guide would allow that beam tube to be used like H11 for a pair of world leading machines, DRACULA plus a new polarized neutron diffractometer D30 with a large area detector that could be used for magnetic studies on both single crystals and powders. Tests with a He3-filter on D1B have already demonstrated the interest of such a machine, and D3 itself was originally located on the thermal beam tube taken for the second cold source. A thermal polarized neutron diffractometer with a large PSD would greatly broaden the user community in this area with little competition from pulsed sources. This scenario would eventually make possible independent instruments D4 and IN1 on separate hot beam tubes, as proposed by the Science Council, and would also remove the conflict between the siting of DRACULA and the Neutron Tomograph.

Finally the limited demand for new cold guides could also be addressed. Calculations show that the best position for the new IN16 would be on it's present guide on the second cold source, which appears to have a flux advantage over the vertical cold source. This might mean the re-location of CRG instruments, but it has always been accepted that public instruments should have priority. Building a complete new cold guide dedicated to IN16 would not give more flux, and would limit possibilities for a future new D33 small angle scattering machine. Calculations also show that the new LADI would best be located on its present position provided that the losses in a small section of that guide could be recuperated – a much less expensive and more efficient solution than building a new vertically curved cold guide.

In short, the proposal to build a 3<sup>rd</sup> cold source instead of upgrading the thermal guides with super-mirrors would be expensive, is not needed in the foreseeable future, and would paint the ILL into a corner dependent on cold neutron TOF machines at a time when such machines will be increasingly challenged by their pulsed source equivalents. It would make the large European diffraction community increasingly dependent on the ISIS pulsed source, which might then become the de facto ESS, even if it is itself uncompetitive with the new American and Japanese accelerators. It would greatly limit future possibilities for the ILL to develop new high flux machines at atomic resolution, using our new skills in constructing large detectors and focusing monochromators to obtain unmatched neutron fluxes on the sample.

I am very proud of the work we have accomplished together in the past 5 years, and in the 20 years that I have served either as Diffraction group co-ordinator or Diffraction group leader, and I am naturally saddened to leave under these circumstances. In the last 5 years we have rebuilt most of the diffraction instruments, often with external money.

My own pet project, D2B attracted grants from the EPSRC (Prof Attfield) and the French ministry (Prof Raveau). It is the world's first high resolution 2D detector, and has already produced a gain of 600% in efficiency, though similar machines have now been constructed at Munich and in Australia. The D19 project was also financed by additional money from EPSRC, and has already produced similar gains, with a projected gain factor of x20 when the full detector is completed this year. The high flux powder machine D20 has also been upgraded with new monochromators and high take-off, allowing high resolution at very high count rates; our experiments on the solid state chemistry of explosive reactions have shown that D20 is currently the fastest diffractometer in the world. These three machines all share a single thermal beam tube, and even in the last 5 years during these upgrades, together produced more scientific papers than all the other thermal beam tubes combined. D2B has also produced most of the ILL' most cited experimental papers.

In the past 5 years, we have lead the world in developments with polarized neutrons with the D3 Millennium project, He3 filters and polarization analysis that is unique for the determination of complex magnetic structures. We have upgraded D9 and D10 with smaller 2D detectors, and exceptional low temperature 4-circle refrigerators. A Diffraction group scientist has lead the development of a new pressure cell, and as a whole the diffraction group has lead in the replacement of the famous orange cryostat by new pulse tube refrigerators. Only a little earlier we rebuilt the liquids and amorphous diffractometer D4, and have now established long term scientific support in this important area.

On the thermal guide tubes in question, we have pioneered new types of single crystal diffractometers, the image plate machine VIVALDI and the CCD camera machine Orient Express. We negotiated directly with Fujii to obtain special neutron image plates, x3 as efficient as those purchased for FRM-2 at the same time; we obtained a sufficient number for VIVALDI and its Australian copy, as well as the new LADI-3 at ILL. These machines demonstrate the great advantage of the continuous reactor source where a white beam can be used, but with continuous high flux on the sample, rather than pulsed.

Again on the thermal guides we have constructed the unique new strain scanner SALSA, using curved perfect crystals to focus on a very small sample volume, a 2D detector to collect the complete diffraction profile, and a novel hexapod system capable of positioning half tonne samples to a precision of 10 microns! We pioneered the first neutron strain scanning experiments on D1A, which together with D1B have formed the basis for the strong growth of the European neutron diffraction user community.

I am not opposed to discussing any new idea, even that of replacing some of these achievements with a new cold neutron guide system. But I am disappointed by the way this was done. The Science Council papers had been finalized before I left France on the 8<sup>th</sup> March, yet barely 1 week later meetings were held to which my official replacement was not invited, and this radical new proposal was finalized for submission to the Science Council at the last minute without telling me or diffraction group scientists. My absence at that time was unfortunate, but it was my only vacation in 2 years, and probably my last chance to take my seriously ill wife to see her mother, herself too old to travel from Australia. You can imagine then my reaction, and my desire to have nothing to do with this proposal conceived in haste and no doubt repented at leisure.

Although I am regretfully resigning as Diffraction group leader, I wish to continue working at ILL until my retirement the year after next. I wish to complete the DRACULA project, which was highly recommended by the last two Instrument Subcommittees and the Science Council itself. This is the kind of machine that represents an important part of the future of ILL, making use of the continuous neutron source to deliver very high fluxes to the sample, fluxes that will not be matched by the Americans and until the complete ESS can be built. This will be achieved by focusing in both real and reciprocal space, using relatively large wavelength spreads, which are not possible on TOF machines because of resolution requirements. Together with the large fast 2D detectors as developed for D19, these kind of machines will allow ILL to continue to lead the world in diffraction.

That is my ambition and my decision, and I will try to make it my achievement.

Sincerely,

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ILL Diffraction Group Leader