Report of the Working Group on Novel Concepts and Materials

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1. MODERATOR THEORY NEEDED

This session was intended as a session to present ideas that had not yet been fully explored, as well as a place for discussion of topics that did not readily fit in any of the other workshop sessions. The first part of the session focused on moderator materials. During the course of the discussions of some novel potential moderator materials it became clear that there was not even agreement on what makes a good moderator for cold neutrons at short-pulse sources. There were two competing diametrically-opposed schools of thought.

One school of thought supported the "conventional" type of moderator materials having large inelastic cross-sections in the energy transfer region comparable to the temperature of the moderator (~20 K for a cold moderator). In this type of moderator, the neutrons will be partially thermalized producing a leakage spectrum with a Maxwell-Boltzmann like distribution with a neutron temperature that is higher than the temperature of the material, but is still very low. Solid methane is an example of this kind of moderator (see poster by Erik Iverson et al.).

The other school of thought supported the "slowing-down" type of moderator materials having a large inelastic cross-section at energies above the temperature of the moderator, but a very small cross-section in the energy region comparable to the temperature of the moderator so that the cold neutrons can easily leak out. In this type of moderator, the leakage spectrum is "colder" than the flux in the moderator, and is not Maxwellian since the neutrons never approach thermal equilibrium with the moderator material. Liquid para-hydrogen is an example of this kind of moderator.

The leakage spectrum for the first type is "hotter" than the temperature of the moderator, while that for the second type is "colder" than the effective temperature of the neutrons in the material. It is clear that we do not yet understand which type of mechanism produces the better results. A much improved understanding of the neutronic performance of these two very different mechanisms for producing cold neutrons is needed before we can really understand what kinds of materials should make the best moderators for cold neutrons.

2. MODERATOR MATERIALS

A number of materials were suggested as candidate moderator materials. Many of these were suggested on the basis that they have many low-frequency modes, giving rise to the large low-energy inelastic cross-section required in the "conventional moderator" model. This category includes the metal hexaamines such as $Ca(NH_3)_6$), mellitene (hexamethyl benzene), krypton in solid methane, and methane-ice clathrate.

Torben Brun pointed out that at 20 K everything except the quantum liquids is solid, so there are no low-frequency diffusive motions for thermalization of the neutrons. Thus we must rely on quantum systems such as free rotation or tunneling for thermalization in cold solid moderators. Torben suggested the metal hexaamines as candidate moderator materials of this type. These materials have free rotations with level spacings in the meV range. For example, in $Ca(NH_3)_6$ all 6 H_3 groups are freely rotating. This material is metallic, and so is easy to cool. The hydrogen density is $\sim 5\times10^{22}$ cm^{-3}, which is higher than that in methane. Potential drawbacks including radiation damage, stability, and possible formation of hydrazine would have to be investigated. The absorption cross-section of nitrogen might also be a problem.

Jack Carpenter suggested mellitene (hexamethyl benzene) as a potential moderator material that also has a high hydrogen density and many low-frequency modes. It has the additional advantages that it is solid at room temperature and so is easy to work with. It should be straightforward to make small pellets which could then be used in a mixed mellitene-liquid hydrogen moderator.

Jack also brought up an idea attributed to Peter Egelstaff, which involves alloying of a small amount of krypton in solid methane. This is known to promote free rotation of the methane molecules, many of which are otherwise orientationally ordered. This should increase the number of low-frequency modes available for energy transfer.

Earlier in the day Frans Trouw suggested the use of methane-ice clathrate for moderators, and this topic was revisited in this session. This is a material that is currently of considerable interest for methane storage. This material can be made as small particles at elevated temperatures (somewhat below the ice freezing point), and is stable as long as it is kept at sufficiently low temperatures. This again might prove useful combined with liquid hydrogen in a mixed moderator.

Tim Broome brought up the idea of using high-pressure (200-300 bar) hydrogen to get higher hydrogen density in supercooled hydrogen moderators. However, he later pointed out that some calculations have indicated that the performance improvements might not be as much as expected.

Jack Carpenter noted that the early calculations of Gary Russell and the more recent calculations of Lowell Charlton have shown the desirable characteristics of a composite water-liquid hydrogen moderator. When the layer of liquid hydrogen is sufficiently thin the water spectrum supplements the liquid hydrogen spectrum, resulting in significantly enhanced intensities around 100K. Such composite moderators may be a viable alternative to liquid methane moderators for use at higher power sources.

Jack Carpenter mentioned that George Stirling had reported a long time ago that adding nitrogen to liquid or solid methane increases the resistance to radiation damage in these materials. Apparently no one has yet followed up on this suggestion for methane moderators.

Metal hydrides may have some possibilities as moderator materials because of the high hydrogen densities, but there are no low-frequency modes of the hydrogen to aid in cooling the neutrons to temperatures needed for cold moderators. However, Günter Bauer pointed out that nanocrystalline metal hydrides have additional hydrogen trapped between the grains, and this gives rise to some lower frequency modes in addition. These materials are resistant to radiation damage and are easy to cool. However, because the number of low frequency modes is still relatively small, these materials are probably more suitable as premoderators than as cold moderators.

László Cser suggested the use of amorphous graphite fibers, which have high thermal conductivity and are easily cooled. They also have an appreciable inelastic scattering intensity at low energies (Jack Carpenter showed data indicating that the density of states varies approximately linearly with energy). Thus they might be useful as moderators. However, Tim Broome pointed out that experience with the ISIS liquid methane moderator indicates that the carbonized amorphous material left behind from radiation damage of the methane has poor moderating properties. Since the material in the ISIS moderators is expected to be rather different from that in the amorphous carbon fibers, this probably does not constitute conclusive evidence against the use of amorphous carbon fibers as moderating material.

3. PREMODERATORS

Evgene Shabalin suggested that a heavy metal be used as the first premoderator, because these materials have a larger cross-section at very high energies and so would be most effective for the first collision after the high-energy neutron is produced. Such materials also attenuate gamma rays. Günter Bauer and Tim Broome pointed out that the target material itself typically fulfills this role at spallation sources, and that this is partially responsible for the softer spectrum produced by uranium targets. Gary Russell mentioned some measurements that have indicated that use of additional heavy metal as a premoderator is not very effective.

Günter Bauer suggested that nanocrystalline metal hydrides, described above under moderators, might be particularly good for use as premoderators. Because of the properties described above, they look very promising for this role.

There was a considerable amount of discussion about the role of the premoderator in reducing the amount of energy deposited in the moderator material. Calculations for the IPNS Upgrade geometry and for the JHP geometry have predicted different magnitudes for this effect. Noboru Watanabe reported that measurements at Hokkaido have indicated that most of the energy deposited in the moderator comes from thermal neutrons, since the energy deposition rises significantly when the decoupler is removed. This would imply that the premoderator should be less effective in reducing energy deposition in the moderator material.

Noboru Watanabe led a discussion of the desired thickness for premoderators. Making the premoderator thick (~3 cm in the Hokkaido measurements) gives maximum reduction of energy deposition in moderator, while a thin premoderator (~1.5 cm in the Hokkaido measurements) gives the shortest pulses. Either of these conditions produces about the same peak flux. Evgene Shabalin stated that the premoderator thickness for the IBR-2 solid methane moderator was 9 cm, since pulse width was not a concern and maximum reduction of energy deposition was important there.

4. DECOUPLERS

Trevor Lucas brought up the topic of fluid decouplers. Fluid decouplers would have the advantage that they are easily cooled, and their decoupling properties can be readily changed. However, they would probably add to the complexity of the moderator assembly and would introduce another potential source of performance instabilities. Some materials suggested include solutions of gadolinium sulfate or boric acid, ^{6}Li-^{7}Li mixtures, and liquid mercury.

Bob Williams noted that sheets of ^{10}B-Al alloy are commercially available from Eagle-Picher in Oklahoma. This material presents some interesting structural possibilities for decouplers, since it is easily cooled, has good thermal conductivity, and could be made as part of moderator can.

Günter Bauer pointed out that the target material itself could be a good decoupler on the side of the moderator facing the target. An example of this is a liquid mercury target.

5. STRUCTURES AND OTHER TOPICS

Tim Broome and Günter Bauer reported that curved guides can completely prevent any fast neutrons from reaching the sample. Thus, for moderators illuminating only curved guides it becomes reasonable to again consider the use of slab moderators. This would provide a gain of ~2 in intensity. With premoderators it may be possible to operate solid methane moderators in this configuration at appreciably higher power target stations, so long as the power remains below some as-yet-undetermined limit. Premoderator thickness can be adjusted to minimize power deposition in the solid methane moderator, so long as the pulse width remains within the desired limits. Use of solid methane will produce a given neutron flux at ~1/3 the source power required to produce the same flux from liquid hydrogen. Thus it may be most effective to actually lower the source power into the range where solid methane moderators are viable.

Operation of high-pressure hydrogen moderators requires relatively thick walls for the moderator container. Even at just supercritical pressures the required wall thickness is substantial. Richard Lanza suggested the use of small diameter thin-wall tubing as the container for the hydrogen moderator. This might lead to substantially less material in the neutron beam.

Jack Carpenter raised the possibility of using single crystal sapphire as a window material, even for windows in high radiation fields. Recent measurements by David Mildner on an existing sapphire filter indicate no degradation in the neutron transmission of the sapphire after irradiation.

Richard Lanza pointed out that single crystal silicon nitride is very strong, and so can be used for very thin windows. However, neutronic and irradiation behavior have not been investigated for this material.

Trevor Lucas described a double aluminum window made by depositing thin aluminum layers on both sides of a piece of aluminum foam. Helium coolant can then be passed through the foam. This construction also adds some stiffness to the window. However, it was pointed out that any rupture would probably spread through both windows, so credit for double containment could not be claimed for such a window.

Grooved moderators were also a topic of discussion. Evgene Shabalin suggested using the sides of moderator grooves as guides to bring out more neutrons from the groove bottoms. It was pointed out that the geometries involved in typical grooved moderators would yield little gain from this approach. Jack Carpenter described recent calculations for moderators with vertical grooves. These calculations showed that for instruments viewing the moderator face at an angle the spectral intensity was essentially the same whether the grooves were horizontal or vertical. This was rather surprising considering that such instruments could not directly view much of the groove bottoms when the grooves were vertical. Careful study indicated that the sides of the grooves played an important role. Jack also pointed out that narrow-beam instruments such as reflectometers can be situated to view only the bottom of a groove, resulting in a significant flux gain at long wavelengths.

Another topic discussed was the effects of cooling the reflector. Jack Carpenter indicated that the reflector was cooled in the configuration initially operated at IPNS. Although no benefits were seen from cooling the reflector in this case, this configuration was not operated very long so such measurements were limited. In principle, cooling the reflector lowers the mean energy of the neutrons in the reflector, so that one can decouple at a lower energy to get more intensity while preserving the pulse width.

László Cser proposed the use of morphous graphite fibers as a replacement for the aluminum foam used to remove the heat from solid methane moderators. He also proposed surrounding the moderator with graphite to provide a reflector for all but the coldest neutrons. This would help ensure better thermalization but would lengthen the pulse, so this appears suitable only for long-pulse or steady-state sources.