JP0150581

JAERI-Conf 2001-002

ICANS-XV
15th Meeting of the International Collaboration on Advanced Neutron Sources
November 6-9,2000
Tsukuba, Japan

17.2

Sharp or Broad Pulse Peak for High Resolution Instruments ? (Choice of Moderator Performance)

[1]M.Arai, [2]N.Watanabe, [2]M.Teshigawara, [3]Y.Kiyanagi, [3]M.Ooi, [1]T.Kamiyama, [1]S.Itoh, [1]M.Furusaka, [4]K.Nakajima, [5]O.Yamamuro, [2]Y.Ikeda

[1]High Energy Accelerator Research Organization, 1-1 Oho, Tsukuba, Japan
[2]Japan Atomic Energy Research Institute, Tokai, Japan
[3]Faculty of Engineering, Hokkaido University, Sapporo, Japan
[4]Institute of Solid State Physics, Tokyo University, Kashiwa, Japan
[5]Faculty of Science, Osaka University, Toyonaka, Osaka, Japan

Abstract

We demonstrate a concept how we should choose moderator performance to realize required performance for instruments. Neutron burst pulse can be characterized with peak intensity, peak width and tail. Those can be controllable by designing moderator, i.e. material, temperature, shape, decoupling, poisoning and having premoderator. Hence there are large number of variable parameters to be determined. Here we discuss the required moderator performance for some typical examples, i.e. high resolution powder instrument, chopper instrument , high resolution back scattering machine.

§1 Introduction

For pulsed neutron source, total optimization in performance is a key issue. Performances of accelerator including intensity, repetition rate, proton beam width in time and space, target-moderator assembly, neutron beam transport including optics and instrument including detector, should be considered systematically and throughout. Even for MW-source, we should be careful to chose these performances. Otherwise, it easily sacrifices intensity and degrades the total performance of neutron source. Especially characteristics of moderator have direct influence to performance of instruments. Hence, in this article we are going to give a concept how we should chose moderator performances, peak height, peak width, rising slope, decay slope, peak tail and integrated intensity.

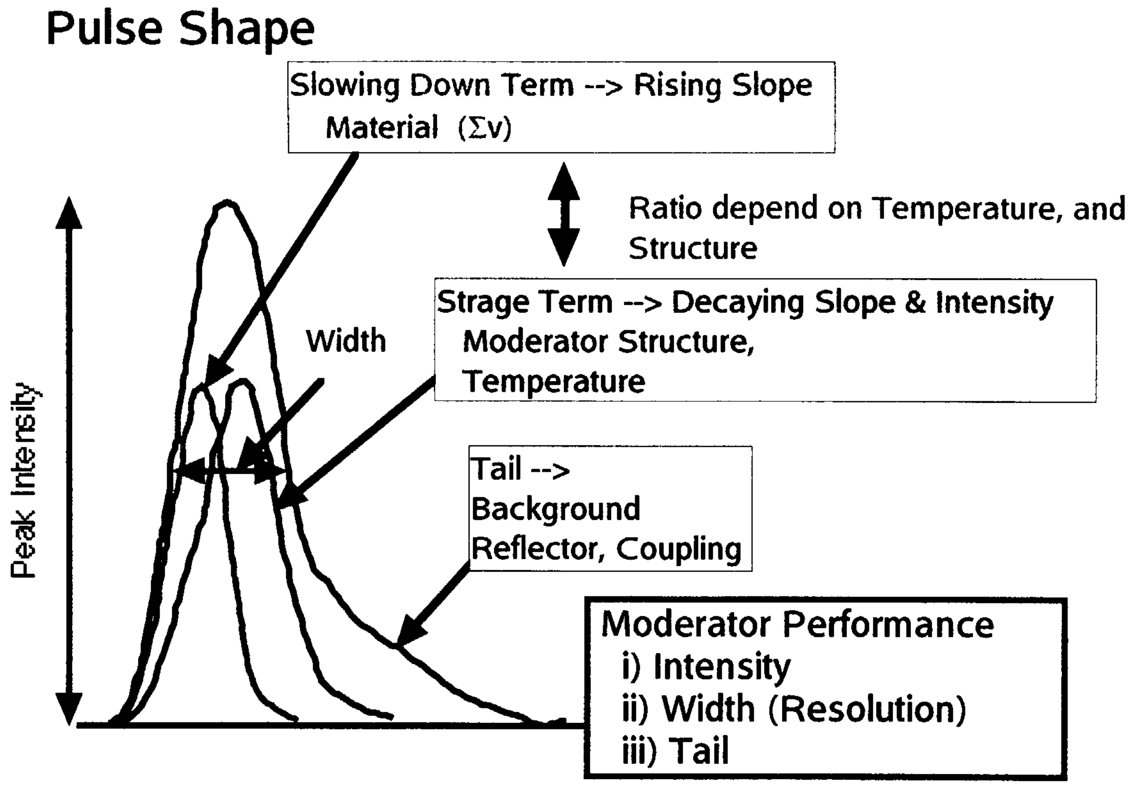

Fig.1 Structure of pulsed neutron peak

§2 Characteristics of pulsed neutron peak

It is a instructive manner to consider that neutron pulse peak is composed from two contributions [1], cf. Fig.1. One is the slowing down term, which determines the rising slope of peak structure. This term is determined by material of moderator and speed of neutron. Since adequate material for neutron moderator is limited, the slowing down term cannot have tailorbility, i.e. once moderator material is determined the slowing down term is determined. On the other hand, the another term, storage term can have tailorbility and the characteristics can be chosen suitably for required performance of instrument. This term can be easily tailored with moderator temperature, shape of moderator, decoupler, poisoning, facilitating pre-moderator etc. The storage term can essentially determine the peak width and peak intensity. Hence, how to control this term is the main task for moderator design work. There is, however, the third character of peak. This is tail, which turned out to be a background after Bragg peak in time-of-flight. Tails push up base line or background level when there are series of Bragg peaks in diffraction. Tail fill out and smear out valley between Bragg peaks. The character of tail can be controlled by choosing decoupling energy of decoupler between moderator and reflector.

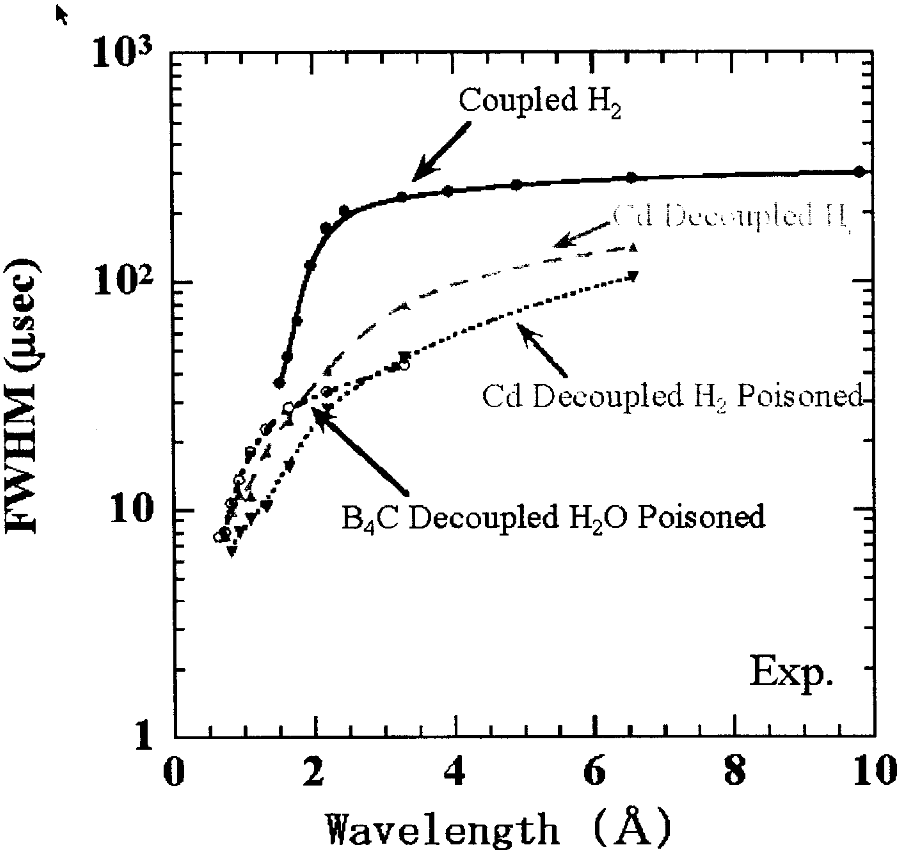

Fig.2 Peak widths for various moderators [2].

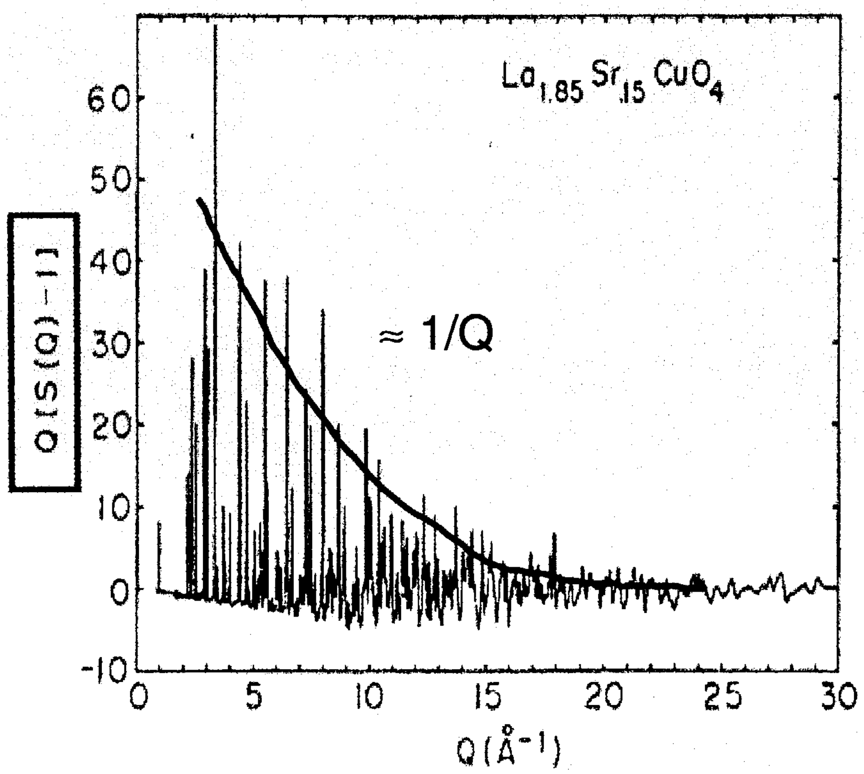

Fig. 3 A typical diffraction pattern on $La_{1.85}Sr_{0.25}CuO_4$ [3].

§3 Required Pulse Structure from instruments

In the previous section we pointed out that there are three issues for peak character, which we should choose them by moderator design for realizing a required performance of instruments. Those are 1) intensity, 2) width, 3) tail. In this secession, we consider several concrete cases of requirement for these issues.

3-1) High Resolution Powder diffraction

The most critical requirement for pulse width is raised from high resolution powder diffractometer. For this kind of instrument, having better resolution is more important than having higher intensity. However, we should set highest resolution is to be as much as intrinsic peak width due to size effect of crystallite. This is about $\Delta d/d \sim 0.03\%$. Therefore, this resolution is the meaningfully highest resolution we should work with. At the highest resolution limit, diffraction measurement should be performed at very high scattering angle, say $2\theta \sim 150°$. In this situation the resolution is dominated by time width of neutron burst peak as we can understand eq.(1).

$$\Delta d/d = \Delta t/t + \Delta\theta \cot\theta \qquad (1)$$

In addition to resolution, because of Lorentz factor $\lambda^4/\sin^3\theta$, it is important to utilize long wave length neutron in order to increase observable intensity. It is, therefore, natural consequence to utilize poisoned decoupled H_2 moderator for high resolution powder diffractometer, cf. Fig.2.

In general, correlation function can be written into two parts, i.e. self term and distinct term.

$$G(r,0) = Gs(r,0) + Gd(r,0) = \delta(r) + g(r) \qquad (2)$$

Therefore, scattering function for homogeneous sample can be written into

$$S(Q) = 1 + 4\pi \int g(r) \sin(Qr)/Q \, dr \qquad (3)$$

At high Q, structure of S(Q) dumps with a factor of 1/Q, Debye-Waller factor accelerates this dumping and S(Q) becomes unity in the end. Therefore, at high Q region, observed intensity becomes structureless and cannot be distinguished from incoherent intensity. This intrinsic character of diffraction data determines the required decoupling energy by itself, which governs tail character. Figure 3 shows a typical example of S(Q) of $La_{1.85}Sr_{0.15}CuO_4$ [3]. Above 15Å^{-1} the character of S(Q) is really dumped away as explained above. This example means that we need sharp decrease of tail up to 100meV and the existence of tail does not affect data quality above this energy. Figure 4 shows results of computer simulation on neutron pulse structure as a function of various kind of reflector material and decoupling energy. The details of calculated results should be consulted with a report by [4]. However, the results clearly shows that 3eV in decoupling energy is sufficient to kills tail up to 120meV. Therefore, from this results, for most of cases of diffraction measurements, decoupling energy 3eV is a good choice.

3-2) Chopper Spectroscopy

One of the typical inelastic scattering instrument in pulsed neutron source is chopper spectrometer. As we will discuss the details of chopper spectrometer in Ref.[5]. Natural choice of the energy resolution is about $\Delta E/E \sim 1\%$ for chopper instrument because of constraint in path length. As we compared performances of chopper instruments with various moderator[6], moderator performance does not affect in inelastic region but seriously affect in elastic peak . Figure 5 shows a comparison between MARI in ISIS and INC in KENS. The moderator for MARI is 100K CH_4 poisoned moderator and that for INC is ambient water non-poisoned moderator. The performance of those moderator has large difference as reported in [6]. However, such a large difference in the performance of moderator does not seriously affect in the inelastic region as shown in Fig.5. This suggests that it is not necessary to be over-sensitive to chose a moderator performance. Decoupled H_2 moderator will do for most of chopper instruments

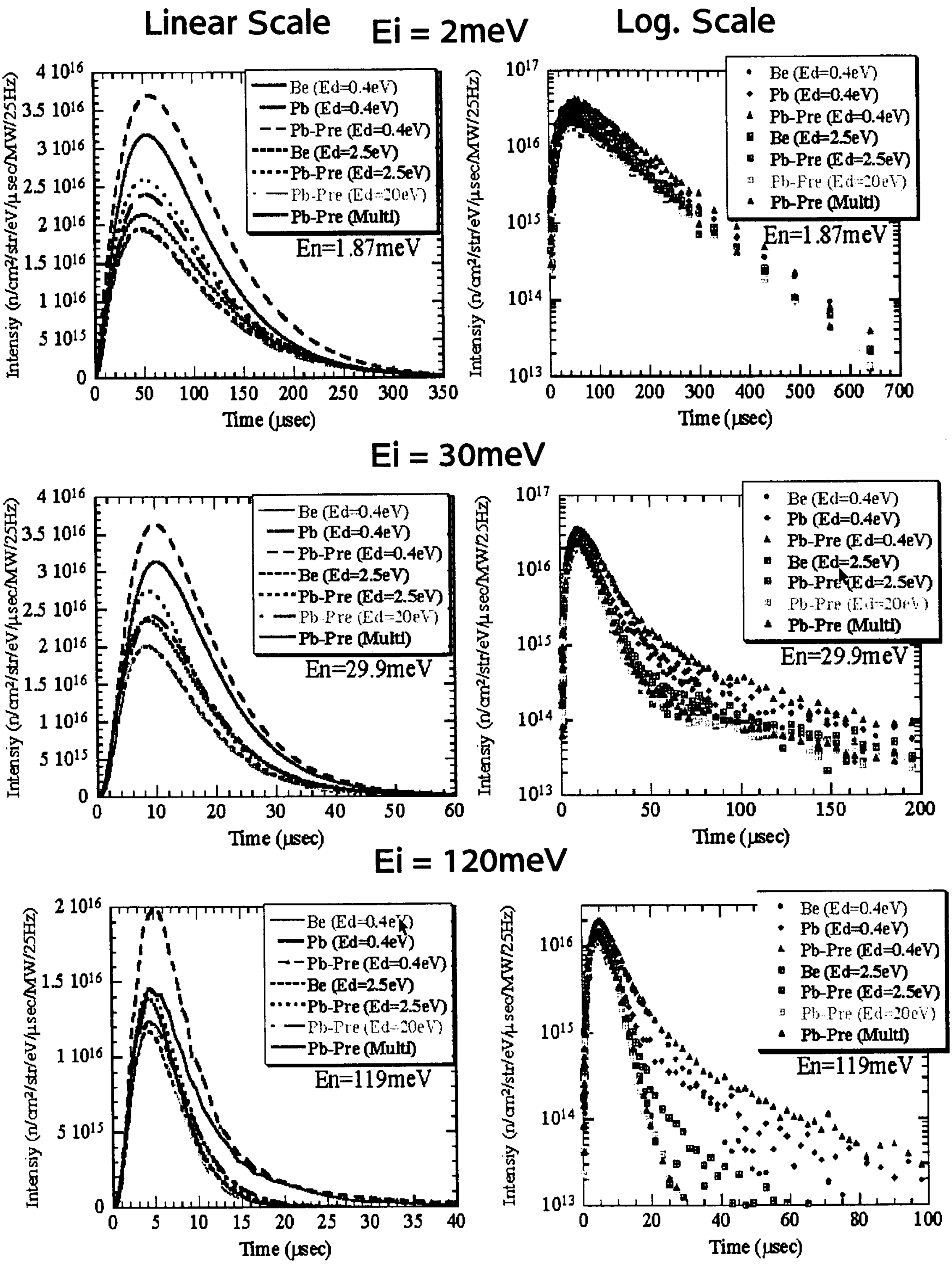

Fig.4 Tail and decoupling energy for various reflector materials.

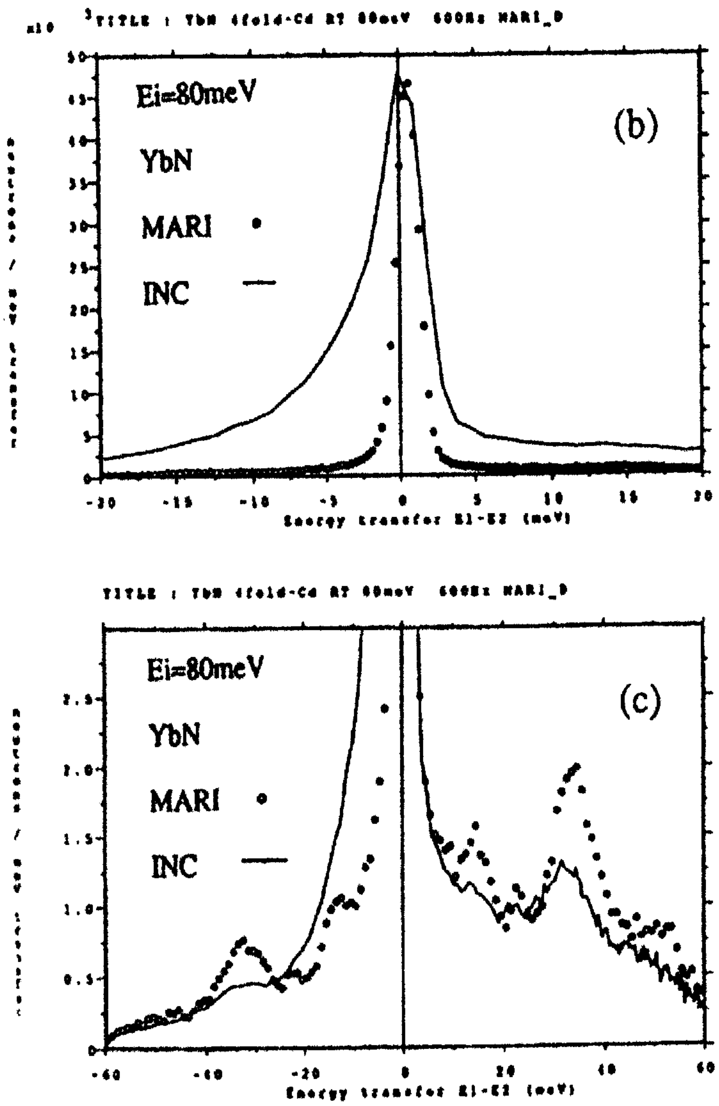

Fig. 5 Comparison of spectrum between MARI and INC [6]

3-3) High Resolution Back Scattering Instrument

Another typical inelastic instrument for pulsed neutron source is a inverted geometry high energy resolution instrument. As it has been proved in actual facilities, this kind of instrument can have a high performance in intensity and resolution by utilizing white neutron beak with time of flight method [7]. The energy resolution of this kind of instrument can be written into

$$\Delta E/E \sim 2(\Delta t/t + Ef/Ei(\cot\theta\Delta\theta)) \qquad (4)$$

and it is $\Delta E/E \sim 2\Delta t/t$ for back scattering high resolution limit. By utilizing Mica (004) reflection, it is easily possible to realize 2μeV resolution by setting $\Delta t/t=0.001$. From common knowledge on moderator performance, one normally take poisoned moderator to realize this required time width and one can decrease flight length to 50m. However, there is a new point of view to realize this performance. Figure 6 shows pulse structure as a function of reduced time by changing flight length by keeping resolution of Δt/t=0.001. As we see in the figure at the bottom, reduced peak width of coupled H_2 moderator with L_1=153m is almost equivalent to that of decoupled H_2 moderator with 54m for 2meV [4]. In addition the former case has one order of magnitude higher intensity. Although this result is preliminary and proceed further careful study, it is worth considering this kind of new idea on moderator performance.

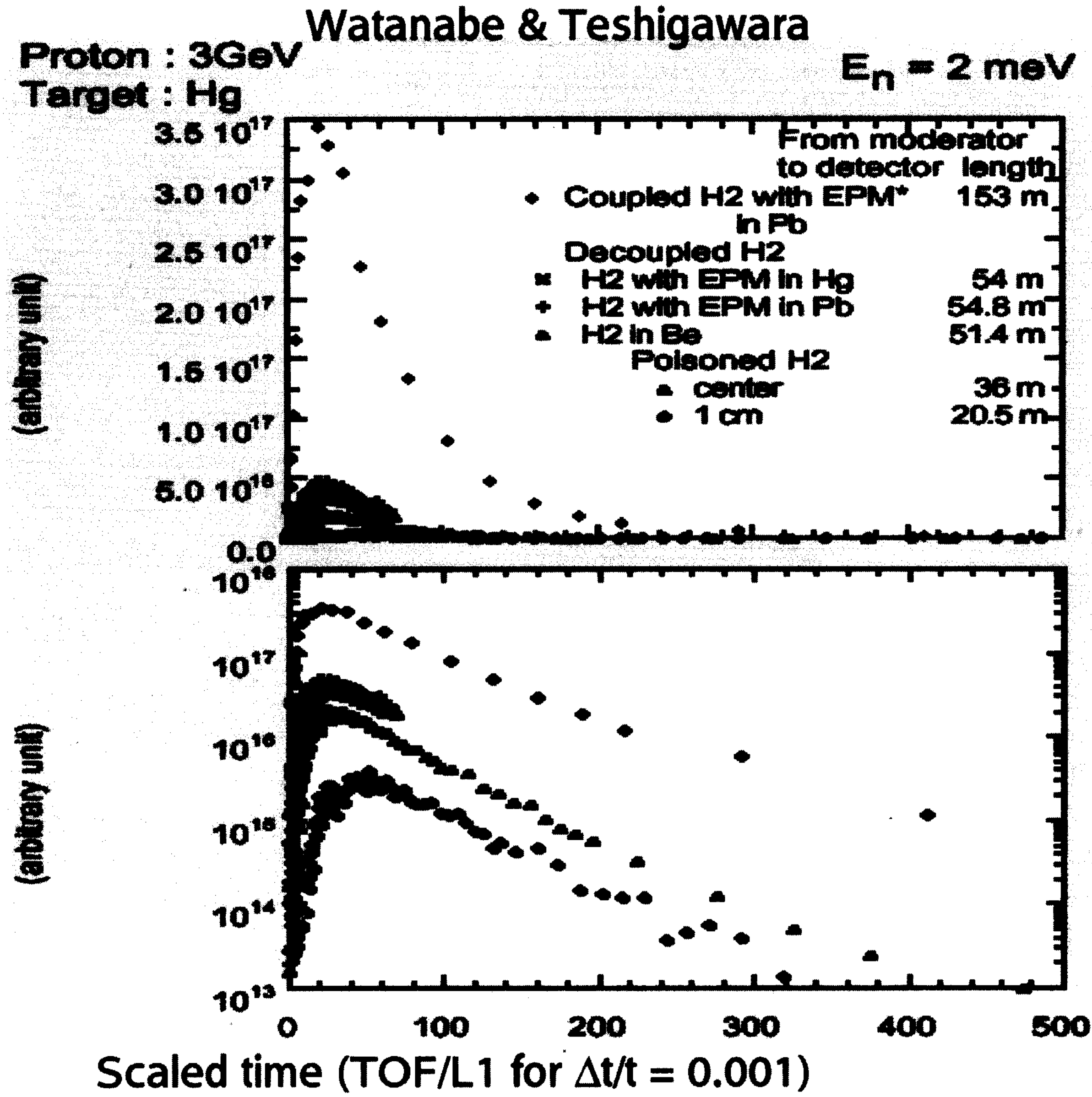

Fig.6 Pulse shape of various moderator as a function of reduce time for various distance by keeping Δt/t=0.001.

§4 Conclusion

In this report we showed a concept how we can choose performance of moderator to be adequate for realizing requirement from instrument performance. Now computer simulation becomes available to obtain detailed information on moderator performance. Of course we should start with scientific requirement to determine the performance of instruments, however, we should know there are various way in moderator design to realize the required performance of instruments.

[1] S.Ikeda and J.M.Carpenter, Nucl. Inst. Meth. in Phys. Res. A239 (1985) 536
[2] Y.Kiyanagi et al., Report in this proceedings.
[3] T.Egami et al., Rev. Solid State Sci. 1 (1987) 247
[4] M.Teshigawara et al., Report in this proceedings.
[5] K.Oyama et al., Report in this proceedings.
[6] M.Arai et al., ICANS-XI, p644
[7] K.Inoue et al., Nucl. Inst and Meth. A309 (1991) 294