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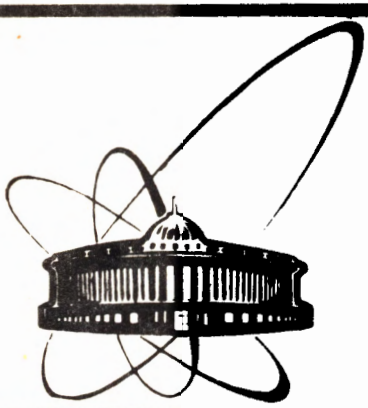

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LOW TEMPERATURE THERMAL PROPERTIES OF PENTANOL-2 - A PERSPECTIVE POLARIZED TARGET MATERIAL

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1. INTRODUCTION

The high polarization of proton targets requires a uniform distribution of the paramagnetic centers. Therefore, the polarization of butanol (C_4H_9OH) or pentanol-1 ($C_5H_{11}OH$) in the glass state of the material is sufficiently larger than in the crystalline one[1-3]. The amorphous structure in these materials can be obtained only after dopening with 5% water and rapid cooling from room temperature to liquid nitrogen temperature[1,2]. In this case the polarization is probably dependent on the cooling rate or on the purity of the target material. Moreover, an accidental warming up of the target to a temperature near the glass transition temperature T_g (T_g of pentanol-1 is about 170K[2]), leads to a drastic reduction of the polarization. Thus the preparation, transport, storage and experiments with these materials are not very convenient.

It will be shown in this paper that there are not these problems with pentanol-2. Pure pentanol-2 (and probably pentanol-3) forms the glass structure independent of the cooling rate, e.g. even after a very weak cooling from 292K to 78K with a cooling rate of about 1K/min.

For the recognition of the glass structure the low temperature heat capacity and the long-time power release were measured. Since the long-time power release is caused by two-level systems (TLS) existing only in glasses, this recognition method is very sensitive. Moreover, according to the tunnelling theory[4,5], a direct determination of the distribution parameter P (and the corresponding density of states of TLS) is possible:

$$P = (24/\pi^2 k^2)\cdot \dot{Q}\cdot t \;/\; V\cdot(T_1^2 - T_0^2) \;, \qquad (1)$$

where $\dot{Q}$ is the power released after a rapid cooling of the sample from the equilibrium temperature T_1 to T_0, t is the time after starting the cooling and V is volume of the specimen.

2. EXPERIMENTAL

A special calorimeter with a low heat leak ($\dot{Q}_B$ = 0.5 nW) to the sample was used in our experiments. A aluminium container (with or without pentanol) hung in a vacuum chamber on 8 kapron

threads. The container was connected with a Ge-thermometer, a heater and a copper wire to provide the thermal contact with a mechanical heat switch.

For the heat release study the resistance drift $\dot{R}$ of the thermometer was measured as a function of time t after the rapid cooling of the specimen from the equilibrium temperature T_1 (where the specimen remained for 24 hr) to $T_0 = 1.5K$. The corresponding power release $\dot{Q}(T_1,T_0,t)$ was then determined from the measured power release $\dot{Q}_m$, the power $\dot{Q}_A$ due to the thermal contact between the specimen and the body of the calorimeter, and the heat leak $\dot{Q}_B$:

$$\dot{Q}(T_1,T_0,t) = \dot{Q}_m - \dot{Q}_A - \dot{Q}_B \ , \qquad (2)$$

where

$$\dot{Q}_m = \dot{R}C/(\delta R/\delta T) \ , \qquad (3)$$

$$\dot{Q}_A = A(T_K - T). \qquad (4)$$

C is the heat capacity of the container with or without the sample, $\delta R/\delta T$ is the sensitivity of the thermometer, and A is the total thermal resistance of the kapron threads and the electric wires to the heater and the thermometer. The sample temperature T was chosen close to the calorimeter temperature T_K, which was kept constant (to $10^{-4}K$). When $T(t) - T_K = 10^{-4}K$, the sample temperature was set to $T_0 = T_K$.

3. RESULTS AND DISCUSSION

First the heat capacity and the power release of the hollow container (174.7g aluminium, 17.4g copper) were measured. As expected, no long-time heat release was observed. After the cooling of the container from $T_1 = 10K$ to 1.5K in 8 min the heat leak $\dot{Q}_B = 0.5$ nW was measured and the constant $A = 0.1$ nW/mK was determined. The accuracy of the power release measurement is given by the fluctuations of $\dot{Q}_B$, which are smaller than 0.1 nW (tested during one weak).

The container with pentanol-1 ($V = 110$ cm^3, $m = 90.12$ g, crystallization temperature: 190 K) or with pentanol-2 ($V = 86.45$ cm^3, $m = 70.28$ g) was cooled down from 292K to 78K with a cooling rate of 3K/min and 1K/min, respectively.

As in the case of the empty container no long-time relaxation was observed in pentanol-1, e.g. 20 min after cooling the container with pentanol-1 from 10K to 1.5K the heat leak $\dot{Q}_B$ = 0.5nW was measured again. Thus in agreement with the heat capacity data (s. fig. 1) pentanol 1 was crystalline. The cooling rate of 3K/min was not fast enough to form the glass structure.

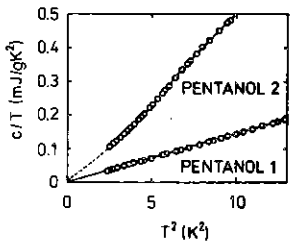

Fig. 1: The heat capacity of pentanol-1 and pentanol-2.

The heat capacity of pentanol-2 is larger than that of pentanol-1 (s. fig. 1) as expected for the amorphous structure. However, determination of linear term typical of glasses requires heat capacity data at lower temperatures.

The power release measurements clearly demonstrate that pentanol-2 is indeed amorphous: the long-time power release typical of glasses was observed (s. fig,2). The power released after cooling from various T_1 to T_0 = 1.5K is proportional to t^{-a} with $a = 0.69 \pm 0.04$. This coefficient is much smaller than

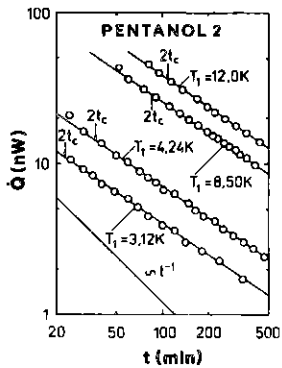

Fig. 2: The power $\dot{Q}$ released in pentanol-2 after rapid cooling from various equilibrium temperature T_1 to T_0 = 1.5K as a function of time t. Solid lines: $\dot{Q}$ is proportional to $t^{-0.69}$.

1 (predicted by the tunneling theory and observed in usual amorphous solids[6]). A similar behavior was observed in another organic material - epoxy resin - where a = 0.76[7]. Thus it is not excluded that the smaller a-values are a typical feature of organic materials probably caused by the side groups. At least our experiment with pentanol-1 and pentanol-2 demonstrate that the replacement of the OH-group from the end of the chain to the side prevent the crystallization, e.g the amorphous structure is caused by the side group.

At $T_1 < 4K$ the power release is proportional to $T_1^2 - T_0^2$ (s. fig. 3) and the distribution parameter $P = 4.1 \cdot 10^{44}/Jm^3$ of pentanol-2 can be determined from eq. (1) with $V = 86.45\ cm^3$ and $t = 1$ hr. This result is in a good agreement with the P-values of other glasses (s. table 1).

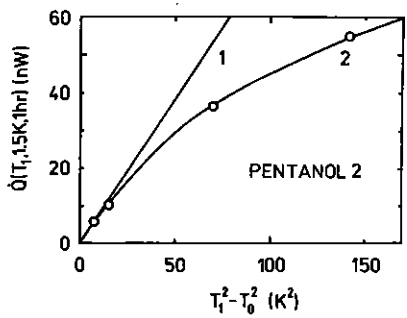

Fig. 3: The power $\dot{Q}$ released in pentanol-2 at $t = 1hr$ after rapid cooling from various T_1 as a function of $T_1^2 - T_0^2$. Curve 1: calculated $\dot{Q}$ according to the tunnelling theory (eq. 1) with $P = 4.1 \cdot 10^{44}/ Jm^3$ and $t = 1hr$. Curve 2: $\dot{Q}$ calculated with the energy dependent density of states (eq. 5) and $P = 4.1 \cdot 10^{44}/Jm^3$, $t = 1hr$, $E_f/k = 23K$, $kT_b/E_f = 0.2$.

At $T_1 > 4K$ the power release data disagree with eq. (1) (s. fig. 3). Similar deviations were observed for all investigated glasses. Using a distribution function with a cut-off energy E_f

$$n(E,t) = (P/2)\ln(4t/\tau_{min})/(1 + \exp((E - E_f/kT_b)) , \qquad (5)$$

where E_f and T_b are constants and τ_{min} is the shortest relaxation time of TLS, a good fit of the T_1-dependence can be

obtained for all investigated amorphous solids[6] including pentanol-2 (s. fig. 3). All obtained parameters a, P, E_f and T_b of pentanol-2 are not far from the corresponding values of other amorphous solids (see table 1), which demonstrates once more the universality of the low temperature anomalies of glasses.

Table 1

Characteristic parameters of the long-time power release in various amorphous solids: a is the coefficient of the time dependence t^{-a}, P is the distribution parameter of TLS, E_f and T_b are constants used for calcuation of the temperature dependence (s. text).

material	a	P , $10^{44}/Jm^3$	E_f/k , K	kT_b/E_f	Ref.
vitr. silica	1.0	1.0 - 3.3	13	0	8,9
$Fe_{80}B_{14}Si_6$	1.0	1.3	20	0	10
$LiCl \cdot 7H_2O$	1.0	10.1	48	0	11
epoxy resin	0.76	7.8	16.5	0.2	7
pentanol-2	0.69	4.1	23	0.2	t.w.

4. CONCLUSIONS

Studying the low temperature long-time energy relaxation showed that pentanol-1 is crystalline and pentanol-2 amorphous after their cooling from 292K to 78K with a cooling rate of about 1K/min. The replacement of the OH-group from the end of the chain to the side prevents the crystallization in pentanol-2. Thus a high polarization of a pentanol-2 target can be expected.

The time dependence of the power release in pentanol-2 differs from the time dependence expected from the tunnelling theory and observed for the most amorphous solids. Since a similar time dependence was observed for epoxy resin it is not excluded that this behaviour is characteristic of the noncrystalline organic materials.

The temperature dependence of the power released in pentanol-2 does not differ from the temperature dependence observed for other glasses. At low temperatures (T_i < 4K) the results agree with the tunnelling theory and the distribution parameter of TLS $P = 4.1 \cdot 10^{44}/Jm^3$ can be obtained. This value is also not far from the distribution parameter of other

amorphous solids. At higher temperatures the results disagree with the tunnelling theory. The assumption of an energy dependent density of states with a cut-off energy E_f/k = 23K yields a good fit of the observed temperature dependence.

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