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Ф И А Н

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Very cold neutron scattering on nanoctructure of various materials.

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Very Cold Neutrons (VCN)

Energy (E)= $2\cdot10^{-7} - 5\cdot10^{-4}$(eV) Velocity (V) = 10 – 100 (m/sec)

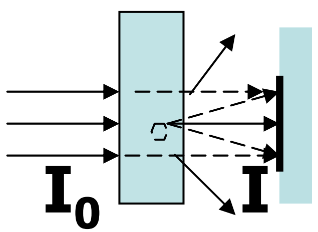
Wave vector module (k) = 0.06 – 6 (nm^{-1}) Wavelength (λ) = 1 - 100(nm)

$U = (2\pi\hbar^2/m)\Sigma_i(N_i b_i)$ – nuclear optical potential ; $\theta \sim \lambda/d$, ΔN, Δb

$$d\Sigma_{SMS}/d\Omega = (A/2\pi)\int_0^\infty K(\rho)[\sin(q\rho)/(q\rho)]\rho^2 d\rho$$

$A=2m^2\hbar^{-4}$, $\rho = |r_1 - r_2|$, $K(\rho)$- correlation function

1. Investigation of SMS by VCN transmission through the sample:

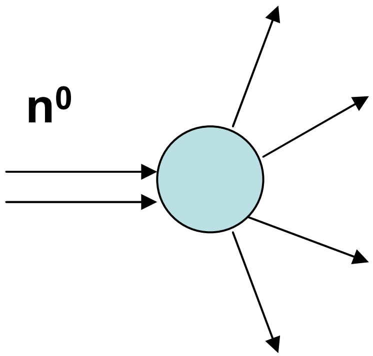


$$I/I_0 = \exp[-d\Sigma_t], \quad \Sigma_t = \Sigma_a + \Sigma_{in} + \Sigma_H + \Sigma_{SMS}$$

Σ_a, Σ_{in}, Σ_H, Σ_{SMS} are the cross-sections for the absorption, inelastic scattering, incoherent nuclear scattering, and scattering on the super molecular structure (SMS).

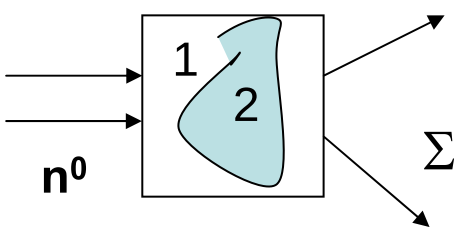
$$\Sigma_{SMS} = Ak^{-2}\int_0^\infty K(\rho)[\cos(2k\rho\sin\theta)-\cos(2k\rho)]d\rho$$

Σ_{SMS}(k) - dependence for VCN scattering on the isolated spheres with radius R:



$$\Sigma_{SMS}=\frac{9\pi N}{2V_0}\left[\frac{m}{2\pi\hbar^2}\right]^2(\Delta U)^2\left[\frac{4\pi R^3}{3}\right]^2\frac{1}{k^2R^2}\left\{\frac{1}{\left(2kR\sin\theta\right)^2}-\frac{\sin\left(4kR\sin\theta\right)}{\left(2kR\sin\theta\right)^3}+\frac{\sin^2\left(2kR\sin\theta\right)}{\left(2kR\sin\theta\right)^4}-\frac{1}{\left(2kR^2\right)}+\frac{\sin 4kR}{(2kR)^3}-\frac{\sin^2 2kR}{(2kR)^4}\right\}$$

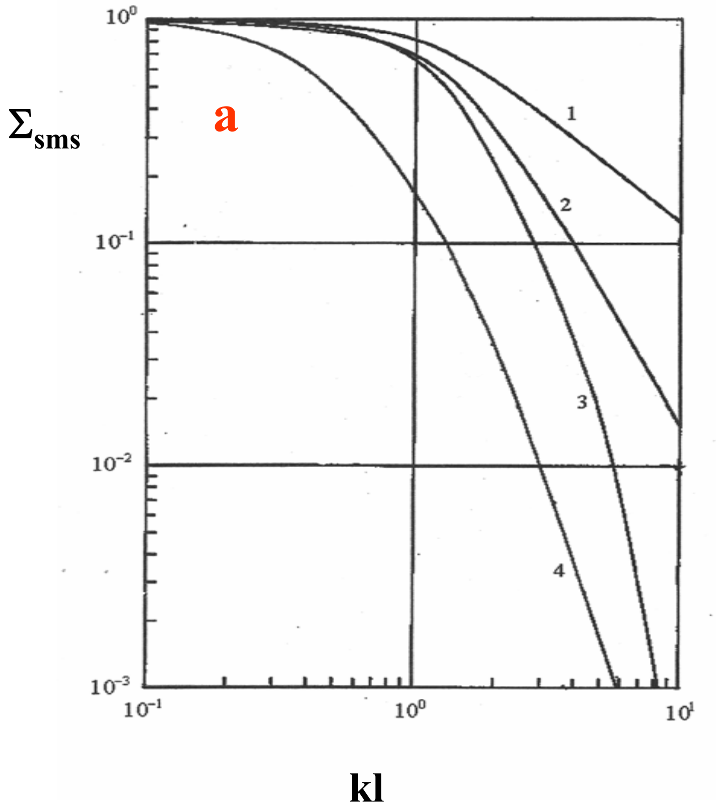
Σ_{SMS}(k) - dependence for VCN scattering on the two phase Poisson SMS:

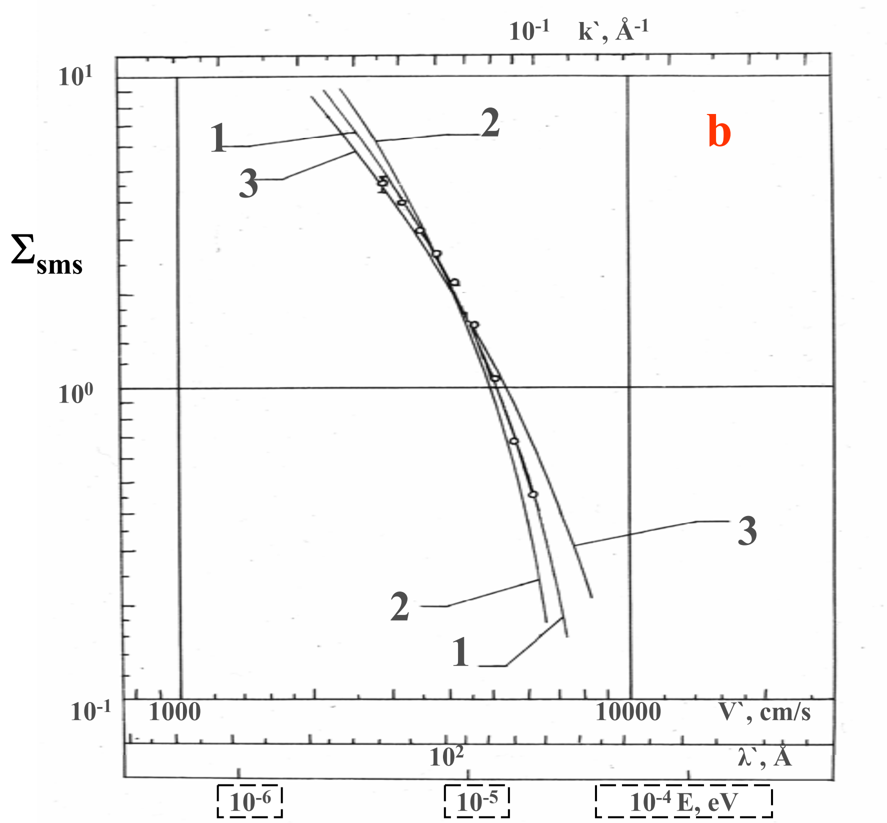


$$\Sigma_{SMS}(k)=AK(0)lk^{-2}\left[\frac{1}{1+\left(kl\sin\theta\right)^2}-\frac{1}{1+\left(kl\right)^2}\right]$$

Where: $K(0)=(1-\varphi)\varphi(\Delta U)^2$ l_1, l_2 - are the average chords of phase-1 and phase-2 domains, φ - voluem part of phase-1

Cross section for the VCN scattering on the particles of various forms (a) and on the porous in thermo pressed Be (b).





Σ_{SMS}(kl) – dependences of VCN scattering on the: 1 – discs, 2 - cylinders, 3 – spheres, 4 – two phase Poisson SMS

Σ_{SMS}(V) – dependences of VCN scattering on $10^{15}cm^{-3}$ pores in thermo pressed Be: ○ - experimental result, model of isolated spherical pores with radius 1 – 5.1 nm, 2 – 6.1 nm, 3 – 4.1 nm [1]

The conditions for BA applicability can be disrupted if the sizes of SMS elements (R) increase.

Faxen-Holtsmark formula:

$$\sigma_{total} = 2\pi \int_0^{\pi} \left(\left|F(\theta)\right|\right)^2 \sin(\theta)\, d\theta$$

$$F(\theta) = \sum_{l}^{\mathbf{max}} \left[(2l+1)F_l P_l(\cos(\theta))\right], \quad F_l = \frac{e^{-2i\delta_l}}{2ik},$$

$$\delta_l = \operatorname{atan}\left(\frac{\frac{k}{\kappa 1}\cdot js(l, x1)\cdot js(l+1, x) - js(l,x)\cdot js(l+1, x1)}{\frac{k}{\kappa 1}\cdot js(l, x1)\cdot ys(l+1, x) - ys(l,x)\cdot js(l+1, x1)}\right)$$

$$\Sigma_{sms} = \frac{n}{k^2}\int_{0.43}^{\pi}\left[\left|\sum_{lmax}\left[(2l+1)ie^{i\delta_l}\sin(\delta_l)P_l(l,\cos(\theta))\right]\right|\right]^2 2\sin(\theta)\,d\theta$$

F(θ) - total scattering amplitude

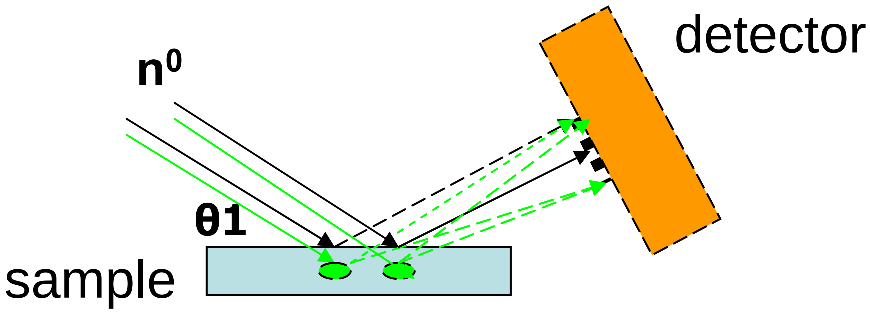
l - orbital moment,
$l_{max} \cong kR$.

x1 = k1R,

n – number of particles

js, ys – Spherical Bessel functions of 1-st & 2-nd kind respectively,
k and k1 - wave vectors out - and inside of the particle,
P_l - Legendre Polynomal function.

VCN reflection



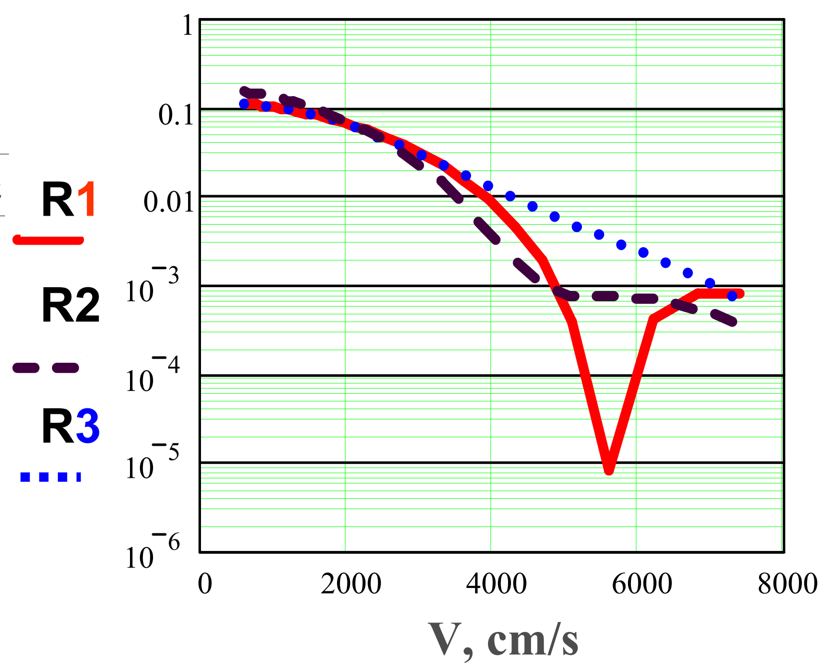
Reflection coefficient Rex include not only VCN reflection from the rough surface of the sample but include the differential cross section of the VCN scattering on SMS.

$$Rex(\lambda)=R_{Fr}\exp(-q^2\delta^2)+\int_{\Omega d}(d\Sigma_{SMS}/d\Omega)d\Omega$$

$$R_{Fr}=\frac{\sqrt{(1-\sin^2\theta_1)}-\sqrt{(n_{12}^2-\sin^2\theta_1)}}{\sqrt{(1-\sin^2\theta_1)}+\sqrt{(n_{12}^2-\sin\theta_1)}} \qquad n_{12}=\sqrt{\frac{E-U_2}{E-U_1}}$$

δ – average height of the surface roughness, Ωd-detector angular dimension, q – 2ksinθ_1, θ_1-VCN full reflection angle

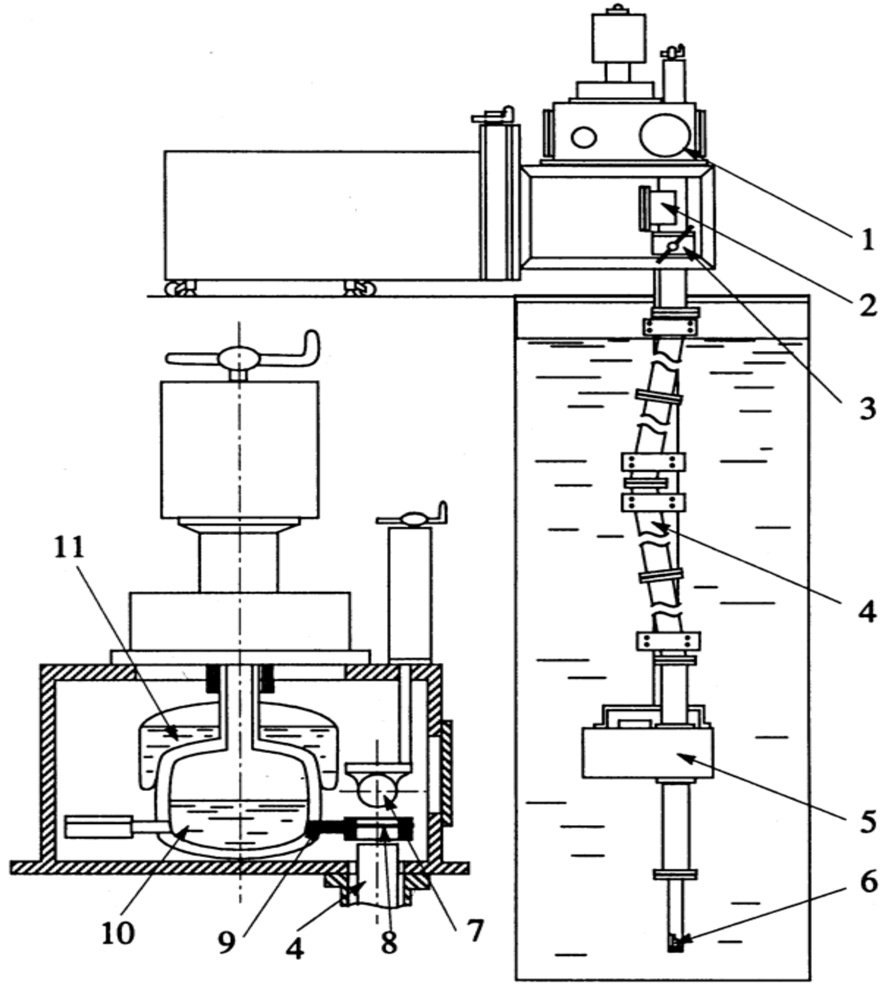
U_1, U_2 – nuclear-optic potentials at the reflection boundary of two mediums.



Intensity of VCN scattering from the sphere to: ideal detector - R1; Ωd = 0.07 - R2; Ωd = 0.15 - R3

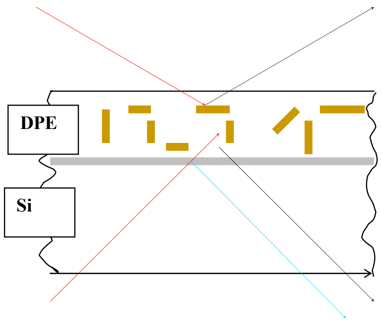
INSTRUMENTS:

The Time-of-Flight Very Cold Neutrons Spectrometer



1 – sample chamber; 2 – monitor; 3 – cut-off valve; 4 – neutron guide tube; 5 – chopper; 6 – converter; 7 – counter; 8 – sample; 9 – sample base; 10 – low-temperature base; 11 – nitrogen screen.

The dependences of the reflected intensity vs. neutron wavelength for Si/DPE material from the both (substrate and vacuum) sides were obtained with reflection angle 30^0..



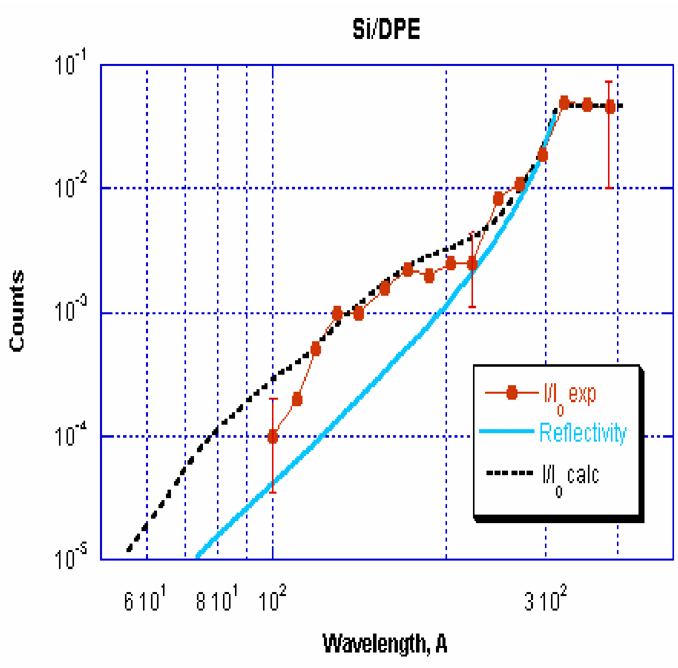


Fig.1. *The reflected intensity profile of two-layer sample from the substrate side.*

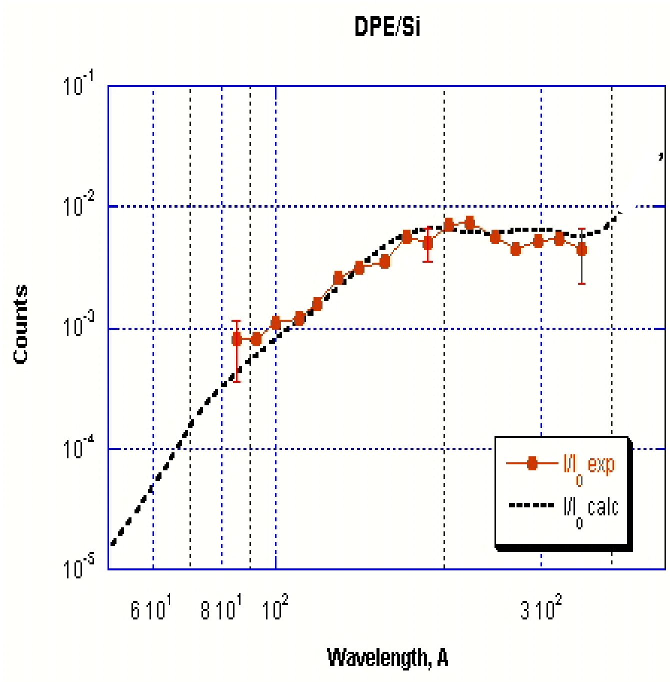


Fig.2. *The reflected intensity profile of two-layer sample from the external PDE side*

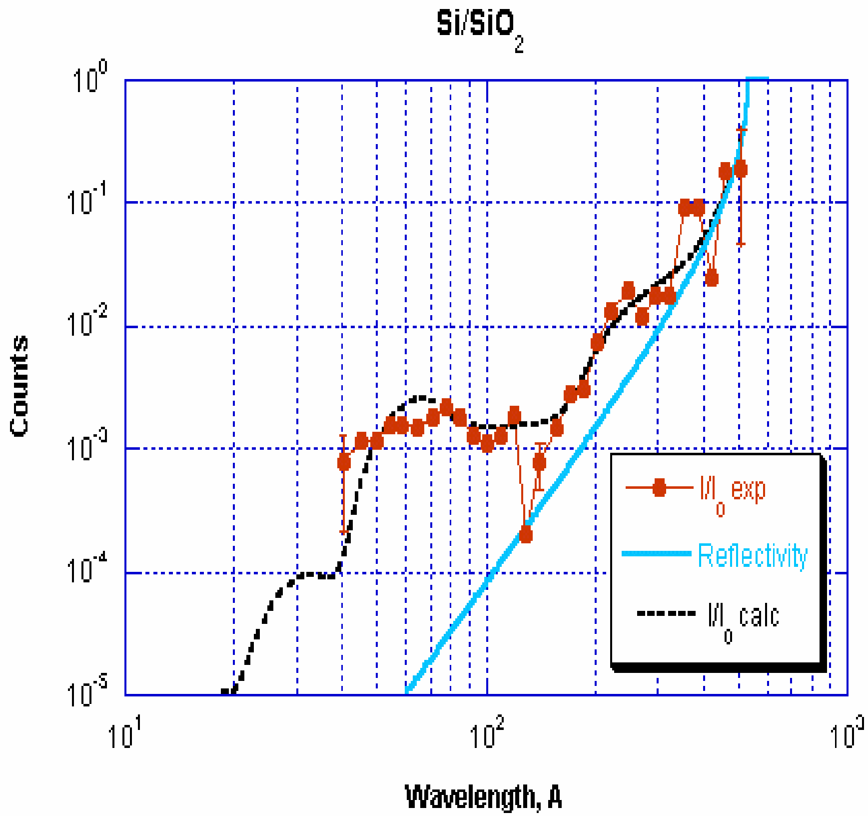


Fig.3. *The intensity profile of nano silicon*

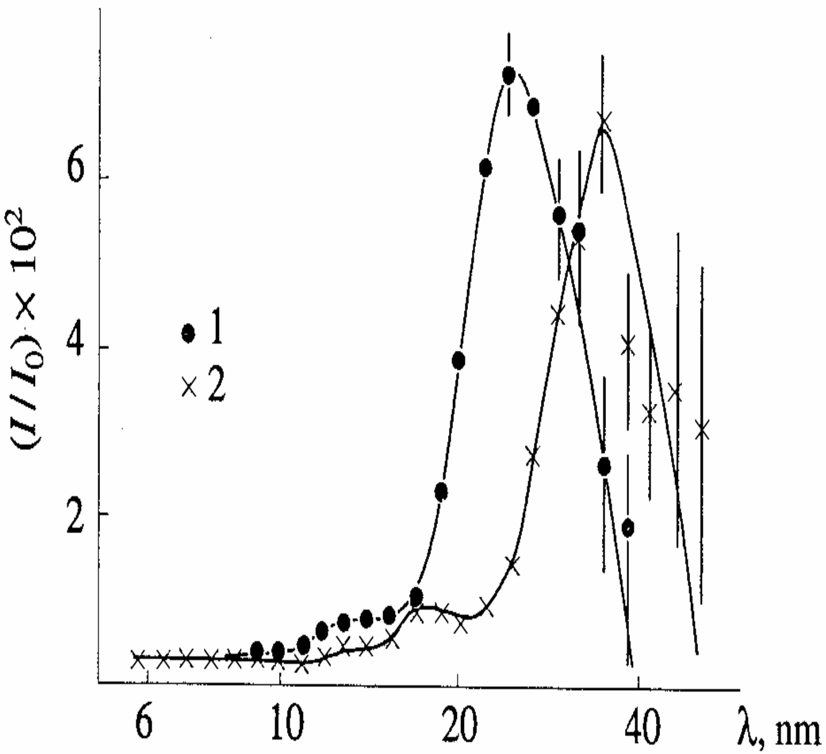


Fig.4. ***VCN reflection from the ordered three bloc co-polymer SMS at reflection angles 30⁰ (1) and 45⁰ (2).***

Differential cross section for the VCN scattering on the porous thermo pressed Be. (θ_1=30, Ωd = 0.15)

1.VCN scattering on the spheres:

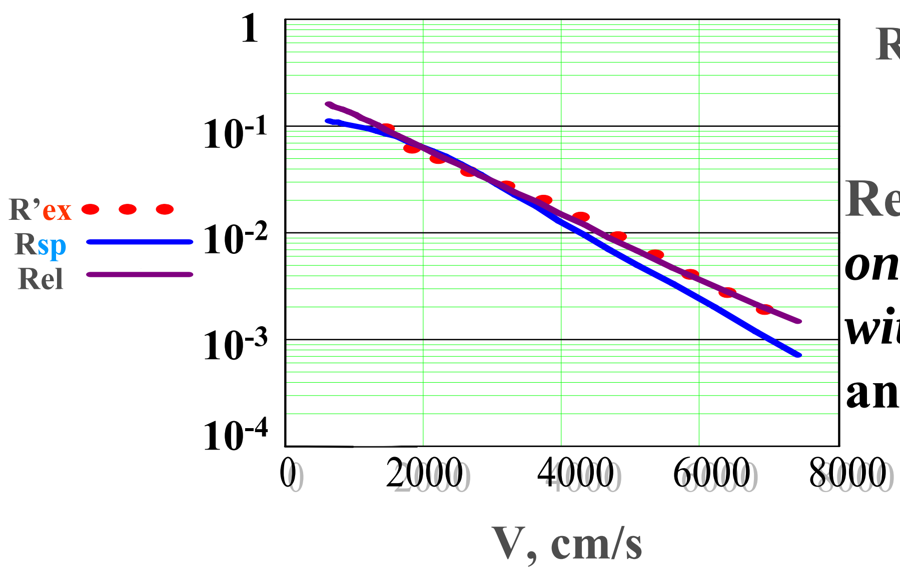
$$R_{sp} = (4\pi R^3/3)^2 \int_{\theta_1-\alpha_1}^{\theta+} \Phi n \tau^2 \sin\alpha \, d\alpha;$$ n - number of spheres, $\tau = N_i b_i$,

$$\Phi = \{[3\sin(2kR\sin\alpha) - 2kR\sin\alpha \cdot \cos(2kR\sin\alpha)]/(2kR\sin\alpha)^3\}^2$$

2.VCN scattering on the ellipsoids:

$$R_{el} = (4\pi\nu R^3/3)^2 \int_{\theta_1-\alpha_1}^{\theta+} \int_0^1 \Phi\{(2kR\sin\alpha)[1+x^2(\nu^2-1)]^{1/2}\} \, n\tau 2\sin\alpha \, d\alpha \, dx$$

R, *R*,ν*R* – half axis of ellipsoid



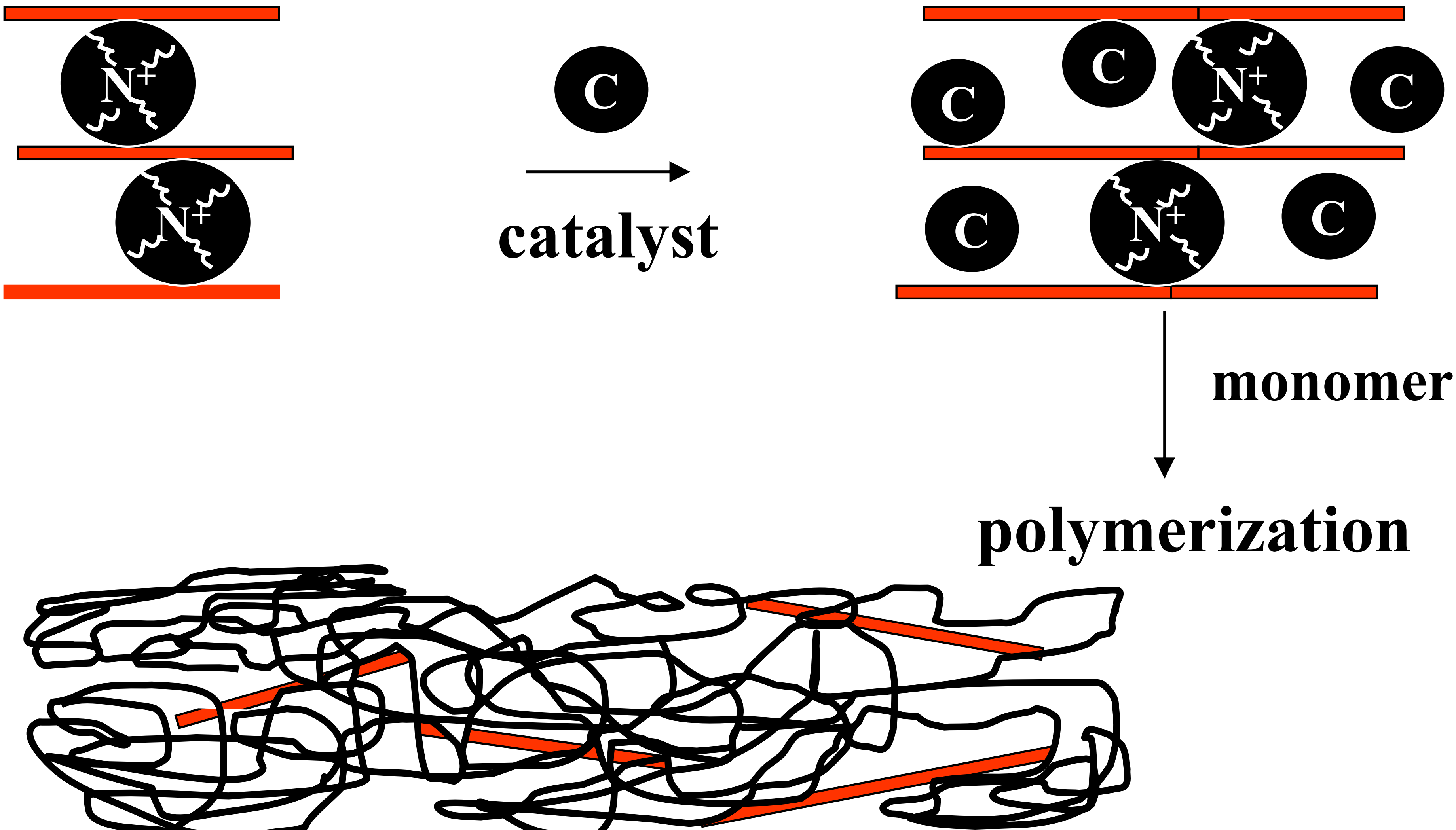
R'ex = Rex- R'_{Fr}

Rel - *scattering on the ellipsoids with R*=3.5nm and ν=3.9

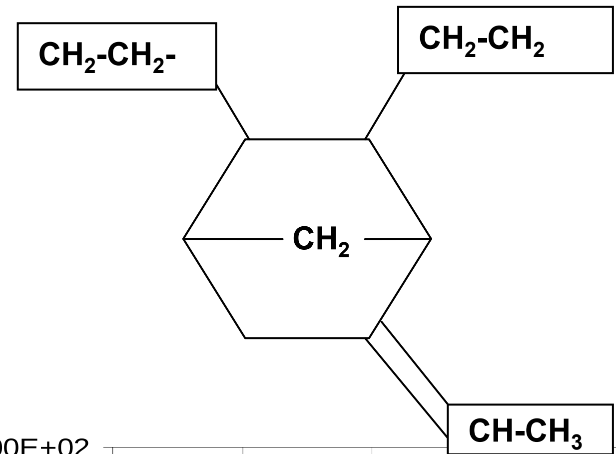
Rsp - *scattering on the spheres with R*=5.1nm *and* n= 10^{15}cm^{-3}

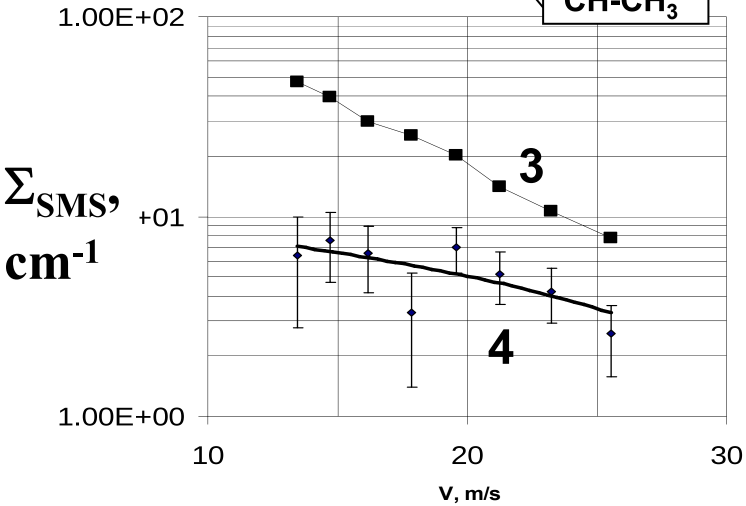
This parameters were obtained by VCN passing through the same sample.

The diagram of polymer-silicate nanocomposite creation



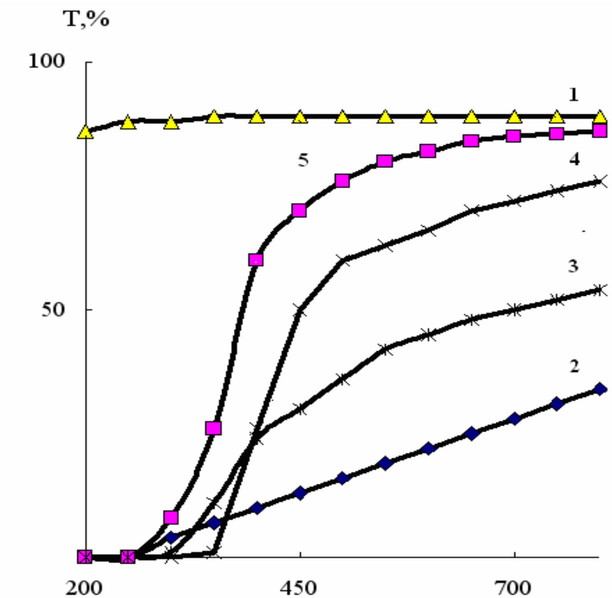
VCN transmission was used to control the nanostructure of copolymers of ethylene and 5-ethylidene-2-norbornene (E/EN).





$\Sigma_{SMS}(V)$ – dependences for E/EN copolymers with EN concentrations:

3 – 5.3, 4 –20 mol%



Transmittance of light as a function of the wavelength for the substrate (1) and ethylene copolymers with 5-ethylidene-2-nonbornene (EN) at contents of EN:
1- substrate2- 0, 3- 5.3, 4- 20, and 5- 50 mol %.

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REFERENCES

[1] Antonov A.V., Isakov A.I., Kuznetsov S.P., Meshkov I.V., Perekrestenko A.D., Shelagin A.V., Fiz.Tverd. Tela, 26, 1585-1587 (1984)

[2] Grinev V.G., Isakov A.I., Krasheninnikov V.G., Kovaleva N.Yu., Kuznetsov S.P., Meshkov I.V., Novokshonova L.A., Perekrestenko A.D., Shelagin A.V., ShelaginD.A., Polymer Science (Vysokomolekulyarnye Soedineniya), Vol 40A, 1763 (1998)

[3] Kuznetsov S.P., Lapushkin Yu.A., Mitrofanov A.V. Shestov S.V. , Udovenko A.I. , Shelagin A.V. , Meshkova I.N. , V.G. Grinev, Kiseleva E.V. , Raspopov L.N. , Shchegolikhin A.N. , Novokshonova L.A. , Crystallography Reports, 2007, in print.

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