Algorithm for preparation of multilayer systems with high critical angle of total reflection

I. Carron[a], V. Ignatovich[b].
[a)] Texas A & M University, College Station, TX, USA
[b)] FLNP JINR, Dubna Moscow region, 141980, Russia

Abstract

The new development of theory of multilayer systems is presented. It shows precisely how to calculate thicknesses and number of layers to get reflectivity close to unity for a given, in principle, arbitrary critical angle. Application of the new approach to real systems is demonstrated.

Алгоритм для приготовления многослойных систем с высоким критическим углом полного отражения

И. Каррон, В. Игнатович.

Аннотация

Излагается новый аналитический подход к анализу многослойных систем. Он позволяет строго рассчитать толщины и число слоев необходимые для получения близкого к полному отражения для заданного, в принципе произвольно высокого, критического угла. Демонстрируется приложение нового подхода к реальным системам.

1 Introduction

We apply a not yet widely known physically transparent analytical method to calculation of thicknesses and number of layers in multilayer systems (MS) to achieve a high critical angle.

Usually MS consist of many bilayers of two materials with different refraction indices, and the thickness a_i of the bilayer varies with its number i according to theoretical prescriptions of [1]. In such a stuck all the bilayers have different thicknesses, and the change of neighboring layers is very small. We consider here a different construction: the MS consists of several periodic chains, and we show how to find the period, number of periods for every chain, and number of chains to achieve the critical angle we wish.

Applications of MS in experiments are discussed in many review papers (see, for instance [2, 3] and references there in), and we do not dwell on it too much. We only want to add some references [4] - [10], which were not mentioned in [3].

In [4, 5, 6, 7] the MS were used for polarization of neutrons by transmission [4] through them, by transportation along magnetized neutron guides [5, 7], and by splitting of unpolarized beam by a magnetized supermirror [6]. In [8] the pulsed beam was produced by reflection from a supermirror periodically magnetized in external field. In [9] supermirrors were used in neutron guides to increase the transmitted flux. Some research on fabrication of supermirrors was presented in [10].

In our present paper we consider MS for polarization of neutrons. This purpose determines materials for bilayers. However our analytical method is not limited to this purpose but is applicable to all MS, even to those that contain more than two materials.

2 Our method

First of all we should mention one difference of our approach comparing to commonly used one. We consider reflection in terms of normal component $k_\perp$ of the incident neutron wave vector instead of the incidence angle. It is more convenient because reflection of a mirror at a given angle depends also on wave length, whereas in terms of the wave vector $\boldsymbol{k}$ it depends only on $k_\perp$ and properties of the mirror. In the following we even omit the index $\perp$, and use simply k, because we deal only with specular reflection and for that the one dimension is sufficient.

To be more precise we consider a neutron propagating along x-axis normal to the supermirror, and calculate its reflection from the supermirror, which is a set of alternating layers of two materials. One of them is represented by a potential barrier of height u_b and width l_b, and another one is represented by a potential well of height u_w and width l_w. The potential barrier with $l_b \to \infty$ totally reflects neutrons with $k^2 < u_b$, and $\sqrt{u_b}$ is called critical number k_c. It is convenient to use $1/k_c$ as a unit of length, then all the variables become dimensionless, the barrier becomes of height $u_b = 1$, and the critical number is also unity. In the following we use a somewhat different normalization. We take for unity the difference $u_b - u_w$, and for the unit length $1/\sqrt{u_b - u_w}$.

We look for such MSs which give total reflection up to some $K_c > k_c = 1$. In principle K_c can be arbitrary large, but practically it is possible achieve K_c not larger than 4.

Our analytical method is based on an observation [11, 12] that every potential can be split by an infinitesimal gap into two separate ones, as shown in fig. 1, and the reflection

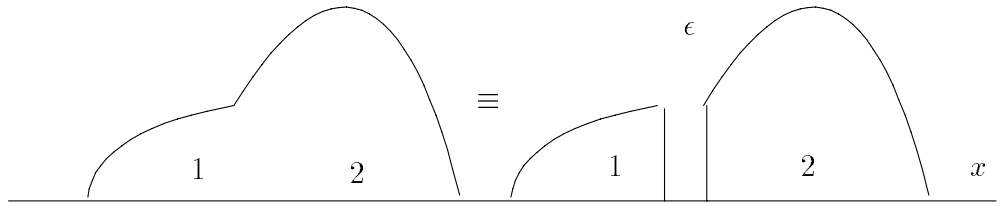

Figure 1: Every potential can be split by an infinitesimal gap of width $\epsilon \to 0$, into two ones, and the splitting does not change their reflection and transmission properties, because of total transmission of the gap.

of the composite potential R_{12} is represented as the combination of reflections R_i and transmissions T_i of the separate barriers:

$$R_{12} = R_1 + T_1^2 \frac{R_2}{1 - R_1 R_2}, \tag{1}$$

where the denominator corresponds to multiple reflections inside the gap. For simplicity in (1) we did not take into account asymmetry of the potentials, we discuss it when needed.

The expression (1) gives immediately the result [13] for a semiinfinite periodic potential. If a single period of the potential is characterized by reflection and transmission amplitudes r and t respectively, then reflection amplitude of the whole potential (denoted R_0 in [1]: eq-s (14-16) there) is

$$R = \frac{\sqrt{(1+r)^2 - t^2} - \sqrt{(1-r)^2 - t^2}}{\sqrt{(1+r)^2 - t^2} + \sqrt{(1-r)^2 - t^2}}, \tag{2}$$

and the Bloch phase factor (denoted by κ in [1]: eq-s (12), (13) there) is

$$\exp(iqa) = \frac{\sqrt{(1+t)^2 - r^2} - \sqrt{(1-t)^2 - r^2}}{\sqrt{(1+t)^2 - r^2} + \sqrt{(1-t)^2 - r^2}}, \tag{3}$$

where a is the period width, and q is the Bloch wave number. At Bragg reflection $R = \exp(i\chi)$ and $\exp(iqa) = \exp(-q'a)$ with real χ, and q'. (We neglect here imaginary part of the potential.)

With the equations (2), (3) we can find [11] reflection, R_N, and transmission, T_N, amplitudes of the periodic chain with finite number N of the periods:

$$R_N = R \frac{1 - \exp(2iqaN)}{1 - R^2 \exp(2iqaN)}, \qquad T_N = \exp(iqaN) \frac{1 - R^2}{1 - R^2 \exp(2iqaN)}. \tag{4}$$

To see how do these formulas work we need to define the single period and its amplitudes r and t. A single period is a bilayer. It consists of a potential well and barrier. This period

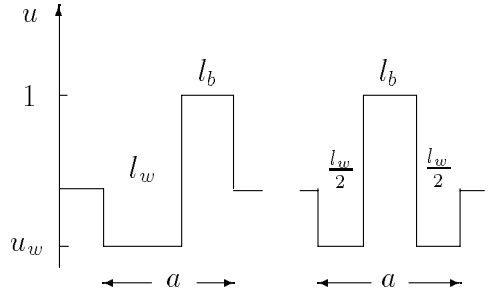

Figure 2: A period containing a well and barrier, can be rearranged to symmetrical form.

is nonsymmetrical, but we can make it symmetrical by shifting the barrier as shown in fig. 2. This rearrangement is not principal, as we see later, but it facilitates our mathematics. For symmetrical period of width $a = l_w + l_b$ we can immediately find amplitudes r and t:

$$r = e^{ik_w l_w} r_{wb} \frac{1 - \exp(2ik_b l_b)}{1 - r_{wb}^2 \exp(2ik_b l_b)}, \quad t = e^{ik_w l_w} e^{ik_b l_b} \frac{1 - r_{wb}^2}{1 - r_{wb}^2 \exp(2ik_b l_b)}, \tag{5}$$

where $k_{w,b} = \sqrt{k^2 - u_{w,b}}$, $r_{wb} = (k_w - k_b)/(k_w + k_b)$ and potentials may contain imaginary part because of losses.

Substitution of them into (2) and (4) gives the result shown in fig. 3 and 4. In fig. 3 we see the Bragg reflection with unit amplitude in the interval Δ called width of the Darwin table. By decreasing l_w and l_b we can shift the interval Δ toward larger k, and, if we can built a system of semiinfinite potentials with different periods in such a way that intervals Δ would overlap as intervals D in fig. 5, we can considerably increase k_c.

However we can build periodic chains only with finite number of periods, so we must use $|R_N|$ of (4), which at Darwin table is smaller than unity because of $\exp(-2q'Na)$ in the nominator. This factor is small when N is large. If we tolerate reflection $|R_N| = 1 - \zeta$ with some small ζ, we must have

$$N = -\frac{\ln \zeta}{2q'a}. \tag{6}$$

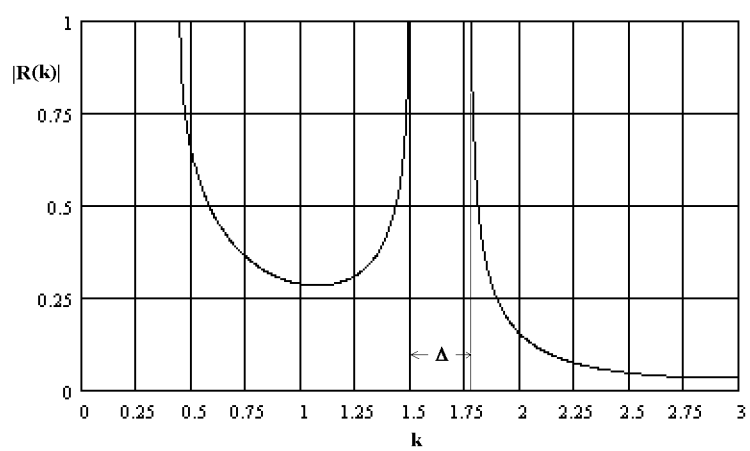

Figure 3: Reflection amplitude $|R(k)|$ of a semiinfinite periodic potential with period containing the potential well of depth $u_w = 0.5$ and width $l_w = 1$, and the barrier of the height 1 and width $l_b = 1$.

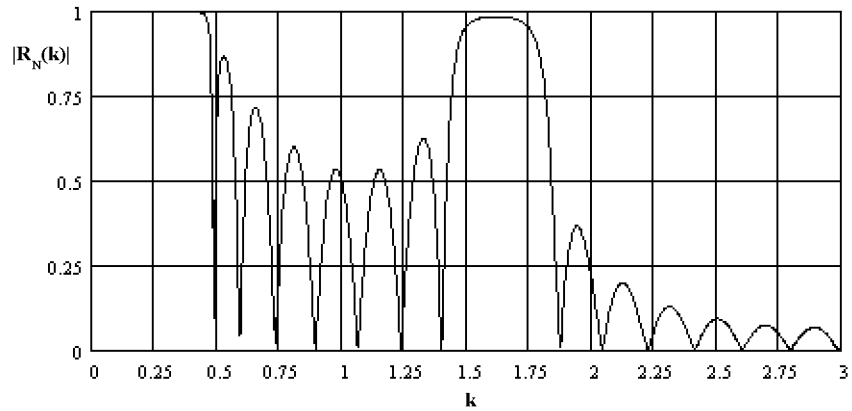

Figure 4: Reflection amplitude $|R_N|$ of the periodic potential with $N = 8$ periods. The parameters of a single period are the same as in fig. 3.

So the strategy is very clear. We step by step cover the range of k, we needed, by overlapping intervals $\Delta' < \Delta$, and tuning parameters l_w, l_b, N find maximal Δ' to minimize the number of required chains, and therefore the total number of layers. To proceed further it is more convenient to transform (2,3) to the form

$$R = \frac{\sqrt{\cos\phi + |r|} - \sqrt{\cos\phi - |r|}}{\sqrt{\cos\phi + |r|} + \sqrt{\cos\phi - |r|}} = \frac{\sqrt{\mathrm{Re}(r) + |r|^2} - \sqrt{\mathrm{Re}(r) - |r|^2}}{\sqrt{\mathrm{Re}(r) + |r|^2} + \sqrt{\mathrm{Re}(r) - |r|^2}}, \tag{7}$$

$$e^{iqa} = \frac{\sqrt{-\sin\phi + |t|} - \sqrt{-\sin\phi - |t|}}{\sqrt{-\sin\phi + |t|} + \sqrt{-\sin\phi - |t|}} = \frac{\sqrt{\mathrm{Re}(t) + |t|^2} - \sqrt{\mathrm{Re}(t) - |t|^2}}{\sqrt{\mathrm{Re}(t) + |t|^2} + \sqrt{\mathrm{Re}(t) - |t|^2}}, \tag{8}$$

where ϕ is the phase and $\mathrm{Re}(r, t)$ are real parts of amplitudes r, t respectively. To derive (7,8) we use the relations valid for arbitrary potential [14]:

$$r = e^{i\phi}|r|, \quad t = \pm i e^{i\phi}|t|, \quad r^2 - t^2 = e^{2i\phi}. \tag{9}$$

From (7) it follows that R is a unit complex number $\exp(i\chi)$, when $|r|^2 > |\mathrm{Re}(r)|$.

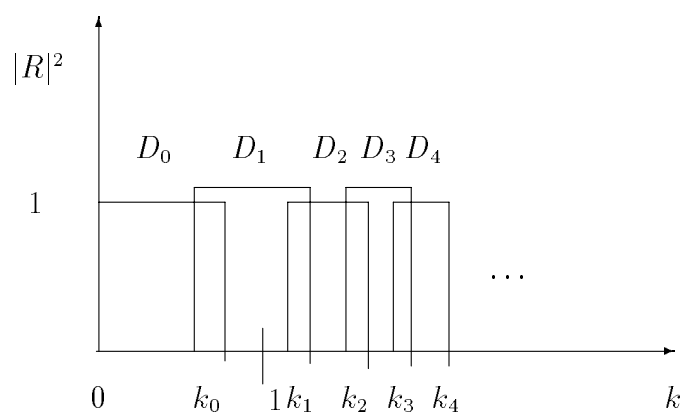

Figure 5: A system of periodic potentials with overlapping Bragg peaks of widths D_i gives total reflection in a range of k considerably wider than the common case $0 \le k \le 1$.

3 Algorithm of calculations of l_b, l_w, N and Δ'.

Substitution of (5) into (7) and (8) in the case $k^2 > u_b$ gives

$$R = \frac{\sqrt{\dfrac{k_b \tan(k_w l_w/2) - k_w \cot(k_b l_b/2)}{k_w \tan(k_w l_w) - k_b \cot(k_b l_b)}} - \sqrt{\dfrac{k_w \tan(k_w l_w/2) + k_b \tan(k_b l_b/2)}{k_b \tan(k_w l_w/2) + k_w \tan(k_b l_b/2)}}}{\sqrt{\dfrac{k_b \tan(k_w l_w/2) - k_w \cot(k_b l_b/2)}{k_w \tan(k_w l_w) - k_b \cot(k_b l_b)}} + \sqrt{\dfrac{k_w \tan(k_w l_w/2) + k_b \tan(k_b l_b/2)}{k_b \tan(k_w l_w/2) + k_w \tan(k_b l_b/2)}}} \tag{10}$$

or

$$R = \frac{\sqrt{\dfrac{\cos\phi_+ + r_{wb}\cos\phi_-}{\cos\phi_+ - r_{wb}\cos\phi_-}} - \sqrt{\dfrac{\sin\phi_+ + r_{wb}\sin\phi_-}{\sin\phi_+ - r_{wb}\sin\phi_-}}}{\sqrt{\dfrac{\cos\phi_+ + r_{wb}\cos\phi_-}{\cos\phi_+ - r_{wb}\cos\phi_-}} + \sqrt{\dfrac{\sin\phi_+ + r_{wb}\sin\phi_-}{\sin\phi_+ - r_{wb}\sin\phi_-}}}, \tag{11}$$

and

$$e^{iqa} = \frac{\sqrt{\cos^2\phi_+ - r_{wb}^2\cos^2\phi_-} - \sqrt{-\sin^2\phi_+ + r_{wb}^2\sin^2\phi_-}}{\sqrt{\cos^2\phi_+ - r_{wb}^2\cos^2\phi_-} + \sqrt{-\sin^2\phi_+ + r_{wb}^2\sin^2\phi_-}}, \tag{12}$$

where $\phi_\pm = (k_w l_w \pm k_b l_b)/2$. It is easy to check that at the limit $l_b \to 0$ we obtain $R \to 0$ and $q \to k_w$, and at $l_w \to 0$ we obtain $R \to r_{wb}$, $q \to k_b$.

If $k^2 < u_b$ instead of (11, 12) we obtain

$$R = \frac{\sqrt{\cos^2\xi_- - \exp(-2k_b' l_b)\cos^2\xi_+} - i\sqrt{\sin^2\xi_- - \exp(-2k_b' l_b)\sin^2\xi_+}}{\sqrt{\cos^2\xi_- - \exp(-2k_b' l_b)\cos^2\xi_+} + i\sqrt{\sin^2\xi_- - \exp(-2k_b' l_b)\sin^2\xi_+}}, \tag{13}$$

$$e^{iqa} = \frac{\sqrt{\dfrac{\sin\xi_- - \exp(-k_b' l_b)\sin\xi_+}{\sin\xi_- + \exp(-k_b' l_b)\sin\xi_+}} - \sqrt{\dfrac{\cos\xi_- - \exp(-k_b' l_b)\cos\xi_+}{\cos\xi_- + \exp(-k_b' l_b)\cos\xi_+}}}{\sqrt{\dfrac{\sin\xi_- - \exp(-k_b' l_b)\sin\xi_+}{\sin\xi_- + \exp(-k_b' l_b)\sin\xi_+}} + \sqrt{\dfrac{\cos\xi_- - \exp(-k_b' l_b)\cos\xi_+}{\cos\xi_- + \exp(-k_b' l_b)\cos\xi_+}}}, \tag{14}$$

where $\xi_\pm = k_w l_w/2 \pm \phi_0$, $\phi_0 = \arccos(k_w/\sqrt{u_b - u_w})$ and $k_b' = \sqrt{u_b - k^2}$.

It is easy to check that in the limit $l_w \to 0$ the periodic potential degenerates to potential step and we obtain $R \to r_{wb} = \exp(-2i\phi_0)$, $q = ik'$. In the limit $l_b \to 0$ barriers disappear, and we obtain empty space with $R = 0$ and $q = k_w$.

Now we consider $k^2 > u_b$. The Bragg reflections take place when expressions under two square roots in (11) have opposite signs. It happens when $|\cos\phi_+| < r_{wb}|\cos\phi_-|$, or $|\sin\phi_-| < r_{wb}|\sin\phi_+|$, i.e. for $\pi n/2 - \delta\phi \le \phi_+ \le \pi n/2 + \delta\phi$, where n is integer. The half width of the Bragg reflection $\delta\phi = r_{wb}|\cos\phi_-|$ for odd n, and $\delta\phi = r_{wb}|\sin\phi_-|$ for even n. To get this width maximal we must have $\phi_- = \pi m$ for odd n and $\phi_- = \pi m \pm \pi/2$ for even n (m is also integer).

From these considerations we obtain, that if we want to have the total reflection at some $k = k_v$ we must require at this point $k_b l_b + k_w lw = \pi$ and $k_w l_w - k_b l_b = 0$, and immediately find two parameters $l_b = \pi/2k_b$, and $l_w = \pi/2k_w$ (as was correctly used in [1], eq. (7)). We can also require $k_b l_b + k_w lw = 2\pi$ and $k_w l_w - k_b l_b = \pi$, and find two other parameters $l_b = \pi/2k_b$, and $l_w = 3\pi/2k_w$.

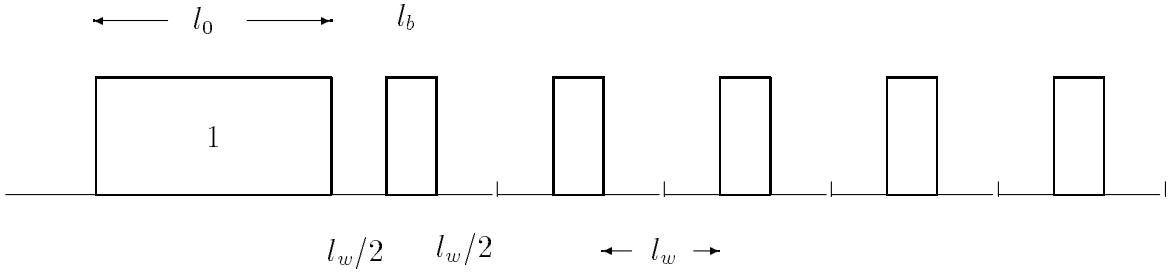

Figure 6: The MS should contain also a barrier of large width l_0 to provide total reflection almost up to $k = 1$

We cannot use the full width Δ of the Darwin table, because the total reflection inside it is possible only for infinite number of periods. We need to find such Δ' and N which will give the maximal effective length $\delta_1 = \Delta'/N$ covered by a single period.

For optimization we represent (12) in the form

$$e^{-q'a} = \frac{1-Q}{1+Q} \approx (-2Q), \quad \text{where} \quad Q = \sqrt{\frac{\cos^2(\phi_-)r_{wb}^2 - \cos^2(\phi_+)}{\sin^2(\phi_+) - \sin^2(\phi_-)r_{wb}^2}}. \tag{15}$$

In the case of small r_{wb} we can expand ϕ_+ near point k_v where $\phi_+ = \pi n/2$ and approximate (15) as

$$Q = r_{wb}\sqrt{1-(x/x_0)^2}, \tag{16}$$

where $x = (k-k_v)/k_v$ and $x_0 \approx 2r_{wb}k_w^2k_b^2/\pi n k_v^2(k_w^2+k_b^2)$. We see, that x_0, and therefore the width of the Darwin table is largest for $n = 1$. Thus it is the best to require $\phi_+ = \pi/2$.

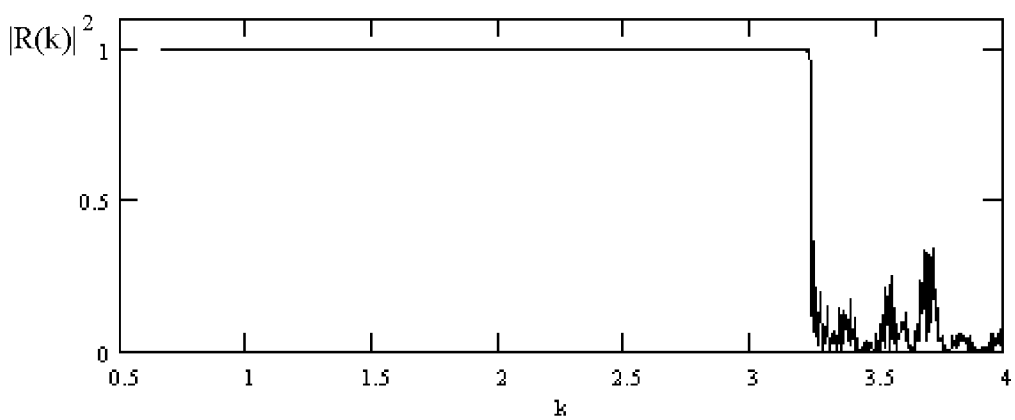

Figure 7: Dependence of reflection coefficient $|R|^2$ of FeCo-Si MS on k. MS consists of a wide barrier of width 20 and 34 chains with different number of periods. Total number of bilayers is 1947. Critical k_c for FeCo is equal to 1. Potentials do not include imaginary parts.

Now we need to find the ends k_{ve} of the Darwin table around k_v. They depend on what deviation from total reflection we tolerate. If we tolerate $|R|^2 = 1 - 2\zeta$, then

$$Q = -\ln(\zeta)/4N. \tag{17}$$

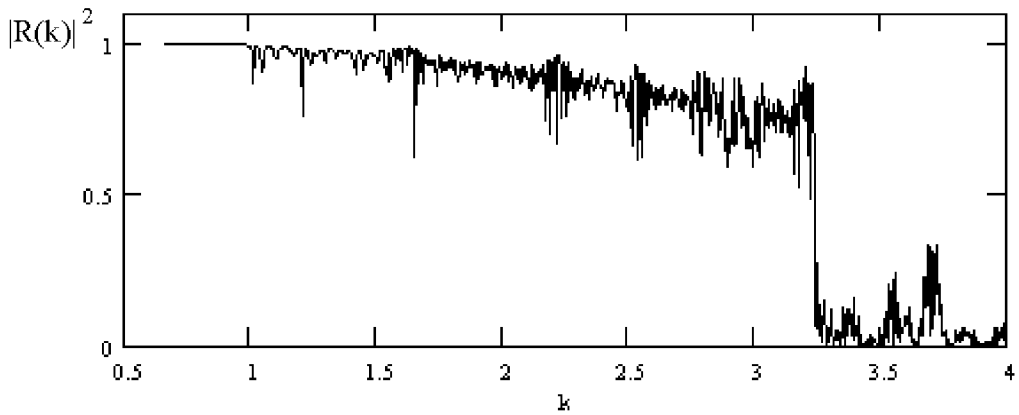

Figure 8: Dependence of reflection coefficient $|R|^2$ of FeCo-Si MS on k. Parameters of MS are the same as for fig. 7. Potentials include imaginary parts

From it we find

$$\left(\frac{x}{x_0}\right)^2 = 1 - \left(\frac{\ln\zeta}{4Nr_{wb}}\right)^2. \tag{18}$$

To find the optimal number N of periods we require the maximal effective width of δk covered by a single period, i.e. we seek a maximum of $(k_{ve} - k_v)/N$. This requirement gives

$$N = \frac{\ln\zeta}{2r_{wb}}, \tag{19}$$

and

$$\delta k = |k_{ve} - k_v| = k_v x_0 \frac{\sqrt{3}}{2} = \frac{\sqrt{3} r_{wb} k_w^2 k_b^2}{\pi k_v (k_w^2 + k_b^2)} \approx \frac{\sqrt{3}}{2\pi} k_v r_{wb}, \tag{20}$$

where k_w, k_b and r_{wb} are determined for $k = k_v$. If we tolerate $2\zeta = 1\%$, then $N = 2.6/r_{wb}$. If we use another condition $\phi_- = \pi/2$ we find that x_0 is approximately 2 times lower. So to use this condition is not profitable.

Now, the interval $\Delta' = 2\delta k = (\sqrt{3}/\pi) k_v r_{wb}$ around k_v is closed, and we can make the step to a new $k_v' = k_v + \Delta'$ and find a new periodic chain around the point k_v'. In practice we made steps $\Delta' = 2\delta k/1.1$ to ensure the overlapping of the intervals, because every next width δk is a little bit lower than the preceding one.

In fig. 7 the reflection coefficient $|R|^2$ is shown for MS consisting of 1947 bilayers with positions of the Bragg peaks chosen as prescribed above. The starting point was $k_v = 1.12$. It was found empirically. We see that reflection coefficient is perfectly equal to one.

Above we did not take into account imaginary part of the potential, however formulas (2 — 5) and (10 — 12)— are valid for arbitrary potentials, so to take into account losses or gains (in the case of active media) we need only substitute in k_w and k_b complex potentials $u_{w,b} = u'_{w,b} - iu''_{w,b}$, where minus sign means losses for $u'' > 0$. Of course, the number and widths of layers in periodic chains and the widths of the Bragg peaks are real numbers so for them we must use absolute magnitudes.

The result of calculations for the real systems FeCo-TiZr, which is similar for FeCo-Si, is shown in fig. 8. Here the number of bilayers is the same as in fig. 7, and we see that

reflection coefficient deviates from unity. It means that our requirement (17) with small ζ is not necessary, because the makes us be tolerable to stronger deviation of the Bragg reflection from unity. So we can strongly decrease the number of periods in every chain.

In fig. 9 we show how reflection coefficient presented in fig. 7 changes, when number of bilayers is decreased to 271. We see that now it becomes alike to the one shown in fig. 8. If we account for imaginary parts of potentials then for the real system FeCo-TiZr with 271 bilayers we obtain the reflection coefficient shown in fig. 10

In the case we are satisfied with smaller increase of the critical angle, we need even smaller number of layers. In fig. 11 we show reflection coefficient for FeCo-TiZr with only 46 bilayers. The parameters of these bilayers are shown in tabl. 1.

4 Reflection from the set of chains

If we have two chains with reflection and transmission amplitudes R_{Ni}, T_{Ni} $(i = 1, 2)$, then reflection R_{21} from two chains from the left (the chain 1 is to the right of the chain 2) is

$$R_{21} = R_{N2} + \frac{T_{N2}^2 R_{N1}}{1 - R_{N2} R_{N1}}. \tag{21}$$

Addition of the third chain to the left side gives the set with reflection amplitude

$$R_{321} = R_{N3} + \frac{T_{N3}^2 R_{21}}{1 - R_{N3} R_{21}}. \tag{22}$$

Four chains will have reflection amplitude R_{4321} and so on. It is a simple algorithm to calculate reflection from all the chains, and at the end we must add a single wide barrier as shown in fig. 6, which provides total reflection for all k almost up to $k = 1$. Because of finite width l_0 of the first barrier, its reflectivity drops near $k = 1$. Indeed, the reflection from the barrier is

$$r = r_{wb} \frac{1 - Q_0}{1 - r_{wb}^2 Q_0}, \quad \text{where} \quad r_{wb} = \frac{k_w - ik_b'}{k_w + ik_b'}, \quad k_w = \sqrt{k^2 - u_w}, \quad k_b' = \sqrt{1 - k^2},$$

and $Q_0 = \exp(-2 l_0 k_b')$.

para-meters	1	2	3	4	5	6	7	8	9	10	11	12
k_v	1.12	1.32	1.44	1.55	1.65	1.73	1.81	1.90	1.96	2.03	2.09	2.15
l_b	3.11	1.84	1.5	1.331	1.20	1.11	1.04	0.98	0.93	0.89	0.86	0.82
l_w	1.40	1.20	1.09	1.01	0.95	0.91	0.87	0.83	0.80	0.78	0.75	0.73
N	3	3	3	3	3	4	4	4	4	5	5	5

Table 1: Parameters of 12 periodic chains with reflection coefficient shown in fig. 8. k_v is position of the Bragg peak, l_w, l_b and N are the widths of Si and FeCo layers and number of bilayers respectively for the chain with the Bragg reflection centered at k_v. Total number of bilayers is 324. The unit of length is equal to 86.2 Å.

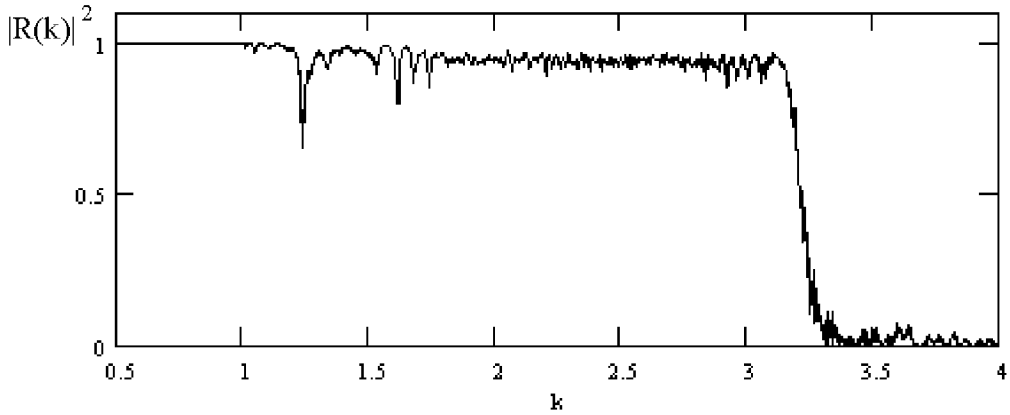

Figure 9: Dependence of reflection coefficient $|R|^2$ of the same system as in fig. 7 with number of periods in every periodic chain strongly decreased. Total number of bilayers is 271.

Suppose, we tolerate, when $|r| = 1 - \zeta$. Near the critical point $k = 1$ reflection coefficient can be approximated as

$$|r|^2 = \frac{(1-Q_0)^2}{(1-Q_0)^2 + 16k_w^2 k_b^2 Q_0} \approx 1 - 4\frac{k^2}{l_0^2},$$

so, if we want to have $|r|^2$ to be everywhere in $0 < k < 1$ larger than $1 - \zeta$, we must choose $l_0 = 2/\sqrt{\zeta}$. In particular, for $\zeta = 0.01$ we must choose $l_0 = 20$. In all the fig-s. 7 — (11 we used this width of the first barrier. However, if we take into account losses, this parameter is not too much critical. To show that we demonstrate fig. 12, which is calculated 12 chains of FeCo-TiZr MS with parameters, shown in table 1, and for $l_0 = 8$. Though reflection of smaller first barrier can be a little bit less the losses in it are also less, so the result is nearly the same. So practically we have no gain, if increase the totally reflecting layer too much.

5 Asymmetry of the period

Above we considered the case when periods of periodical chains are symmetrical, i.e. barrier of width l_b is surrounded on both sides with wells of width $l_w/2$, i.e. it is represented as a threelayer. In practice it is more simple to consider the period as a bilayer consisting of the well of width l_w and the barrier of the width l_b. Such a period is not symmetrical. Its reflection from the left r_l is not equal to reflection from the right, r_r, though transmissions from both sides is equal and is given by formula (5). The amplitudes r_l and r_r for the bilayer are

$$r_l = e^{2ik_w l_w} r_{wb} \frac{1 - \exp(2ik_b l_b)}{1 - r_{wb}^2 \exp(2ik_b l_b)} = e^{ik_w l_w} r, \quad r_r = r_{wb} \frac{1 - \exp(2ik_b l_b)}{1 - r_{wb}^2 \exp(2ik_b l_b)} = e^{-ik_w l_w} r, \tag{23}$$

where r is reflection of the symmetrical period shown in (5). With nonsymmetrical period expression (2) should be modified. For instance, reflection from the semiinfinite periodic

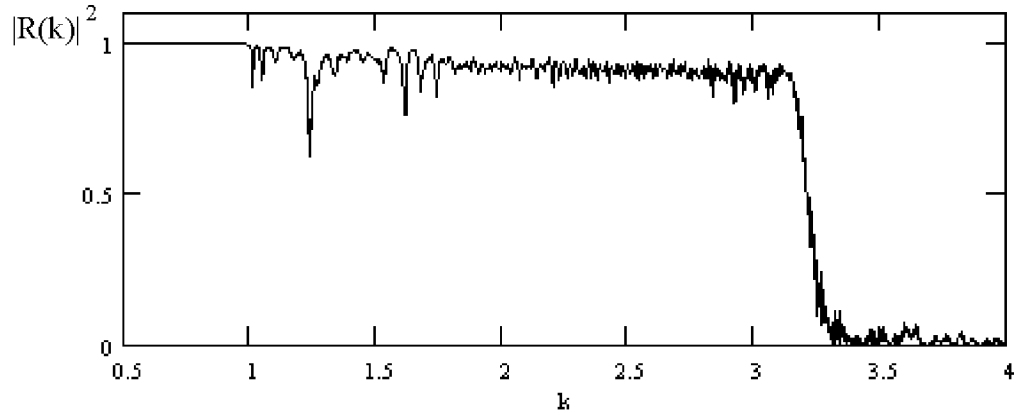

Figure 10: Dependence of reflection coefficient $|R|^2$ of FeCo-TiZr MS on k. Parameters of MS are the same as for fig. 8, but the number of bilayers is only 271.

potential beginning with the well we have $R_l =$

$$\sqrt{\frac{r_l}{r_r}}\frac{\sqrt{(1+\sqrt{r_r r_l})^2-t^2}-\sqrt{(1-\sqrt{r_r r_l})^2-t^2}}{\sqrt{(1+\sqrt{r_r r_l})^2-t^2}+\sqrt{(1-\sqrt{r_r r_l})^2-t^2}} = e^{ik_w l_w}\frac{\sqrt{(1+r)^2-t^2}-\sqrt{(1-r)^2-t^2}}{\sqrt{(1+r)^2-t^2}+\sqrt{(1-r)^2-t^2}}, \tag{24}$$

or it is $\exp(ik_w l_w)R$, where R is symmetrical amplitude given by (2). The reflection from semiinfinite periodic potential beginning with the barrier will be $\exp(-ik_w l_w)R$, i.e. asymmetry of r is inherited by R.

Equation (3) for the Bloch phase factor does not change, because instead of r^2 it contains $r_l r_r$, which is identical to r^2. Now it is easy to understand that reflection of a finite number periods R_N for asymmetrical period will change in the same way as R, i.e. for reflection from the left and right we have $R_{Nl,r} = \exp(\pm ik_w l_w)R_N$, where R_N is for the symmetrical period. Now we need to see what happens when we stack two nonsymmetrical chains. For that we need to generalize expression (1) for nonsymmetrical potentials 1 and 2 shown in fig. 1. This generalized expression is

$$R_{l12} = R_{l1} + T_1^2\frac{R_{l2}}{1-R_{r1}R_{l2}}, \tag{25}$$

where indices l, r denote reflection from the left and right respectively.

Taking into account this generalization we represent (21) in the form

$$R_{l21} = e^{ik_w l_{w2}}\left[R_{N2} + \frac{T_{N2}^2\exp(ik_w[l_{w1}-l_{w2}])R_{N1}}{1-R_{N2}\exp(ik_w[l_{w1}-l_{w2}])R_{N1}}\right], \tag{26}$$

where asymmetry is explicitly represented by the factor $\exp(ik_w[l_{w1}-l_{w2}])$. It is easy to prove that, if the chain 1 at some k gives total reflection, i.e. $R_{N1} = \exp(i\chi)$, then inclusion of chain 2 will not destroy this total reflection, i.e. R_{l21} for these k is also a unit complex number: $R_{l21} = \exp(i\chi')$. Indeed, taking into account relations (9), which are valid for R_N and T_N, we can transform (26) as follows

$$R_{l21} = -e^{ik_w[l_{w2}+l_{w1}]+i\chi+2i\phi_2}\frac{1-|R_{N2}|\exp(-ik_w[l_{w1}-l_{w2}]-i\phi_2-i\chi)}{1-|R_{N2}|\exp(ik_w[l_{w1}-l_{w2}]+i\phi_2+i\chi)}, \tag{27}$$

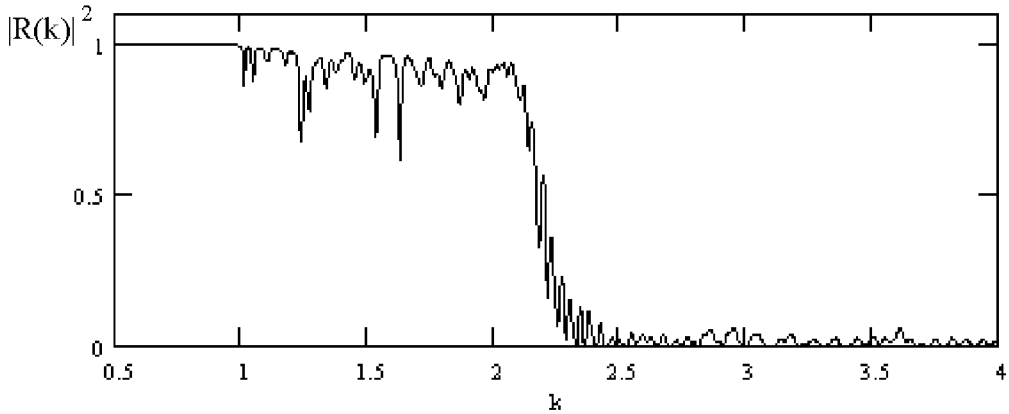

Figure 11: Reflection of 46 bilayers of FeCo-TiZr system with account of losses. Parameters of layers are shown in table 1.

where ϕ_2 is the phase of the amplitude R_{N2}. Since the last factor is of the form $\exp(i\psi)$ the whole R_{l21} is also of the form $\exp(i\chi')$ which corresponds to the total reflection.

Of course, all these relations are precise only for real potentials. Imaginary part of the potentials gives a correction to them, and the smaller is imaginary part the smaller is the correction.

6 Similarity of all the MS systems

All the MS can be represented as a system with barriers of height 1, and wells of height 0. Indeed, if in a real system barriers have the potential u_b, and wells — the potential u_w, then the potential step between well and barrier is $u_b - u_w$, and we can normalize this difference to unity, and take as a unit length the critical wave length $\bar{\lambda} = \hbar/\sqrt{2m(u_b - u_w}$. So, calculations for all the real systems is the same. The only difference is that at the end we need to include reflection amplitude from the potential step from vacuum to the well. This potential step is now has normalized potential $\tilde{u}_w = u_w/(u_b - u_w)$. If reflection amplitude from MS without this correction is R, then after correction it will be

$$r_{0w} + \frac{(1 - r_{0w}^2)R}{1 + r_{0w}R}, \quad \text{where} \quad r_{0w} = \frac{k - k_w}{k + k_w}, \quad k_w = \sqrt{k^2 - \tilde{u}_w}.$$

We applied our method to real physical system, and considered only 34 chains, though it is not principal. With these chains we are able to triple the critical angle. To double it it is sufficient to have only 12 chains. Their parameters are presented in Table 1. The first row shows the points k_v which are centers of the Bragg peaks. The first number $k_v = 1.12$ was chosen empirically. Next two rows show the width of the wells l_w and barriers l_b for those k_v, And the last line shows the number of periods in every chain. We do not present here the numbers of periods that give the perfect reflection for real potentials and requires 324 bilayers. We show here the numbers of periods that give reflection fig. 11 and 12 with 46 bilayers, and which is nearly the same as reflection for real system with 324 bilayers as can be seen from comparison with fig. 8.

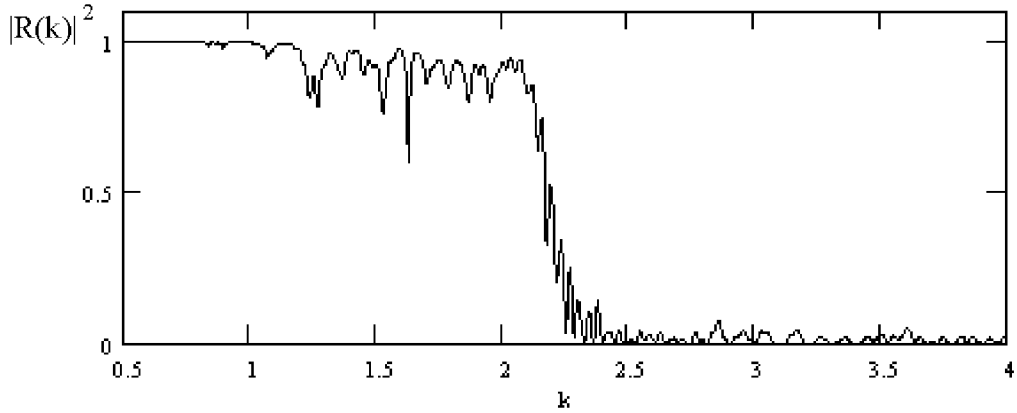

Figure 12: Reflection of 46 bilayers of FeCo-TiZr system with account of losses. Parameters of layers are shown in table 1. The width of the first barrier is 8.

Imaginary parts for potentials of real systems were normalized to difference of real parts of $u_b - u_w$. Thus for FeCo-Si system in which Si are wells with $u_w = 54.4 - i6.25 * 10^{-4}$ neV and FeCo are barriers with $u_b = 330.7 - i6.40 * 10^{-2}$ neV, the normalised potentials are $u_b = 1 - i2 \cdot 10^{-4}$ and $u_w = 0 - i2.3 \cdot 10^{-6}$.

In FeCo-TiZr system the normalized imaginary part of FeCo is $\approx 3 \cdot 10^{-4}$, and that of TiZr $\approx 1 \cdot 10^{-4}$. The main effect of losses comes from imaginary part of FeCo, so the results of calculations for real systems with Si and TiZr give nearly the same result.

The width of the first wide barrier for real systems can be taken equal to 8 instead of 20, required for perfect system with no losses. Accounting for losses shows that the increase of the first barrier only increases losses in the whole range of energies and decreases the total reflection.

7 Conclusion

We presented the method of calculation of a supermirror, having high critical angle of total reflection. We suppose that our method has some advantage, because it is analytical, and therefore more controllable. Change of parameters δl_b and δl_w from chain to chain is sufficiently large and therefore is less prone to errors related to technology of layers preparation. There is only few change of parameters comparing to common way, when the parameters change almost continuously, and δl_b, δl_w become lower than a monolayer. Such a small change of width is almost impossible to control.

We want also to add that though our analytical method is very good for analysis, it is too slow for calculations. So, the calculation of reflection coefficient, after all the parameters were defined, was performed numerically with the matrix method.

We have shown here how to prepare MS by increasing the range of total reflection step by step. However it is possible to proceed differently. We can put one bilayer on a substrate and calculate its reflection. Then put another bilayer with parameters scanned in some intervals, choose parameters, which give the larger increase of the reflectivity. Then look for parameters of third bilayer and so on. If we do not restrict thickness of layers, we can get with 200 bilayers a good reflectivity as shown in fig. 13 for some

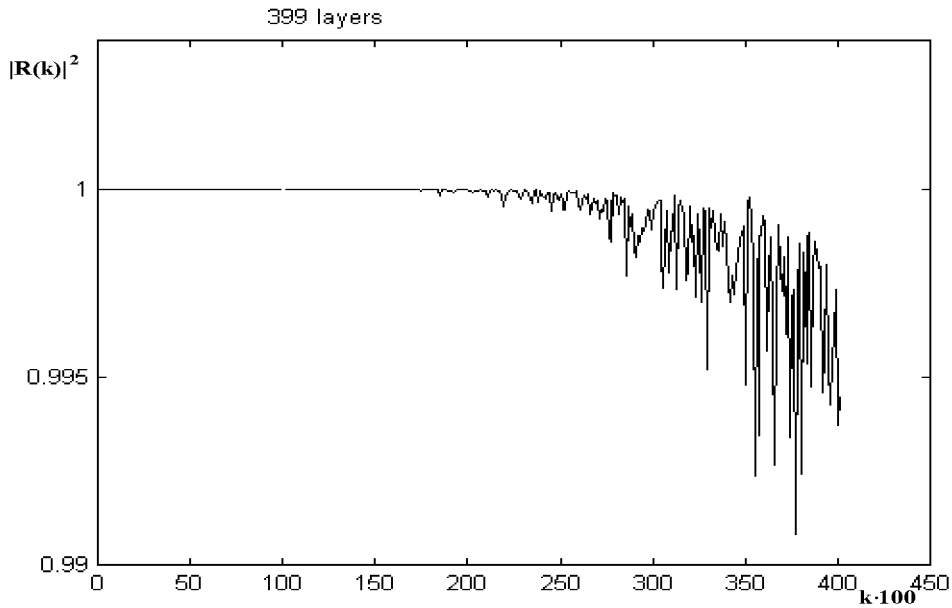

Figure 13: Reflection of 399 layers for a model system with $u_w = -1$

model system with $u_w = -1$ even for interval $k = 4k_c$[1]. However in these bilayers some thicknesses are of the order 0.1 of interatomic distance. It is clear that it is impossible to achieve a good homogeneity for such thicknesses. We can restrict thicknesses to some values when scanning in the parameter space. It may give a multilayer system with smaller number of layers and with not perfect, but well tolerable reflectivity in a wide enough interval of k.

Though this try and error method may give a tolerable reflection with smaller number of periods, the step by step method is promising for improving the technology for preparation of MSs. When we know exact thickness of a single monolayer we can prepare layers with better surfaces, and we can control the perfectness of the layers by comparing calculated and really obtained reflectivities in a wide range of energies.

We considered here only reflection of neutrons from MSs. There is no problem to apply our method also to x-rays. However to do that we should find a better way to optimize number of layers when we account for imaginary parts of the potentials. In the case of neutrons the number of layers can be easily found somewhat empirically. In the case of x-rays we can do the same, however because the imaginary parts for x-rays are considerably higher the analytical analysis must be more reliable.

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