RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 49, NUMBER 15 15 APRIL 1994-I

Direct observation of neutron-guided waves in a thin-film waveguide

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(Received 29 December 1993)

Guided propagation of neutrons in thin films was directly observed in a TiO_2/Ti/Si waveguide by exciting one of its discrete guided modes from an external neutron beam. The condition found experimentally for exciting this particular mode agrees well with theory. The measured intensity of the guided neutrons was also in good agreement with a calculation based on a previous coupling theory.

Total reflection of neutrons[1] from smooth interfaces has a wide range of applications in neutron optical devices. Macroscopic neutron guide tubes have been successfully constructed to transport neutrons emerging from a nuclear reactor to experimental stations situated tens of meters away, reducing the background level of radiation considerably.[2] Hollow glass capillaries of micrometer diameters have been used to form a neutron focusing lens.[3,4] In both cases, the propagation of neutrons can be described by geometrical optics, provided an effective refractive index for neutrons is used. A neutron of an arbitrary momentum is allowed to be guided so long as it strikes the guide or capillary wall below the relevant critical angle. More importantly, due to the large transverse dimensions of the guide tubes or glass capillaries, the interference effect of neutron waves does not manifest in these devices.

If the transverse size of the guiding device is sufficiently small, the wave nature of neutrons becomes essential, such as in a planar waveguide[5] composed of a thin film sandwiched between media of lower refractive indices. Similar to guides for electromagnetic radiation at both optical[6] and x-ray[7] wavelengths, a neutron thin-film guide can sustain only a discrete set of guided modes, each corresponding to two coherent neutron waves with well-defined momenta that are equal in amplitude but opposite in sign. To effectively excite these modes from an external neutron beam, a scheme of resonant coupling analogous to the prism coupling[8] for light can be used.[5] For a lossless coupler, the coupling efficiency can be as high as 81% for a monochromatic and infinitely coherent beam. Here, we present experimental measurements illustrating neutron-guided propagation in a TiO_2/Ti/Si thin-film guide excited by a resonant coupler. We have excited the uppermost mode of the guide at an angle agreeing very well with our calculations. The measured intensity of the guided waves could be explained by a calculation based on a previous theory.

In the absence of any Bragg diffraction, neutron propagation in a medium can be described by an effective refractive index $n=1-\delta_N=\sqrt{1-V/E_0}$, where E_0 is the neutron kinetic energy and V the average potential of the medium. For nonmagnetic materials with negligible incoherent and absorption processes, $V=2\pi\hbar^2\rho b_{\text{coh}}/M_n$, where M_n is the neutron mass, b_{coh} the coherent scattering length, and ρ the number of neutrons per unit volume. At an interface between vacuum and a medium characterized by V, the critical angle for neutron total reflection $\theta_c=\sin^{-1}(\sqrt{V/E_0})$. To form a neutron guide, a thin film is surrounded by media of higher scattering potential (thus lower refractive indices), allowing neutrons to be guided by total reflection at both interior interfaces. For an asymmetric guide whose boundary media have *slightly* different scattering potentials, the total number of guided modes N_{total} is given by

$$N_{\text{total}} \sim 1+(d_2/\lambda)\sqrt{8\Delta\delta_N} \, , \tag{1}$$

where d_2 is the film thickness, λ the neutron de Broglie wavelength, and $\Delta\delta_N$ the difference between δ_N of the thin film and the average of the boundary media.[9] Since typically $\delta_N \sim 10^{-6}$, d_2 needs to be 10^2-10^3 Å to allow for more than one mode. Thus, in general, $d_2 \gg \lambda$, permitting a device to function as a waveguide even in the presence of interfacial roughness comparable to or even greater than λ.

We have fabricated a thin-film guide structure composed of a coupling, guiding, and decoupling sections as shown in Fig. 1. The guiding layer was a 1200-Å-thick Ti film evaporated on an optically flat 4-in.-diameter silicon wafer. A roughly 150-Å- (d_1) thick TiO_2 film was then formed electrochemically from this Ti film, reducing its thickness d_2 to about 1050 Å. By masking off the coupling and decoupling regions, a 6000-Å-thick SiO_2 layer was evaporated onto the center of the TiO_2 film, completing the main body of the guide which is asymmetric due to the different δ_N for Si and the TiO_2/SiO_2 bilayer. For practical purposes, the SiO_2 overlayer in the guiding region can be regarded as infinite. The roughness of the Si/Ti, Ti/TiO_2, and TiO_2/SiO_2 interfaces was estimated to be about 25, 45, and 65 Å, respectively, based on a reflectivity measurement and the corresponding analysis using a slicing method.[10]

The physics of a thin-film waveguide can be mapped into that of a one-dimensional potential well as illustrated in Fig. 2: the wave functions in the z direction of the guided modes are equivalent to those of the bound states of the well. Using $\delta_N = 1.82\times10^{-6}$, -1.71×10^{-6}, 1.11×10^{-6} (Ref. 11), and 3.07×10^{-6} for Si, Ti, TiO_2, and SiO_2, respectively, our calculation showed that there are three guided modes as shown in Fig. 2(a) by the three bound states Σ_0, Σ_1, and Σ_2, agreeing with Eq. (1). Because of the negative scattering potential of Ti, $V_3<0$, both Σ_0 and Σ_1 are negative.

External neutrons can be coupled into a guide by making one of its boundary layers sufficiently thin as depicted in Fig. 2(b).[5] This process corresponds to the resonant tunneling by an incident beam impinged on the potential barrier V_2 of the TiO_2 layers as a function of $k_z = k_0 \sin\theta_{in}$, the z component of the neutron wave number in vacuum, where θ_{in} is the incident angle.[5] We note that a desired V_2 is one that is higher than all the bounds states. In the present device, however, V_2 is lower than Σ_2, and thus no true resonant coupling (tunneling) can be achieved. It is nevertheless possible to excite the Σ_2 mode quasiresonantly, if T_1 matches exactly Σ_2, where $T_1 = E_0 \sin^2\theta_{in} = \hbar^2 k_z^2/2M_n$ is the neutron kinetic energy in the z direction in vacuum. On this condition, the incident neutrons can be "trapped" in the well (Ti layer) with a finite probability P_m. If the neutron energy is fixed, this quasiresonance can be achieved by adjusting θ_{in}. By making the TiO_2 layer suddenly very thick or covering the TiO_2 layer with a thick SiO_2 overlayer as in the present case, the neutrons dwelling inside the Ti layer will remain trapped and become guided neutrons. These guided neutrons can escape from the guiding layer from another region of thin TiO_2 layer in the decoupling section, whose action is a complete reversal of that of the coupler. Since T_1 is always positive, only the Σ_2 mode can be directly excited as depicted in Fig. 2(b). This was indeed confirmed experimentally.

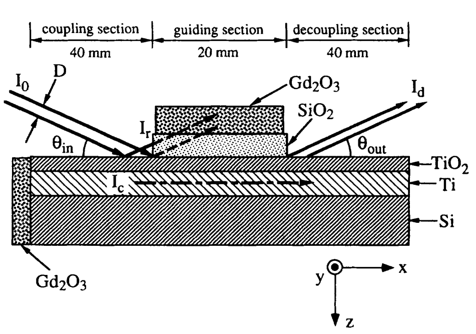

FIG. 1. Schematic diagrams of a thin-film neutron waveguide structure: the section covered by the SiO_2 film is the main body of the waveguide, while the sections on the left and on the right function as two resonant beam couplers, allowing the incident beam to be coupled into the guiding layer and then subsequently decoupled from the guiding layer for detection. The Ti film is about 1050 Å thick, and the TiO_2 layer is about 150 Å thick. The length of the guiding region is about 20 mm.

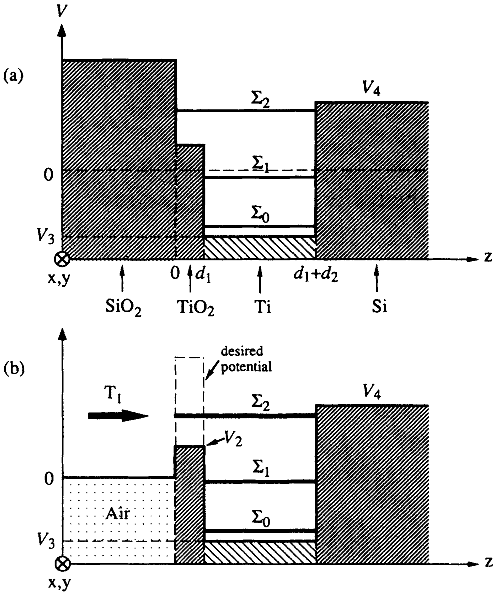

FIG. 2. The quantum-mechanical representations of (a) the waveguide where there are three bound states (Σ_0, Σ_1, and Σ_2) corresponding to the three guided modes, and (b) beam coupling when the energy T_1 of incident neutrons matches that of the Σ_2 mode, allowing them to become "trapped" in the guiding media of TiO_2 and Ti layers. A true resonant trapping is achieved only when the potential V_2 has the desired height above Σ_2. Note that only the Σ_2 mode is directly accessible because T_1 is always positive.

Our measurements were carried out on the BT-7 reflectometer of NBSR at the National Institute of Standards and Technology. A filtered monochromatic neutron beam with an average value of 2.35 Å and 1% spread in wavelength was used. The angular divergence $\Delta\Theta$ of the beam in the x-z plane was calculated to be 2.4×10^{-4} rad. The effective beam size D was calculated to be 62 μm, projecting out a footprint of $D/\sin\theta_{in} = 37$ mm at $\theta_{in} = 0.095°$ on the coupling surface. The beam size $D_y = 25.4$ mm in the y direction and is irrelevant in our analyses. The total measured intensity I_0 of the incident neutrons was 1700 counts/sec. Since an incident neutron has a finite probability to be reflected even at resonance and a certain fraction of the incident neutrons does not match the resonance condition, there is a considerable intensity in the directly reflected beam I_r. To block I_r so that it did not obscure our measurements, we have painted the front end of the guide and the top surface of the SiO_2 layer by highly absorbing Gd_2O_3 paste as shown in Fig. 1.

The guided neutron waves were observed by systematically varying the incident angle θ_{in} and then scanning the detector angle θ_{out} about the direction where they were expected to escape from the guide. In Fig. 3, three such scans are shown where θ_{out} was varied between 0.04° and 0.16° with θ_{in} being fixed at 0.09°, 0.10°, and 0.11°, respectively. A well-defined peak centered at $\theta_{out}=0.095°$ is clearly shown for the scan at $\theta_{in}=0.10°$, indicating that the Σ_2 mode was excited and propagated through the guide. Whereas at $\theta_{in}=0.11°$, no peaks can be resolved above a sloping background. This background was present in all three scans and is attributed to a refracted beam running nearly parallel to the surface of the guide. This spurious effect is caused by the large angular divergence of the beam that allowed certain neutrons to impinge on the coupler at angles higher than the critical angle of the Ti/Si interface, and thus to get refracted. We note that at $\theta_{in}=0.09°$, only a very weak anomaly can be seen. However, the shapes and the center positions of these two anomalies at $\theta_{in}=0.09°$ and 0.10° are essentially identical, indicating that the decoupled beam, if any, would come off the decoupler at the exactly same angle characteristic of the Σ_2 mode.

The "resonant" nature of the coupling was confirmed in Fig. 4, where the decoupled intensity I_d extracted at a fixed $\theta_{out}=0.095°$ was plotted for seven scans of different θ_{in}'s. The "resonant" line shape was best fit to a Lorentzian centered at $\theta_2=0.098°$ with a half-width $(\Delta\theta_2)_{exp}$ of 0.009° or 1.6×10^{-4} rad. This resonance at $\theta_{in}=\theta_2=0.098°$ agrees well with our calculation to within the experimental resolution. We have calculated the width $2\Gamma_2$ of resonant coupling to be 1.6×10^{-3} Å^{-1}, corresponding to an angular width $(\Delta\theta_2)_{cal}$ of 6×10^{-4} rad for a fixed neutron energy. The measured width $(\Delta\theta_2)_{exp}$ was, however, determined by both the intrinsic linewidth $(\Delta\theta_2)_{int}$ of the Σ_2 mode inside the guiding section and $\Delta\Theta$. We note that $(\Delta\theta_2)_{int}$ is much smaller than $(\Delta\theta_2)_{cal}$ and depends only on the broadening mechanisms such as absorption and diffuse scattering from interfacial roughness.

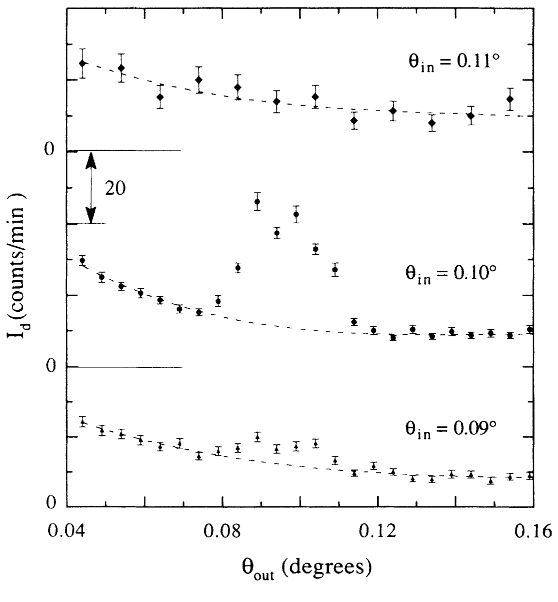

FIG. 3. Detector scans of the tunneled neutron beam I_d with incident angle θ_{in} fixed at a value of 0.09°, 0.10°, and 0.11° separately. The sloping background shown by the dashed lines is due to a refracted beam (see text).

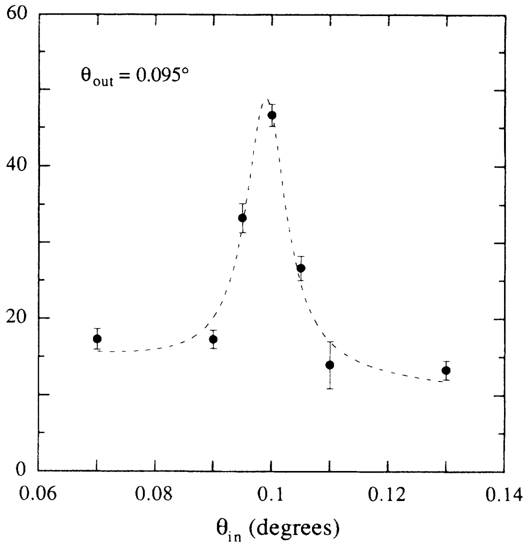

FIG. 4. Resonant coupling of the Σ_2 mode. Plotted is the measured intensity of the decoupled neutrons at a fixed angle θ_{out} for various incident angles. The dashed line represents an empirical fit to a Lorentzian line shape with a full width at half maximum of 0.009° and a center angle of 0.098°.

To account for the measured intensity I_d, we make the assumptions that losses during coupling due to absorption and incoherent scattering processes are negligible and that the incident beam is coherent over a distance D_{coh} along D such that $D_{coh}\leq D$. We also assume that the coupling theory based on the desired potential $(V_2>\Sigma_2)$ remains valid. At resonance, the probability for the incident neutrons to remain in the well is given by

$$P_m \approx \left[\frac{D_{coh}}{D}\right]\frac{8\sinh^2(\Gamma_m D_{coh}/2)}{\Gamma_m D_{coh}}e^{-\Gamma_m D_{coh}} , \qquad (2)$$

where Γ_m is the half-width of the mth resonance.[9] Clearly, P_m depends crucially on the parameter $\Gamma_m D_{coh}$, and reaches a maximum of 81% if $\Gamma_m D_{coh}=1.26$ and $D_{coh}=D$. Using the calculated $\Gamma_2=8\times10^{-4}$ Å^{-1} and assuming that $D_{coh}=D=62$ μm, we found that $\Gamma_2 D_{coh}=496$ and the coupling efficiency $P_2=0.4\%$, much smaller than the ideal value of 81%. The small value of P_2 is a direct result of the large Γ_2 that allows the coupled neutrons to escape easily from the guide before reaching the guiding section.

If the effect of interfacial roughness is neglected, the expected intensity of the Σ_2 mode emerging from the decoupling section is given by

$$I_d \approx F P_2 Q_2 e^{-\alpha_a L} I_0 , \tag{3}$$

where F represents the fraction of the incident beam that falls within the width $(\Delta\theta_2)_{\text{int}}$ and thus can be accepted by the guide after having been coupled into the Ti layer, $Q_2 = 1$ is the escaping probability[9] of a Σ_2 mode neutron from the decoupling section, and the factor $\exp(-\alpha_a L)$ arises from attenuation due to absorption and incoherent scattering, with $L = 20$ mm being the length of the guiding section. For simplicity, we estimated $(\Delta\theta_2)_{\text{int}}$ by the measured width $(\Delta\theta_2)_{\text{exp}}$ and $F \sim (\Delta\theta_2)_{\text{exp}}/\Delta\Theta \sim 0.67$. The constant α_a of the Σ_2 mode can be approximated by that of the Ti layer, i.e., $\alpha_a = l_a^{-1} = 0.063$ mm^{-1}, where $l_a = 16$ mm is the $1/e$ length of Ti for 2.35-Å neutrons. Hence, $I_d = 1.3$ counts/sec, agreeing well with the measured value of 0.6 counts/sec.

The interfacial roughness in the guide structure will cause mode mixing[12] between the Σ_2 mode and other guided modes and unbound modes above Σ_2. Since both the Σ_0 and Σ_1 modes were negative and could not be decoupled like the Σ_2 mode, we did not directly observe mixing between these three guided modes. The mixing probability is related to the average reflectivity of the boundary interfaces of the guide. In light of the large roughness (> 20 Å) at the boundary interfaces, we expect that the three guided modes were *fully* mixed at the end of the guiding section so that there was an equal population of neutrons in each mode. This would reduce the expected decoupled intensity of the Σ_2 mode by roughly a factor of 3 to 0.4 counts/sec, in even better agreement with the observed value. Of course, neutrons in the Σ_2 mode could also be transferred to the unbound modes, causing additional losses not included in Eq. (3). Based on the close agreement between the calculated and measured I_d, we believe, however, that these losses were quite small.

If the coherence length D_{coh} of the incident beam was shorter than its geometrical width D, we must reconsider the above analysis. As evident from Eq. (2), D_{coh} sets the upper limit for the portion of the beam that can be resonantly coupled, while $1/\Gamma_m$ sets the upper limit for the actual portion that will be coupled if $D_{\text{coh}} > 1/\Gamma_m$. A previous direct measurement has found that D_{coh} was of the order of 20 μm.[13] Since $2/\Gamma_2 = 0.25$ μm, the useful portion of the beam was only about 0.25 μm, leading to a small probability $P_2 = 0.4\%$. The fact that we did observe resonant coupling and guided waves rules out the possibility that $D_{\text{coh}} \ll 0.25$ μm, because such a short D_{coh} would give too small a P_2 to be consistent with the measurement.

In summary, guided propagation of neutrons has been directly observed in a thin-film waveguide, and quantitative analysis of the guided wave intensity indicates that the transverse coherence length of the incident beam is at least 0.25 μm and that the losses due to the large interfacial roughness (> 20 Å) in the device is quite small.

We acknowledge useful conversations with D. Weitz.

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[1] E. Fermi and W. Zinn, Phys. Rev. **70**, 103 (1946).

[2] H. Maier-Leibnitz and T. Springer, J. Nucl. Energy A/B **17**, 217 (1963).

[3] M. A. Kumakhov and V. A. Sharov, Nature **357**, 390 (1992).

[4] H. Chen *et al.*, Nature **357**, 391 (1992).

[5] R. E. De Wames and S. K. Sinha, Phys. Rev. B **7**, 917 (1973).

[6] J. Kane and H. Osterberg, J. Opt. Soc. Am. **54**, 347 (1964).

[7] Y. P. Feng, S. K. Sinha, H. W. Deckman, J. B. Hastings, and D. P. Siddons, Phys. Rev. Lett. **71**, 537 (1993).

[8] P. K. Tien and R. Ulrich, J. Opt. Soc. Am **60**, 1325 (1970).

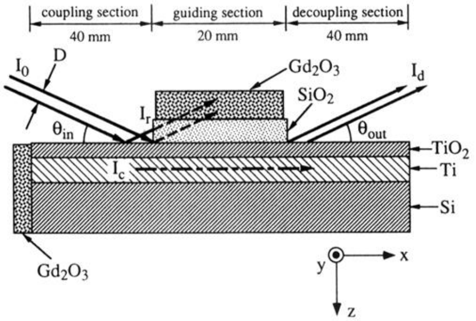
[9] Y. P. Feng (unpublished).

[10] D. G. Wiesler (unpublished).

[11] This value of δ_N for TiO$_2$ was obtained from a reflectivity measurement (Ref. 10) and is about two times lower than that expected.

[12] Mode mixing is a very common phenomenon that has been observed in optical and x-ray thin-film waveguides.

[13] C. G. Shull, Phys. Rev. **179**, 752 (1969).



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