X-Ray Flux Enhancement in Thin-Film Waveguides Using Resonant Beam Couplers

Y. P. Feng,[1] S. K. Sinha,[1] H. W. Deckman,[1] J. B. Hastings,[2] and D. P. Siddons[2]
[1]*Exxon Research and Engineering Company, Annandale, New Jersey 08801*
[2]*National Synchrotron Light Source, Brookhaven National Laboratory, Upton, New York 11973*
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We present experimental evidence for achieving significant x-ray flux enhancement by coupling a highly collimated and monochromatic synchrotron x-ray beam into a Si/polyimide/SiO_2 thin-film waveguide. The observed 20-fold flux increase agrees with theoretical predictions and was limited only by absorption of the 1 Å x rays in the waveguide structure.

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It is well known that a thin-film optical waveguide can support a discrete set of guided modes in which the light is confined mainly to the guiding film [1]. Such guided waves can be excited from an external source via a prism coupler [2], whose efficiency can be as high as 81% for coupling a laser beam. It is thus possible to effectively compress a laser beam into a thin film and increase its flux by orders of magnitude.

Coupling and subsequent guided propagation of radiation at very short wavelengths in thin-film waveguides should also be possible as was first proposed for neutrons by De Wames and Sinha [3], by using a resonant beam coupler (RBC) analogous to a prism coupler. For x rays, the refractive index of a medium is given by $n=1-\delta+i\beta$, where $\delta\sim10^{-6}$ is proportional to the electron density, and $\beta\sim10^{-8}$ is proportional to the x-ray absorption coefficient [4]. An x-ray waveguide can thus be formed by surrounding a thin film by media of higher electron densities, allowing x-ray guided propagation by total reflections within the guide. Experimentally, x-ray propagation in a thin-film waveguide that used a RBC was first observed by Spiller and Segmüller [5]. Because of the low intensity and large angular divergence of the x-ray source used, the observed coupling efficiency was quite small, and consequently no flux enhancement was demonstrated.

Because of the high brightness of modern synchrotron sources, highly collimated and monochromatic x-ray beams with an energy spread of ~1 eV can be obtained without severely sacrificing the beam intensity. For an ideal RBC illuminated by a perfectly monochromatic beam, theory [3] has predicted a maximum coupling efficiency of 81% and a possible flux enhancement of 10^2- to 10^3-fold. In a real RBC, however, the effects of absorption and surface roughness must be considered. A recent calculation [6] showed that they both reduce the coupling efficiency while increasing the bandwidth of the coupling.

In this Letter, we present measurements and analysis of the resonant coupling of a synchrotron x-ray beam into a Si/polyimide/SiO_2 thin-film waveguide structure and show that it is possible to achieve near theoretical performance in an absorbing RBC with interface roughness of ~6 Å. The measured coupling efficiency ranges from 0.7% to 22% depending on the mode, producing a maximum flux enhancement of over 20-fold in the RBC within a bandwidth less than 0.6 eV.

The performance of the RBC was determined by studying the complete guide structure shown in Fig. 1. The guiding layer of thickness d_2 was formed by spin coating a polyimide (PIQ) [7] film on an optically flat Si wafer. The roughness of the PIQ film was measured to be ~6 Å from x-ray reflectivity experiments. A thin SiO_2 overlayer of thickness d_1 was evaporated onto the PIQ film, followed by the deposition of a second but very thick SiO_2 stripe on the center of the wafer, forming the coupler (RBC), guiding, and decoupler sections.

The principle of the x-ray RBC is similar to that of optical prism couplers [2]. An x-ray beam is impinged on the thin SiO_2 layer in the RBC at an angle $\theta_{in}<\theta_c$ (the critical angle of the air/SiO_2 interface), creating an evanescent wave below the interface. This evanescent wave can resonantly excite a guided mode, if the vertical component of the incident wave vector k_z $(=2\pi\sin\theta_{in}/\lambda)$ exactly matches that required for that mode [3,6]. At resonance, a part of the incident x rays is not reflected but tunnels into the guiding layer. For a beam of *a vertical width W,* the x-ray intensity in the guiding layer of the RBC builds up continuously, reaching a maximum I_m^c at a point directly below where the incident footprint ter-

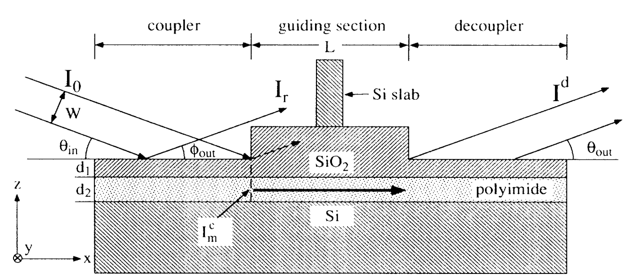

FIG. 1. Cross section of a planar x-ray waveguide structure and the experimental setup (not drawn to scale). The coupling (RBC) and the decoupling sections function as two "air" prism couplers.

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minates [8]. By making the SiO_2 layer suddenly thick, the tunneled x rays will remain in the guiding layer and propagate through the guiding section. For optimal coupling, the incident footprint is arranged to end just before the thick layer as depicted in Fig. 1. The guided x rays could be decoupled from the guide either by terminating the waveguide and letting them spill out at the end or via a decoupling section that reverses the action of the RBC.

The experiment was carried out at beam line X27C of the National Synchrotron Light Source at Brookhaven National Laboratory. By reflecting an unfocused white beam off a dispersive Si (220) monochromator assembly, a highly monochromatic 11.83 keV ($\lambda = 1.048$ Å) x-ray beam with an energy spread ΔE of 0.6 eV was obtained. The beam was then collimated by slits to have a vertical width W of 20 μm and a horizontal width W_y of 8 mm (irrelevant here since the plane of reflection is vertical). The incident footprint in the x direction was 7.6 mm at $\theta_{\text{in}} = 0.15°$ and the incident angular divergence $\Delta\theta_{\text{in}}$ was estimated to be 14 μrad. The vertical coherence length (along W) of the beam is determined by $L_t = \lambda D/\sigma = 14$ μm, where $\sigma = 115$ μm is the vertical size of the source and $D = 15$ m is the distance between the source and the sample. The longitudinal coherence length of the beam depends on the monochromaticity and is given by $L_l = \lambda(E/\Delta E) = 2$ μm.

To observe resonant coupling, the reflectivity of the RBC was first measured by varying the incident angle θ_{in} (without the Si slab in place as in Fig. 1). As shown in Fig. 2, the reflectivity (I_r/I_0, where I_0 is the incident intensity) is very close to unity for $\theta_{\text{in}} < 0.16°$, except at angles very near 0.122°, 0.128°, 0.136°, 0.145°, and 0.154°. The dips at these angles are the signatures of the resonant modes (TE_0 through TE_4) [9] in an absorbing waveguide, where absorption is greatly enhanced at each resonance because of the prolonged duration of the tunneled x rays in the film [6]. Other reflectivity minima for $\theta_{\text{in}} > 0.16°$ correspond to the usual interference fringes. Apart from the intensity that tunneled into the guiding section and the fact that W is finite, the full reflectivity curve can be approximated using the standard electromagnetic theory for an infinite plane wave incident on a multilayer sample. The solid line in Fig. 2 represents a fit in which d_2, d_1, and δ of each layer were varied and the incident angular divergence $\Delta\theta_{\text{in}}$ was folded in [10]. It was found that $\delta = 3.3\times10^{-6}$, 2.2×10^{-6}, and 3.6×10^{-6} for SiO_2, polyimide, and Si, respectively, and that $d_2 = 1230$ Å, and $d_1 = 378$ Å, agreeing with the values measured during fabrication. The values of β were not varied; instead the calculated values of 2.3×10^{-8}, 2.3×10^{-9}, and 4.0×10^{-8} were used for SiO_2, polyimide, and Si, respectively.

The width Γ_m in k_z of the resonant coupling was best measured by tuning the x-ray energy E at a fixed θ_{in} and detecting x rays exiting the decoupler. The x rays that reflected directly off the RBC were blocked by a Si slab placed on top of the thick SiO_2 stripe. Figure 3 shows the decoupled intensity I^d of the TE_2 mode versus E, when the same mode was excited at $\theta_{\text{in}} = 0.136°$. The solid line is a fit by a Lorentzian with a full width of 74 eV [11] or equivalently $2\Gamma_2^{\text{exp}} = 8.9\times10^{-5}$ Å^{-1}. Other measured widths are given in Table I. A recent calculation [6] shows that $\Gamma_m = \Gamma_m^e + \Gamma_m^a$, where Γ_m^e is proportional to the evanescent wave amplitude that causes x rays to leak in and out of the guiding layer and depends exponentially on d_1, and Γ_m^a is due to absorption and diffuse scattering losses. Inside the guide, Γ_m^a becomes the intrinsic width of the TE_m mode. By treating the guide structure as a symmetric one and solving the mode equations numeri-

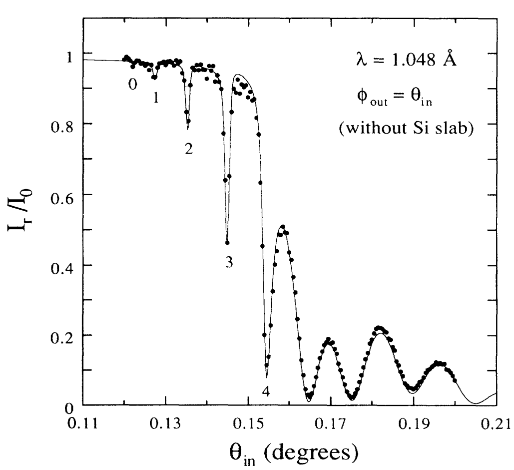

FIG. 2. Reflectivity I_r/I_0 of the input RBC. The five dips for $\theta_{\text{in}} < 0.16°$ signify the five TE modes. The solid line represents a fit using the standard electromagnetic theory in multilayers.

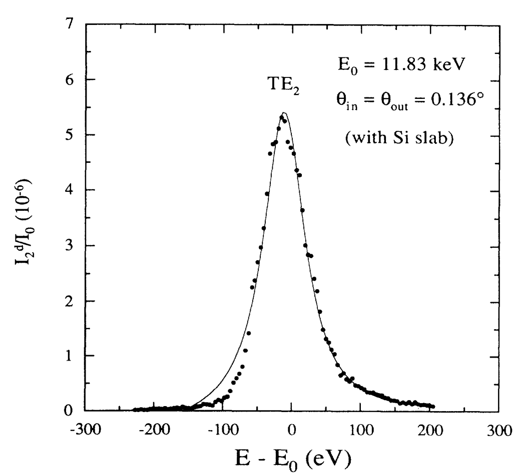

FIG. 3. Resonant coupling of the TE_2 mode measured by tuning the incident x-ray energy E at a fixed $\theta_{\text{in}} = 0.136°$. The solid line represents a fit by a Lorentzian with a full width of 74 eV, equivalent to a coupling width of $2\Gamma_2 = 8.9\times10^{-5}$ Å^{-1}.

TABLE I. The calculated and measured quantities of each guided mode. The measured $2\Gamma_m$ was limited by the incident resolution of $\Delta k_z = 8.56\times10^{-5}$ Å^{-1}. Note that Γ_4 and α_4 were obtained by extrapolation from those of the lower order modes [9].

	$2\Gamma_m(10^{-5}$ Å$^{-1})$		α_m	I_m^d	η_m (%)		$M_{\max}$
Mode	Calculated	Measured	(cm^{-1})	(10^{-7})	Calculated	Measured	Estimated
TE_0	1.38	8.8	2.92	8.3	0.6	0.7	1.1
TE_1	1.62	8.8	3.47	54	3.0	2.5	4.1
TE_2	2.44	8.9	5.12	61	7.5	6.0	9.8
TE_3	4.24	11.8	7.88	19	12.3	13.4	22
TE_4	~8.86	~20	~11.7	1.1	~11.3	~22	~36

cally with the parameters found from the fit in Fig. 2, Γ_m was calculated as given in Table I, in particular, $2\Gamma_2^{calc} = 2.44\times10^{-5}$ Å^{-1}, much smaller than the measured value. The larger width in Fig. 3 can be fully accounted for by the incident divergence $\Delta\theta_{in}$, which amounted to a spread of $\Delta k_z = 8.56\times10^{-5}$ Å^{-1} in k_z.

The efficiency η_m of the RBC for the TE_m mode is defined as I_m^c/I_0^m, where I_m^c is the intensity of the TE_m mode entering the guiding section, and $I_0^m \cong I_0(2\Gamma_m/\Delta k_z)$ is the incident intensity within the coupling bandwidth Γ_m, if $\Delta k_z \geq 2\Gamma_m$. As shown below, η_m could be determined from the intensity of the TE_m mode I_m^d exiting the decoupler while it is being excited in the RBC. As shown in Fig. 4, when the TE_1 mode was excited at $\theta_{in} = 0.128°$, the same TE_1 mode was observed exiting the decoupler at $\theta_{out} = 0.128°$. However, there were four additional peaks at $\theta_{out} = 0.122°$, 0.136°, 0.145°, and 0.154°, corresponding to the other four modes TE_0, TE_2, TE_3, and TE_4. This effect is commonly known as mode mixing in optical

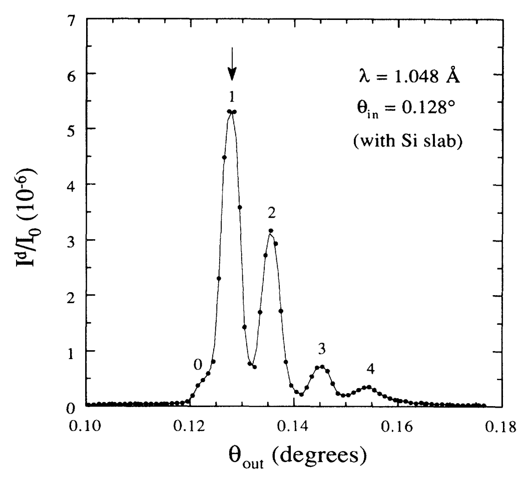

FIG. 4. X-ray intensity I^d exiting the decoupler with $\theta_{in} = 0.128°$ set to excite TE_1 only (the line is a guide to the eye). The four peaks and one shoulder correspond to all five guided TE modes present in the guide due to mode mixing. The intensity of the TE_1 mode is in fact much greater than that of the other modes. The small magnitude of I^d is due primarily to absorption in the guide.

systems [1] and is caused primarily by density inhomogeneities and interface roughness in the guide. Mode mixing was always observed regardless which mode was being excited. Note that the angular width of the various peaks in Fig. 4 does not reflect the true Γ_m, because they were smeared by the instrumental resolution of the detector slits.

If mode mixing is *not* considered, the decoupled intensity of the TE_m mode I_m^d is simply given by

$$I_m^d \cong I_m^c e^{-\alpha_m L}\xi_m = I_0\left(\frac{2\Gamma_m}{\Delta k_\perp}\right)\eta_m e^{-\alpha_m L}\xi_m\,, \qquad (1)$$

where η_m is the coupling efficiency, $L = 1$ cm is the length of the guiding section, $\xi_m \approx \eta_m$ is the decoupling efficiency [6], and α_m is the calculated attenuation constant of the TE_m mode. For the TE_0 mode, α_0 should be roughly equal to the absorption coefficient of the PIQ, because nearly all the x rays in this mode are confined to the guiding layer. For high order modes, however, x rays penetrate more into the more absorbing boundary layers, yielding greater α_m. It was found that $\alpha_m \approx a_0 + a_1 m^2$, where $a_0 = 2.92$ cm^{-1} and $a_1 = 0.276$ cm^{-1} [6]. By inverting Eq. (1), η_m can be obtained by

$$\eta_m \cong \left\{\left[\frac{I_m^d}{I_0(2\Gamma_m/\Delta k_\perp)}\right]e^{\alpha_m L}\right\}^{1/2}. \qquad (2)$$

As shown in Table I, η_m ranges from 0.7% to 22% within the respective bandwidth of the modes, much lower than the 81% efficiency achievable in a nonabsorbing RBC [3]. In a more elaborate analysis [12], mode mixing was considered using a phenomenological approach. The observed intensity distribution such as that in Fig. 4 was found to be consistent with uniform mixing occurring primarily between nearest neighbor modes. This analysis yielded a set of coupling efficiencies in good agreement with those obtained from Eq. (2).

For the given waveguide structure, η_m can be calculated from theory [6] which showed that $\eta_m \propto \Gamma_m^e/(\Gamma_m^e + \Gamma_m^a) = \Gamma_m^e/\Gamma_m$, where Γ_m^e and Γ_m^a are the evanescent wave and absorption contributions to the coupling width Γ_m, respectively. Since Γ_m^e depends exponentially and Γ_m^a only quadratically on the mode number m, η_m has a strong mode dependence. The predicted η_m's are listed in

Table I, agreeing well with those obtained from Eq. (2). For lower order modes, calculation showed that $\Gamma_m^e \ll \Gamma_m^a$, yielding rather small efficiencies. This means that the rate at which the x rays tunnel across the SiO_2 layer is not fast enough to build a large intensity up because they are being rapidly absorbed. We point out that, in calculating η_m, the beam was assumed to be coherent across W. This would overestimate η_m slightly. However, the symmetric waveguide approximation made for calculating Γ_m^e would underestimate η_m, because a larger value for δ was used for the thin SiO_2 layer, resulting in an underestimation of the evanescent wave amplitudes.

The flux enhancement factor M of the RBC (defined as the ratio of the flux of the TE_m mode in the guiding layer over that of the incident beam within the bandwidth Γ_m) is determined from the coupling efficiency. At the entrance of the guiding section the TE_m mode has the maximum intensity I_m^c, giving rise to a maximum M given by

$$M_{\max} = \frac{I_m^c/d_2 W_y}{[I_0(2\Gamma_m/\Delta k_z)]/WW_y} = \eta_m \frac{W}{d_2} = 163\eta_m , \quad (3)$$

where W_y naturally drops out because the RBC compresses the beam only in the direction parallel to W. As given in Table I, $M_{\max}$ was found to range from 1.1 to 36 within the respective bandwidths, which is just $2\Gamma_m/\Delta k_z$ times the incident bandwidth of 0.6 eV. This small energy bandwidth was obtained because the RBC accepted only a fraction of the angular spread of the incident beam [11]. In particular, $M_{\max} = 22$ within a 0.3 eV bandwidth for the TE_3 mode.

To obtain even higher flux enhancement, it is necessary to reduce or eliminate absorption in the RBC. Low or negligible absorption may be achieved by using higher energy (30–40 keV) x rays or replacing the PIQ film with empty space. Furthermore, making a guide with even smaller d_2 spacing would not only increase $M_{\max}$, but reduce mode mixing as well since fewer modes are then allowed to propagate. Under these conditions, a flux enhancement of 10^2- to 10^3-fold may be realized with the existing fabrication technology.

Even with the present level of absorption, the unique properties of the RBC can be exploited to make two different types of x-ray optical elements. A RBC may be constructed as a hard x-ray monochromator with a 10^2–10^3 Å d spacing capable of producing an energy bandpass of 100 eV and μrad angular resolutions, if L in Fig. 1 is reduced to $\lesssim 250$ μm to limit absorption loss. This provides an alternative to the usual multilayer monochromators, of which the angle that satisfies the first-order Bragg condition would fall below the critical angle and thus is inaccessible. Possible applications for this include small angle x-ray scattering, x-ray microtomography, etc. Second, by eliminating the decoupling section, intense x rays emerging from the end of the guiding section may be used as a coherent source (in the z direction only) for x-ray radiography, or for studying structures of thin films sandwiched between bulk solids.

Finally, we note that photon flux enhancement may also be achieved in a thin film without an overlayer at incident angles beyond the critical angle of the air/film interface, as has been shown by Wang, Bedzyk, and Caffrey [13]. Such a flux enhancement utilizes the virtual resonance because of the partial reflection by the air/film interface; whereas in our waveguide, resonance is established by total reflections from both the Si/film and film/SiO_2 interfaces.

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[7] The PIQ series polyimide is a product of Hitachi Chemical Co., Ltd.
[8] The magnitude of I_m^c depends on W and the bandwidth Γ_m of the resonant coupling, and is maximized for $W\Gamma_m = 1.26$ if the x rays are coherent across W.
[9] The symmetric guide theory used in the paper does not predict the TE_4 mode as a guided one. The actual guide, however, has an asymmetric structure.
[10] The electromagnetic theory overestimates the size of absorption dips by about a factor of 2. The observed dip size is partially accounted for by the coupled intensity into the guide.
[11] This is due to a peculiar property of the RBC. Since resonant coupling only occurs when $k_z = k_0 \sin\theta_{\rm in} \pm \Gamma_m$, with $\theta_{\rm in}$ being very small, the acceptance range for energy $\Delta E/E$ at a fixed $\theta_{\rm in}$ is much greater than the angular acceptance range $\Delta\theta_{\rm in}$ at a fixed energy.
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