Multilayer phase diffraction gratings modeled as a structure in three dimensions

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ABSTRACT

X-ray phase diffraction gratings can be designed to behave in a fashion similar to blazed gratings, directing the majority of the energy into certain desired orders. They should be easy to fabricate using conventional semiconductor production technology, and offer advantages in design flexibility and efficiency over conventional amplitude grating or blazed grating structures. As a multilayered structure, a phase grating has structure in depth as well as across the surface. Most theoretical analyses in the literature treat the embedded structure through simplifying approximations or assumptions. We will discuss a model which treats the embedded structure explicitly using the Fresnel-Kirchoff integral in the Fraunhofer diffraction limit. This approach produces a set of equations which are identical to the result for an amplitude diffraction grating except for an additional factor which depends on the phase relationships of the various surfaces in the multilayer stack.

1. INTRODUCTION AND BACKGROUND

A multilayer x-ray phase grating is a multiple surface diffraction grating. Unlike an amplitude grating, which causes diffraction by varying the amplitude across the wavefront by absorption or scattering part of the impinging wave, it attempts to place the energy contained in the entire impinging wavefront in the diffraction pattern. While so doing, multilayer phase gratings also establish control over the distribution of diffracted energy by providing direct influence over phase relationships in the diffracted wavefronts. The ability to manipulate the phase relationships by the choice of design parameters in the phase grating makes it possible to selectively enhance or diminish certain diffraction orders, subject to the constraints of multilayer reflection. This behavior is in a sense similar to that of a conventional optical blazed grating where the blaze angle places most of the energy in the diffracted wavefronts into a narrow range of diffraction orders.

The manufacture of useful multilayer x-ray diffraction gratings depends on the smoothness of substrates, the regularity of the grating periods, and the size of the grating periods. We have been working on a manufacturing process based on techniques common to the semiconductor industry that we feel offers significant advantages in these areas. This process is

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intended to initially produce a two surface laminar multilayer diffraction grating with grating periods as small as 0.3 μm. When perfected this process will be able to produce multiple copies of a desired grating period and multilayer spacing with only a little more effort than is required to produce multiple copies of a multilayer mirror. The effective grating area will be on the order of 5 square centimeters. This process will also offer considerable design flexibility since a change in the grating characteristics will require just a simple change in the lithography or multilayer characteristics. With improved substrate smoothness, we expect to see an enhancement in energy efficiency due to the improved utilization of the impinging wavefront inherent in a structure of this type.

Multilayer diffraction gratings have been discussed in the literature for several years. There have been reports of gratings produced by building a multilayer structure on ruled and blazed gratings, by laying multilayers over etched structures, and by etching into a multilayer structure.[1,2,3,4,5] There have also been theoretical discussions of the expected behavior of x-ray gratings produced in these ways.[3,4,6] Several of these papers have treated phase gratings, or, as Warburton terms them, two-surface laminar gratings. Very few of them treat the internal structure of a multilayer grating in great detail. One of the best treatments of the interior detail of one-surface (amplitude) and two-surface (phase) laminar gratings was done by Warburton in 1990.[7]

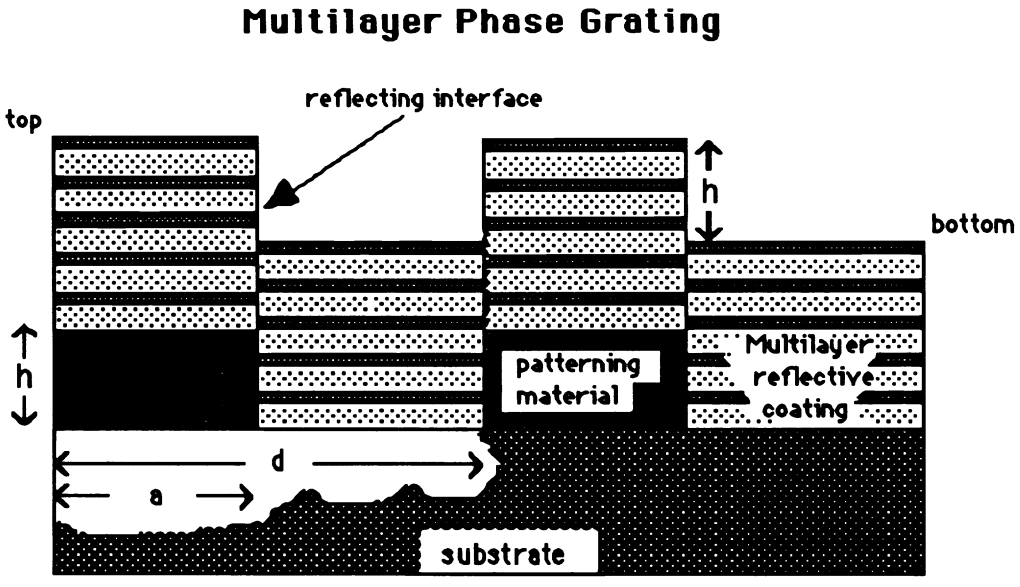


Fig. 1. Interior detail of a multilayer phase grating.

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2. THEORETICAL APPROACH

The interior or embedded detail in a multilayer phase grating is very important in correctly understanding the behavior of the device. As shown in Fig. 1 a phase grating consists of a large number of interspersed reflecting interfaces which have a very complicated phase relationship. Definition of a unique phase relationship for all reflecting interfaces is, in general, impossible. The phase relationship which describes one grouping of interfaces is not applicable to another grouping. This can be seen in Fig. 2 where we have illustrated two of the several different phase relationships which exist for the same structure.

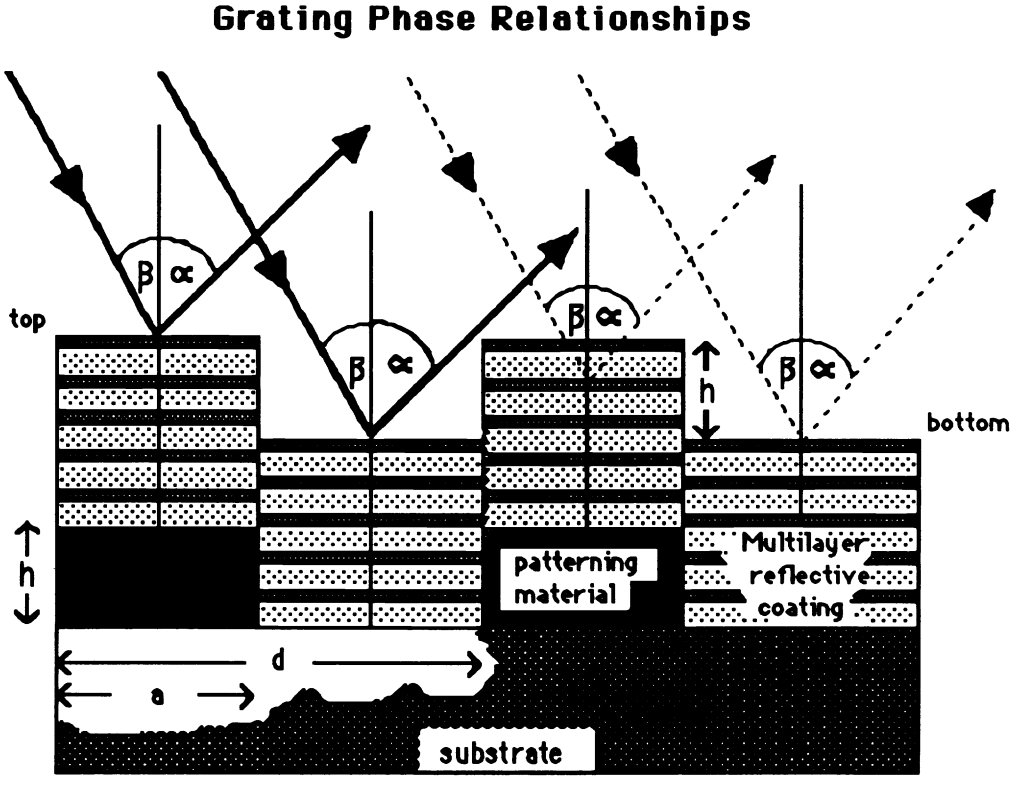


Fig. 2. The dashed and solid lines indicate different phase relationships which exist between the various reflecting interfaces.

2.1 Significance of phase relationships

A simple argument can be made that all these multiple phases are important to a full understanding of the diffraction effects of the phase grating, and not just the phase relationship between the exposed surfaces as is done in conventional visible phase gratings, for example. If we were to remove the topmost layer pair from all the raised surfaces in Fig. 1, as shown in Fig. 3, we change the appearance of the grating and the phase relationship of the top surfaces of the grating. However, this change is mostly superficial. Since all the

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other reflections still have the same phase relationships they had before the one layer pair was removed, with just slight alterations in relative intensities and phases because radiation is no longer reflected, attenuated, and phase shifted by the removed layer pair, we should see a radiation distribution substantially similar to what we observed before. In other words, removing just one set of reflecting interfaces from the many sets that compose the diffracted radiation reflected from the phase structure introduces only a slight perturbation, and we therefore expect that the new diffraction pattern will be only slightly different from the former pattern. Since this slight alteration will not greatly affect the distribution of radiation reflected from the device, we conclude that the apparent phase difference, or the phase difference between the tops of the two multilayer stacks, is not the only phase relationship significant to the behavior of multilayer phase gratings.

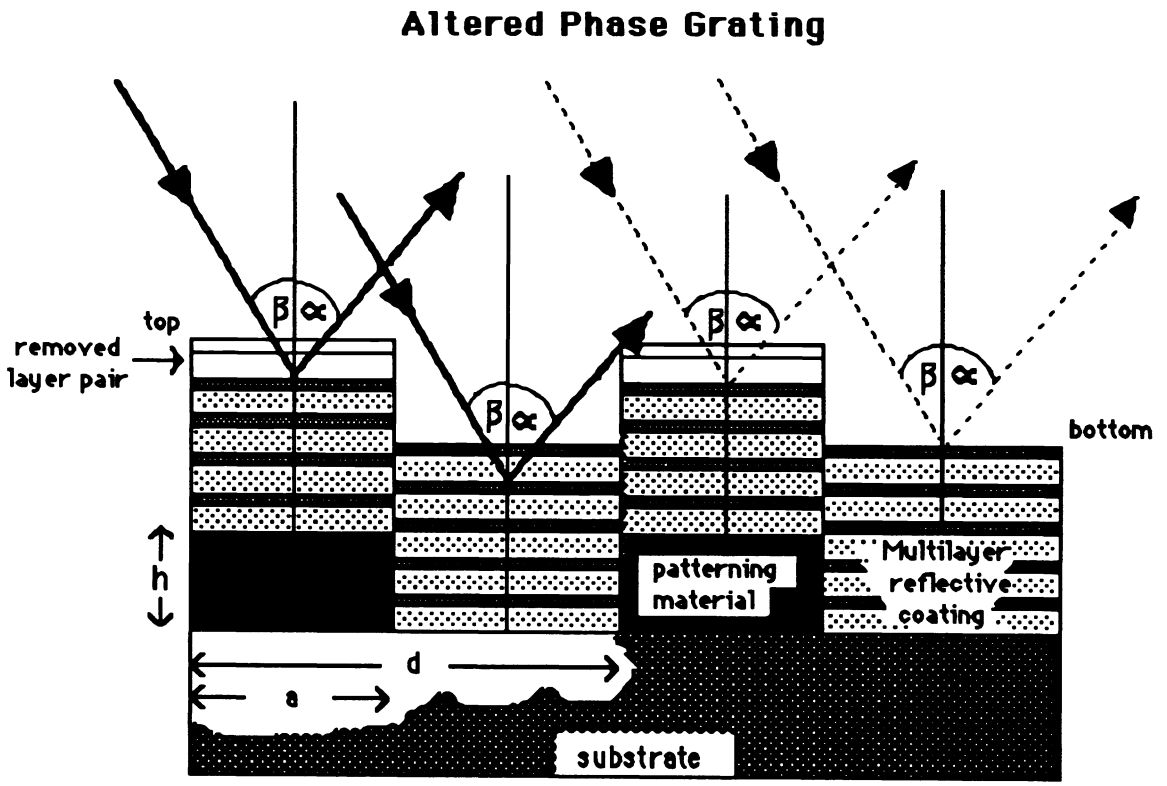


Fig. 3. The same phase relationships outlined in Fig. 2 are still present, even though one layer pair is missing.

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2.2 Nested diffraction gratings

Having concluded that there are multiple phase relationships which must be considered in an analysis of a structure of this type, we are left with the question of how to proceed. Conceptually, we wish to determine the amplitude of the incident x-ray radiation reflected from each interface, and then add these amplitudes with the relevant phase and attenuation relationships together to determine the resultant amplitude for the structure as a whole. An interesting alternate derivation of the diffraction properties of multilayer amplitude gratings which is helpful in understanding the approach we are taking was recently done by Warburton.[7]

To make the problem tractable, we need to take advantage of the geometrical order of the structure. The first simplification takes advantage of the vertical and horizontal ordering of the structure. We do not need to consider each interface individually, but can group them into sets determined by their vertical location in the multilayer stacks. Interfaces located at the same vertical position in the high stacks will be grouped together and, similarly, for the low stacks. Considered in this way, the multilayer phase grating becomes a set of amplitude diffraction gratings which are nested together and illuminated in such a way that the intensity of illumination decreases and the incident phase changes as we move down through the stack of gratings.

Treating the problem in this fashion, and applying the Fresnel-Kirchoff equations in the usual manner for a diffraction grating, [8] while preserving the phase information, which is usually integrated out since it provides no useful information for most applications, we can arrive at the following expression for the diffracted radiation amplitude U as a function of position:

$$U(p) = \frac{sin(kpa)}{kpa}\left(\frac{sin(\frac{Mkpd}{2})}{sin(\frac{kpd}{2})}\right)exp(\frac{-i(M-1)kpd}{2})\left(\sum_{n=1}^{N} A_n exp(ik_n(\delta r + \delta s))\right). \quad (1)$$

p is a function of the angular position of the source and the detector and can be defined:

$$p = sin\alpha - sin\beta,$$

Where α and β are defined in the figures.

k is the wave number of the incident radiation, which we can treat as being in vacuum with reasonable accuracy, since the function is insensitive to small variations in the value of k.

k_n is the wave number corresponding to the element or compound compos-

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ing layer n. We do not assume this to be the vacuum value because small differences here will be important in determining the reflectivity.

M is the number of apertures distributed horizontally in one layer of the grating or the number of apertures illuminated by the incident radiation beam.

N corresponds to the number of layers in the phase grating.

a is the width of a reflecting interface or aperture, and d is the period of the grating.

δr and δs are the angle dependent path lengths for the layers.

A_n is the amplitude of the incident beam reflected from the nth interface.

The intensity I as a function of position can be written

$$I(p) = \left(\frac{sin(kpa)}{kpa}\right)^2 \left(\frac{sin(\frac{Mkpd}{2})}{sin(\frac{kpd}{2})}\right)^2 \left|\left(\sum_{n=1}^{N} A_n exp(ik_n(\delta r + \delta s))\right)\right|^2. \quad (2)$$

With the equation now in a more familiar form, we can see that the diffraction pattern is the product of three factors. The first factor is the single slit diffraction pattern determined by aperture width. This particular form of the equation assumes that the phase grating has equal width steps. If this is not the case, then the sum will have to be altered to account for the different types of gratings. This involves a straightforward extension of the theory we have outlined and we will not discuss it further.

The second factor is the standard amplitude diffraction grating pattern,[8] third factor is the phase relationship term. This term is not simply the multilayer reflectivity, but is a combination of the multilayer behavior and the phase behavior introduced by the stepped structure of the grating. The diffraction pattern is obviously more complex than that of an amplitude diffraction grating. One way of understanding this equation is to think of it as describing a diffraction grating modulated by a phase dependent term which expresses the phase and amplitude relationships between the nested amplitude gratings. Depending on the phase relationships, this third term can be used either to modulate the envelope of the diffraction pattern, or to alter the structure inside the envelope of the diffraction pattern. Which use is made of the third term would depend on the intended application.

By judicious choices of the initial layer thickness, the reflection angles, and the grating parameters, the third term can be used to cancel undesired reflections and enhance desired

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ones. An analogy can be drawn to the behavior of a blazed grating, in which most of the reflected energy is placed into a small number of diffraction orders by the choice of blaze angle. With a phase grating we can adjust the radiation distribution in a similar manner by choosing the phase relationships which will set the location of maximum intensity in the diffraction pattern. A typical application would be to remove the first order reflections and enhance the zero order reflection by using this property. Using the relationships between the layer pair thicknesses and the multilayer stack offsets, it will be possible to significantly alter the reflected radiation pattern. It should be possible using these relationships, for example, to produce reflection peaks that would be forbidden on the basis of the multilayer relationships alone.

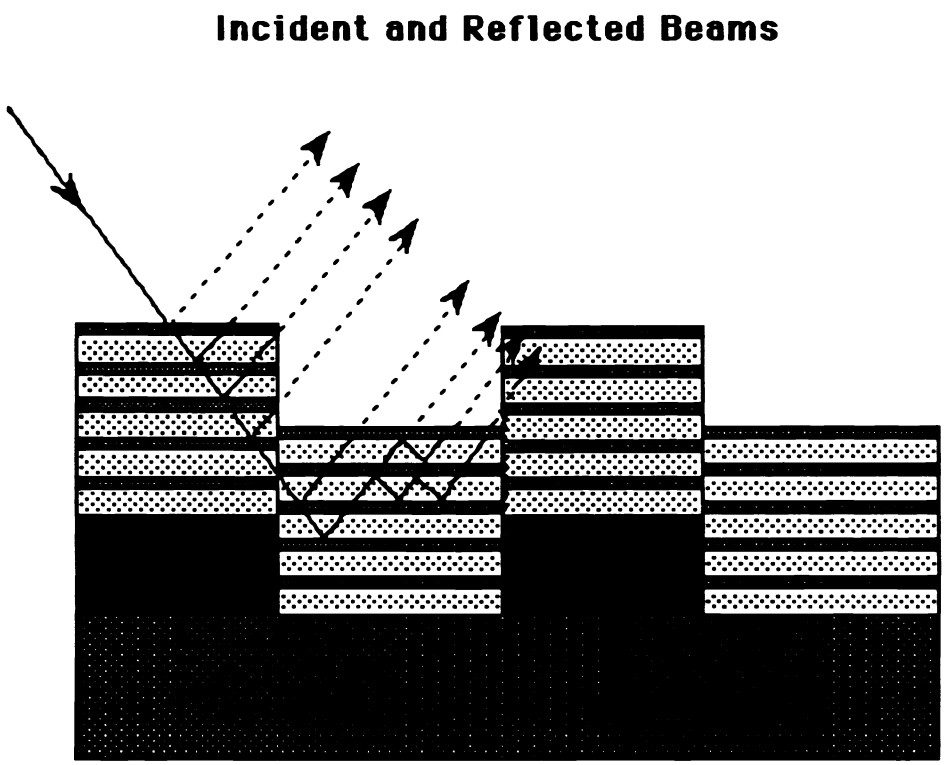


Fig. 4. Propagation of the incident and reflected beam is complicated. Notice that only a few of the many possible multiple reflections are indicated.

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2.3 Interface reflectivity

The phase factor contains a term which describes the reflection of radiation from each interface. This reflected amplitude term, A_n, hides a multitude of physics. If we consider the reflection from the nth layer in the stack, we find, as illustrated in Fig. 4, that propagation of the incident beam into the multilayer structure and propagation of the reflected beam back out is complex. This problem has been solved for ordinary multilayer structures using a recursive formula derived initially by Parratt[9], and extended by Underwood and Barbee[10], or by using matrix expressions as described by Perkins[11,12]. These solutions, unfortunately, do not preserve the information we need, which is the amplitude and phase shift as reflected from each interface. However, using the approach of matching fields at the interface boundaries, as discussed in detail by Parratt, we can calculate the amplitude and phase for each interface directly by starting at the substrate and iterating through the layers to the top, or we can take solutions as provided by Perkins or Underwood and Barbee and iterate from the top surface down to the substrate. Since the amplitude from any given interface is so small, we can neglect multiple reflections in most cases.

3. EXPERIMENTAL WORK AND FUTURE EFFORTS

Part of our research effort has been to develop a method of producing multilayer phase gratings, and eventually more complex phase structures, using thin film and lithography techniques borrowed from the microelectronics industry. To date we have succeeded in producing lithographic structures with a feature size on the order of 0.16 μm (Fig. 5) which are suitable for the production of phase gratings with 0.32 μm period.

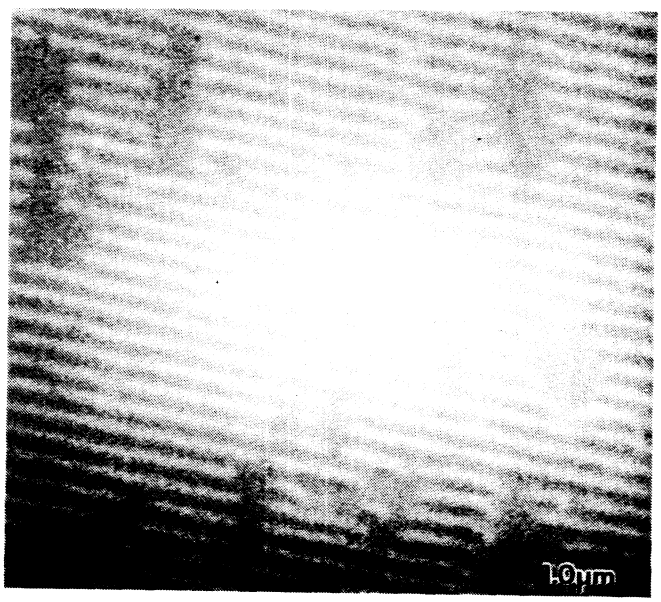


Fig.5 0.32 μm period etched into 120 Å of silicon dioxide on silicon.
These structures would serve as the substrate for a multilayer phase grating.

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These structures were produced by holographic lithography. We are also exploring the feasibility and affordability of using other lithographic techniques for producing preliminary phase structures. A comparison of x-ray diffraction from these structures with calculations based on this model is of great interest and will be the subject of a future report.

4. ACKNOWLEDGMENTS

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