Diffraction Grating Handbook - 5th Edition

DIFFRACTION GRATING HANDBOOK

*fifth edition*

Christopher Palmer

Erwin Loewen, *Editor (first edition)*

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The *Diffraction Grating Handbook* is supplemented by Thermo RGL's *Grating Catalog*, which lists the standard plane and concave gratings available.

If the Catalog does not offer a diffraction grating that meets your requirements, please contact us for a listing of new gratings or a quotation for a custom-designed and -fabricated grating.

Thermo RGL remains committed to maintaining its proud traditions - using the most advanced technology available to produce high-quality precision diffraction gratings, and providing competent technical assistance in the choice and use of these gratings.

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1. REPLICATED GRATINGS

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  5. **INTRODUCTION** [top]

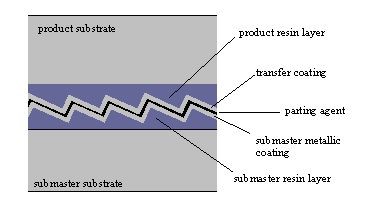
Decades of research and development at Thermo RGL have contributed to the process for manufacturing replicated diffraction gratings (*replicas*). This process is capable of producing thousands of duplicates of master gratings which equal the quality and performance of the master gratings. The replication process has reduced the price of a typical diffraction grating by a factor of 100 or more, compared with the cost of acquiring a master grating.

* 1. **THE REPLICATION PROCESS** [top]

The process for making replica gratings results in a grating whose grooves are formed in a very thin layer of resin that adheres strongly to the surface of the substrate material. The optical surface of a reflection replica is usually coated with aluminum, but gold or platinum is recommended for greater diffracted energy in certain spectral regions. Transmission gratings have no reflective coating.

The production of a replicated diffraction grating is a sequential process. ●*Submaster selection.* The replication process starts with the selection of a suitable *submaster* grating that has the desired specifications (groove frequency, blaze angle, size, …). [A submaster grating is a grating replicated from a master, or from another submaster, but is itself used not as an final optical product but as a mold for the replication of product gratings.]

* + - *Application of parting agent.* A parting agent is applied to the surface of the master grating. The parting agent serves no optical purpose and has no optical effects but aids in the separation of the delicate submaster and product grating surfaces.
    - *Application of transfer coating.* After the parting agent is applied, a reflective coating (usually aluminum) is applied as well. This coating will form the optical surface of the product grating upon separation. To obtain an optical quality coating, this step is performed in a vacuum deposition chamber. [Since this coating is applied to the submaster, but transfers to the product grating upon separation, it is called a *transfer coating*.] Typical transfer coating thicknesses are about one micron.
    - *Cementing.* A substrate is then cemented with a layer of resin to the grooved surface of the master grating; this layer can vary in thickness, but it is usually tens of microns thick. It is the resin that holds the groove profile and replicates it from the submaster to the product; the transfer coating is much too thin for this purpose. The "sandwich" formed by the substrate and submaster cemented together is shown in Figure 5-1.



*Figure 5-1. The replication "sandwich",* showing the substrates, the resin layers, the metallic coatings, and the parting agent.

Since the resin is in the liquid state when it is applied to the submaster, it must harden sufficiently to ensure that it can maintain the groove profile faithfully when the product grating is separated from the submaster. This hardening, or curing, is usually accomplished by a room-temperature cure period (lasting from hours to days) or by heating the resin to accelerate the curing.

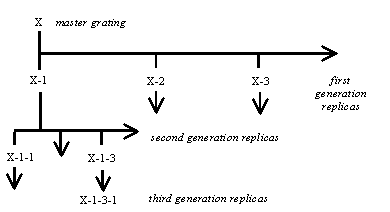
* + - *Separation.* After the resin is fully cured, the groove profile is faithfully replicated in the resin when the submaster and product are separated. The parting agent serves as the weak interface and allows the separation to take place between the submaster coating and the transfer metallic coating. The groove profile on the product is the inverse of the groove profile on the submaster; if this profile is not symmetric with respect to this inversion, the efficiency characteristics of the two gratings will generally differ. In such cases, an additional replication must be done to invert the inverted profile, resulting in a profile identical to that of the original submaster. However, for certain types of gratings, inversion of the groove increases efficiency significantly.

At this stage, if a transmission grating is desired, the transfer coating is removed from the product, leaving the groove structure intact in the transparent resin.

* + - *Inspection.* After separation, both the submaster and the product gratings are inspected for surface or substrate damage. The product grating may also be tested for key performance characteristics (*e.g.*, efficiency, wavefront flatness (or curvature), scattered light, alignment of the grooves to a substrate edge) depending on requirements.

The product grating formed by this replication process may be used as a grating, or it may serve as a mold (replication tool) by being considered a submaster. In this way, a single master grating can make several submasters, each of which can make several more submasters, *etc.*, to form a replication tree (see Figure 5-2).

The replication tree shown in Figure 5-2 illustrates two important features of replication: extension horizontally (within a generation) and vertically (to subsequent generations). Replication within a generation is accomplished by the successive replication of a single grating (much as a parent can have many children). Replication to additional generations is accomplished by forming a replica (child), which itself forms a replica (grandchild), *etc.* Thus replication can extend both within generations (X-1, X2, X-3, X-4, …) and to subsequent generations (X-1, X-1-3, X-1-3-1, X-1-3-14, …) to create a large number of replicas from a single master grating.



*Figure 5-2. A replication tree.* Master X is replicated to create several firstgeneration replicas (X-1, X-2, …), which themselves are replicated to form second-generation replicas (X-1-1, …), &c.

As an example, consider a master grating X from which five firstgeneration replicas are made (X-1 through X-5). Each of these is used as a submaster to form five replicas: X-1 forms X-1-1 through X-1-5, X-2 forms X2-1 through X-2-5, and so on. This forms twenty-five second generation replicas. If each of these replicas is itself replicated five times, we arrive at 125 third-generation products (X-1-1-1, X-1-1-2, …, through X-5-5-5). This example illustrates that a large number of replicas can be made from a single master grating, assuming a conservative number of replicas and a reasonable number of generations.

The number *N* of replicas of a particular generation that can be made from a single master can be estimated using the following formula,

*(5-1)*

where *R* is the number of replications per generation and *g* is the number of generations. Reasonable values of *R* are 5 to 10 (though values well above 20 are not unheard of), and *g* generally ranges from 3 to 9. Conservatively, then, for *R* = 5 and *g* = 3, we have *N* = 125 third-generation replicas; at the other end of the ranges we have *R* = 10 and *g* = 9 so that *N* = 1,000,000,000 ninthgeneration replicas. Of course, one billion replicas of a single grating has never been required, but even if it were, Eq. (5-1) assumes that each replica in every generation (except the last) is replicated *R* times, whereas in practice most gratings cannot be replicated too many times before being damaged or otherwise rendered unusable. That is, some branches of the replication tree are truncated prematurely. Consequently, Eq. (5-1) must be taken as an upper limit, which becomes unrealistically high as either *R* or *g* increase. In practice, *N* can be in the thousands, and can be even higher if care is taken to ensure that the submasters in the replication tree are not damaged.

**5.2. REPLICA GRATINGS VS. MASTER GRATINGS** [top]

There are two fundamental differences between master gratings and replica gratings: how they are made and what they are made of.

* *Manufacturing process.* Replica gratings are made by the replication process outlined in Section 5.1 above - they are resin castings of master gratings. The master gratings themselves, though, are not castings: their grooves are created either by burnishing (in the case of ruled gratings) or by optical exposure and chemical development (in the case of holographic gratings).
* *Composition.* Replica gratings are composed of a metallic coating on a resin layer, which itself rests on a substrate (usually glass). Master gratings also usually have glass substrates, but have no resin (the grooves of a ruled master are contained entirely within a metallic layer on the substrate, and those of a holographic master are contained entirely within a layer of photoresist or similar photosensitive material).

The differences in manufacturing processes naturally provide an advantage in both production time and unit cost to replica gratings, thereby explaining their popularity, but the replication process itself must be designed and carried out to ensure that the performance characteristics of the replicated grating match those of the master grating. Exhaustive experimentation has shown how to eliminate loss of resolution between master and replica - this is done by ensuring that the surface figure of the replica matches that of the master, and that the grooves are not displaced as a result of replication. The efficiency of a replica matches that of its master when the groove profile is reproduced faithfully. Other characteristics, such as scattered light, are generally matched as well, provided care is taken during the transfer coating step to ensure a dense metallic layer. [Even if the layer were not dense enough, so that its surface roughness caused increased scattered light from the replica when compared with the master, this would be diffuse scatter; scatter in the dispersion plane, due to irregularities in the groove spacing, would be faithfully replicated by the resin and does not depend significantly on the quality of the coating.] Circumstances in which a master grating is shown to be superior to a replicated grating are quire rare, and can often be attributed to flaws or errors in the particular replication process used, not to the fact that the grating was replicated.

In one respect, replicated gratings can provide an advantage over master gratings: those cases where the ideal groove profile is not obtainable in a master grating, but the inverse profile is obtainable. Echelle gratings, for example, are ruled so that their grooves exhibit a sharp trough but a relatively less sharp peak. By replicating, the groove profile is inverted, leaving a firstgeneration replica with a sharp peak. The efficiency of the replica will be considerably higher than the efficiency of the master grating. In such cases, only odd-generation replicas are used as products, since the even-generation replicas have the same groove profile (and therefore the same efficiency characteristics) as the master itself.

The most prominent hazard to a grating during the replication process, either master or replica, is scratching, since the grating surface consists of a thin metal coating on a resin layer. Scratches involve damage to the groove profile, which generally leads to increased stray light, though in some applications this may be tolerable. Scratches faithfully replicate from master to submaster to product, and cannot be repaired, since the grating surface is not a polished surface, and an overcoating will not repair the damaged grooves.

Another hazard during replication is surface contamination from fingerprints; should this happen, a grating can sometimes (but not always) be cleaned or recoated to restore it to its original condition. [In use, accidentally evaporated contaminants, typical of vacuum spectrometry pumping systems, can be especially harmful when baked on the surface of the grating with ultraviolet radiation.]

**5.3. STABILITY OF REPLICATED GRATINGS** [top]

*Temperature.* There is no evidence of deterioration or change in standard replica gratings with age or when exposed to thermal variations from the boiling point of nitrogen (77 K = –196 °C) to 50 °C. Gratings that must withstand higher temperatures can be made with a special resin whose glass transition temperature is high enough to prevent the resin from flowing at high temperatures (thereby distorting the grooves). In addition to choosing the appropriate resin, the cure cycle can be modified to result in a grating whose grooves will not distort under high temperature.

Gratings replicated onto substrates made of low thermal expansion materials behave as the substrate dictates: the resin and aluminum, which have much higher thermal expansion coefficients, are present in very thin layers compared with the substrate thickness and therefore do not expand and contract with temperature changes since they are fixed rigidly to the substrate.

*Relative Humidity.* Standard replicas generally do not show signs of degradation in normal use in high relative humidity environments, but some applications (*e.g.*, fiber-optic telecommunications) require extended exposure to very high humidity environments. Coatings and epoxies that resist the effects of water vapor are necessary for these applications.

Instead of a special resin, the metallic coating on a reflection grating made with standard resin is often sufficient to protect the underlying resin from the effects of water vapor.

*Temperature and Relative Humidity.* Recent developments in fiber optic telecommunications require diffraction gratings that meet harsh environmental standards, particularly those in the Telcordia (formerly Bellcore) document GR1221, "Generic Reliability Assurance Requirements for Passive Optical Components". Special resin materials, along with specially-designed replication techniques, can be used so that replicated gratings can meet demanding requirement with no degradation in performance.

*High Vacuum.* Even the highest vacuum, such as that of outer space, has no effect on replica gratings. Concerns regarding outgassing from the resin are addressed by recognizing that the resin is fully cured.

*Energy Density of the Beam.* For applications in which the energy density at the surface of the grating is very high (*e.g.*, some pulsed laser applications), it may be necessary to make the transfer coat thicker than normal, or to apply a second metallic layer (an overcoat) to increase the opacity of the metal film(s) sufficiently to protect the underlying resin from exposure to the light and to permit the thermal energy absorbed from the pulse to be dissipated without damaging the groove profile. Using a metal rather than glass substrate is also helpful in that it permits the thermal energy to be dissipated; in some cases, a water-cooled metal substrate is used for additional benefit.

Pulsed lasers often require optical components with high damage thresholds, due to the short pulse duration and high energy of the pulsed beam. For gratings used in the infrared, gold is used as the reflective coating, and a standard gold-coated replica grating can tolerate an energy density at 10 microns of about 10 J/cm2; for a 10 nsec pulse this corresponds to a power density of 1 GW/cm2. The damage threshold for a subnanosecond 1 micron is about 400 mJ/cm2. Doubling the thickness of the reflective layer can greatly increase the damage threshold of a replicated grating used in pulsed beams.

Experimental damage thresholds for continuous wave (cw) beams, reported by Loewen and Popov4, are given in Table 5-1.

*Grating Type*

*Damage Threshhold*

*(*

*energy density*

*)*

Standard replica grating

on glass substrate

40

to 80 W/cm

2

Standard replica grating

on copper substrate

c. 100 W/cm

2

Standard replica grating

on water-cooled copper substrate

150

to 250 W/cm

2

*Table 5-1. Damage thresholds for continuous wave (cw) beams.*

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1. PLANE GRATINGS AND THEIR MOUNTS

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  3. **GRATING MOUNT TERMINOLOGY** [top]

The auxiliary collimating and focusing optics that modify the wavefronts incident on and diffracted by a grating, as well as the angular configuration in which it is used, is called its *mount*. Grating mounts are a class of *spectrometer*, a term which usually refers to any spectroscopic instrument, regardless of whether it scans wavelengths individually or entire spectra simultaneously, or whether it employs a prism or grating. For this discussion we consider grating spectrometers only.

A *monochromator* is a spectrometer that images a single wavelength or wavelength band at a time onto an exit slit; the spectrum is scanned by the relative motion of the entrance (and/or exit) optics (usually slits) with respect to the grating. A *spectrograph* is a spectrometer that images a range of wavelengths simultaneously, either onto photographic film or a series of detector elements, or through several exit slits (sometimes called a *polychromator*). The defining characteristic of a spectrograph is that an entire section of the spectrum is recorded at once.

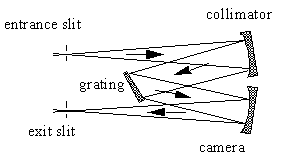
* 1. **PLANE GRATING MONOCHROMATOR MOUNTS**

[top]

A *plane grating* is one whose surface is flat. Plane gratings are normally used in collimated incident light, which is dispersed by wavelength but do not focused. These mounts require auxiliary optics, such as lenses or mirrors, to collect and focus the energy. Some simplified plane grating mounts illuminate the grating with converging light, though the focal properties of the system will then depend on wavelength. For simplicity, only plane reflection grating mounts are discussed below, though each mount may have a transmission grating analogue.

* + 1. **The Czerny-Turner Monochromator**

This design involves a classical plane grating illuminated by collimated light. The incident light is usually diverging from a source or slit, and collimated by a concave mirror (the *collimator*), and the diffracted light is focused by a second concave mirror (the *camera*); see Figure 6-1. Ideally, since the grating is planar and classical, and used in collimated incident light, no aberrations should be introduced into the diffracted wavefronts. In practice, aberrations are contributed by the off-axis use of the concave spherical mirrors.



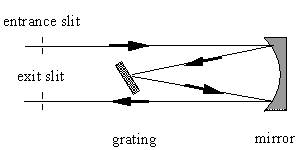
*Figure 6-1. The Czerny-Turner mount.* The plane grating provides dispersion and the concave mirrors provide focusing.

Like all monochromator mounts, the wavelengths are imaged individually. The spectrum is scanned by rotating the grating; this moves the grating normal relative to the incident and diffracted beams, which (by Eq. (21)) changes the wavelength diffracted toward the camera. For a Czerny-Turner monochromator, light incident and diffracted by the grating is collimated, so the spectrum remains at focus at the exit slit for each wavelength, since only the grating can introduce wavelength-dependent focusing properties.

Aberrations caused by the auxiliary mirrors include astigmatism and spherical aberration (each of which is contributed additively by the mirrors); as with all concave mirror geometries, astigmatism increases as the angle of reflection increases. Coma, though generally present, can be eliminated at one wavelength through proper choice of the angles of reflection at the mirrors; due to the anamorphic (wavelength-dependent) tangential magnification of the grating, the images of the other wavelengths experience subsidiary coma (which becomes troublesome only in special systems).

**6.2.2. The Ebert-Fastie Monochromator**

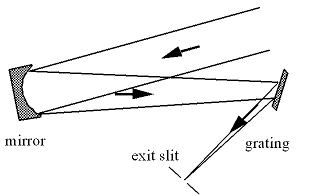
This design is a special case of a Czerny-Turner mount in which a single relatively large concave mirror serves as both the collimator and the camera (Fig. 6-2). Its use is limited, since stray light and aberrations are difficult to control.



*Figure 6-2. The Ebert-Fastie mount.* A single concave mirror replaces the two concave mirrors found in Czerny-Turner mounts.

**6.2.3. The Monk-Gillieson Monochromator**

In this mount (see Figure 6-3), a plane grating is illuminated by converging light (*r* < 0). Usually light diverging from an entrance slit (or fiber) is rendered converging by off-axis reflection from a concave mirror (which introduces aberrations, so the light incident on the grating is not composed of perfectly spherical converging wavefronts). The grating diffracts the light, which converges toward the exit slit; the spectrum is scanned by rotating the grating to bring different wavelengths into focus at or near the exit slit. Often the angles of reflection (from the primary mirror), incidence and diffraction are small (measured from the appropriate surface normals), which keeps aberrations (especially off-axis astigmatism) to a minimum.

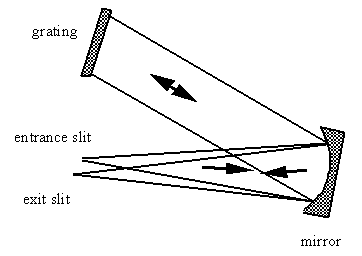


*Figure 6-3. The Monk-Gillieson mount.* A plane grating is used in converging light.

Since the incident light is not collimated, the grating introduces wavelength-dependent aberrations into the diffracted wavefronts (see Chapter 7). Consequently the spectrum cannot remain in focus at a fixed exit slit when the grating is rotated (unless this rotation is about an axis displaced from the central groove of the grating, as pointed out by Schroeder5). For low-resolution applications, the Monk-Gillieson mount enjoys a certain amount of popularity, since it represents the simplest and least expensive spectrometric system imaginable.

**6.2.4. The Littrow Mount**

A grating used in the Littrow or autocollimating configuration diffracts light of wavelength λ back along the incident light direction (Fig. 6-4). In a *Littrow monochromator*, the spectrum is scanned by rotating the grating; this reorients the grating normal, so the angles of incidence α and diffraction β change (even though α = β for all λ). The same auxiliary optics can be used as both

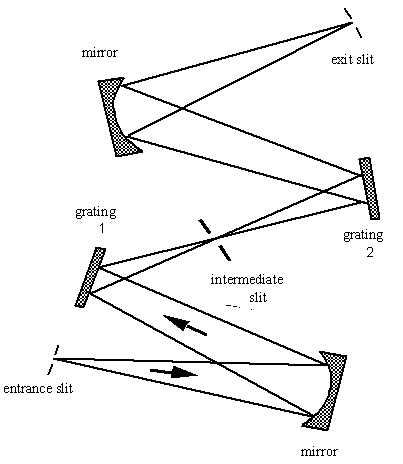


*Figure 6-4. The Littrow monochromator mount.* The entrance and exit slits are slightly above and below the dispersion plane, respectively; they are shown separated for clarity.

collimator and camera, since the diffracted rays retrace the incident rays. Usually the entrance slit and exit slit (or image plane) will be offset slightly along the direction parallel to the grooves so that they do not coincide; of course, this will generally introduce out-of-plane aberrations. As a result, true Littrow monochromators are quite popular in laser tuning applications (see [Chapter 12)](http://www.gratinglab.com/library/handbook5/chapter12.asp).

**6.2.5. Double & Triple Monochromators**

Two monochromator mounts used in series form a *double monochromator*. The exit slit of the first monochromator usually serves as the entrance slit for the second monochromator (see Figure 6-5). Stray light in a double



*Figure 6-5. A double monochromator mount.*

monochromator is much lower than in a single monochromator: it is the product of ratios of stray light intensity to parent line intensity for each system. Also, the reciprocal linear dispersion of the entire system is the sum of the reciprocal linear dispersions of each monochromator.

A *triple monochromator* mount consists of three monochromators in series. These mounts are used only when the demands to reduce stray light are extraordinarily severe (*e.g.*, Raman spectroscopy).

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